

wwPDB EM Validation Summary Report (i)

Jun 21, 2023 – 05:28 pm BST

PDB ID	:	8BX8
EMDB ID	:	EMD-16312
Title	:	In situ outer dynein arm from Chlamydomonas reinhardtii in the post-power stroke state
Authors	:	Zimmermann, N.E.L.; Noga, A.; Obbineni, J.M.; Ishikawa, T.
Deposited on	:	2022-12-08
Resolution	:	30.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 30.30 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 $(\#Entries)$	${f EM\ structures}\ (\#{f Entries})$		
Clashscore	158937	4297		
Ramachandran outliers	154571	4023		
Sidechain outliers	154315	3826		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Q	uality of chain	
1	А	4620	16%		23% • •
2	В	4595	13%		25% ••
3	С	4168	18%	%	16% • 5%
4	D	657	8%	49%	• 12%
5	Е	670	37%	45%	• 17%
6	F	133	18%	48%	• •
7	G	159	30% 51%	35%	• 7% 5%
8	Н	92	37%	62%	

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Mol	Chain	Length	Quality	of chain	
9	Ι	110	35%	61%	• •
10	J	95	34%	65%	•
11	Κ	93	40%	57%	·
12	L	111	42%	58%	
13	М	87	43%	57%	
14	N	117	57%	40%	•
15	0	132	42%	46% •	9%
16	Р	122	• 57%	26% 5% • 1	1%
17	Q	202	72% 65%	29%	• 5%
18	R	160	64%	15% •	6%

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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
19	ADP	А	4701	-	-	Х	-
19	ADP	А	4703	-	-	Х	-
19	ADP	В	5405	-	-	Х	-
19	ADP	С	4305	-	-	Х	-
20	ATP	А	4702	-	-	Х	-
20	ATP	В	5403	-	-	Х	-
21	MG	А	4705	-	-	Х	-



2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 119530 atoms, of which 156 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 heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	4453	Total 33975	C 21575	N 5801	O 6441	${ m S}$ 158	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	4488	LYS	GLY	conflict	UNP Q22A67

• Molecule 2 is a protein called Outer arm dynein beta heavy chain.

Mol	Chain	Residues		Α		AltConf	Trace		
2	В	4519	Total 34713	$\begin{array}{c} \mathrm{C} \\ 22055 \end{array}$	N 5945	O 6563	S 150	0	0

• Molecule 3 is a protein called Dynein-1-alpha heavy chain, flagellar inner arm I1 complex protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	С	3947	Total 30427	C 19395	N 5159	0 5724	S 149	0	0

• Molecule 4 is a protein called Dynein intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	579	Total 4680	C 2975	N 791	0 883	S 31	0	0

• Molecule 5 is a protein called Flagellar outer dynein arm intermediate protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Е	555	Total 4440	C 2798	N 762	0 858	S 22	0	0



• Molecule 6 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues		At	oms	AltConf	Trace		
6	F	128	Total 996	C 625	N 176	O 193	${ m S} { m 2}$	0	0

• Molecule 7 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	G	151	Total 1024	C 636	N 184	O 203	S 1	0	0

• Molecule 8 is a protein called Dynein light chain.

Mol	Chain	Residues		At	oms	AltConf	Trace		
8	Н	91	Total 750	C 483	N 124	0 139	$\frac{S}{4}$	0	0

• Molecule 9 is a protein called Dynein light chain.

Mol	Chain	Residues		At	oms	AltConf	Trace		
9	Ι	106	Total 827	C 526	N 134	0 161	S 6	0	0

• Molecule 10 is a protein called Dynein light chain.

Mol	Chain	Residues		At	oms	AltConf	Trace		
10	J	95	Total 807	C 527	N 135	0 140	${f S}{5}$	0	0

• Molecule 11 is a protein called Dynein light chain.

Mol	Chain	Residues		At	oms	AltConf	Trace		
11	K	90	Total 754	C 489	N 124	0 137	${S \atop 4}$	0	0

• Molecule 12 is a protein called Dynein light chain.

Mol	Chain	Residues		At	oms			AltConf	Trace
12	L	111	Total 855	C 555	N 145	0 152	${ m S} { m 3}$	0	0

• Molecule 13 is a protein called Dynein light chain.



Mol	Chain	Residues		At	oms			AltConf	Trace
13	М	87	Total 735	C 477	N 123	O 130	${ m S}{ m 5}$	0	0

• Molecule 14 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues		At	oms	AltConf	Trace		
14	Ν	114	Total 852	C 542	N 142	0 165	${ m S} { m 3}$	0	0

• Molecule 15 is a protein called Dynein light chain 2A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	0	120	Total 994	C 639	N 173	0 179	${ m S} { m 3}$	0	0

• Molecule 16 is a protein called Thioredoxin.

Mol	Chain	Residues		Ato	ms		AltConf	Trace
16	р	109	Total	С	Ν	Ο	0	0
10	1	105	541	323	109	109	0	0

• Molecule 17 is a protein called Dynein light chain 1.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
17	Q	191	Total 1001	$\begin{array}{c} \mathrm{C} \\ 607 \end{array}$	N 202	O 192	0	0

• Molecule 18 is a protein called Dynein light chain 4A.

Mol	Chain	Residues		Α	toms			AltConf	Trace
18	R	150	Total 895	C 439	Н 156	N 150	O 150	0	0

• Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).





Mol	Chain	Residues		Ate	oms			AltConf
10	Δ	1	Total	С	Ν	Ο	Р	0
19	A	1	27	10	5	10	2	0
10	Δ	1	Total	С	Ν	Ο	Р	0
19	Л	1	27	10	5	10	2	0
10	В	1	Total	С	Ν	Ο	Р	0
15	D	T	27	10	5	10	2	0
10	В	1	Total	С	Ν	0	Р	0
15	D	1	27	10	5	10	2	0
10	С	1	Total	С	Ν	Ο	Р	0
15	U	1	27	10	5	10	2	0
19	C	1	Total	С	Ν	Ο	Р	0
1.5			27	10	5	10	2	0

• Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).





Mol	Chain	Residues		Ate	oms			AltConf
20	Λ	1	Total	С	Ν	Ο	Р	0
20	A	1	31	10	5	13	3	0
20	В	1	Total	С	Ν	Ο	Р	0
20	D	1	31	10	5	13	3	0
20	С	1	Total	С	Ν	Ο	Р	0
20	U	1	31	10	5	13	3	U

• Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
21	А	3	Total Mg 3 3	0
21	В	3	Total Mg 3 3	0
21	С	3	Total Mg 3 3	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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, outer arm protein







PROTEIN DATA BANK

E2065 12066 K2067	D2069	S2084 D2089	N2095 L2098	A2099 D2100 12101 F2102	P2103 K2104	L2105 K2106	E2107 V2108 P2109	L2112	Y2113 P2114	V2115 V2116 F2117	K2118	K2119 12120 P2121	E2122	12141 Q2142 L2143	L2155	<mark>G2162</mark> K2163	S2164	T2171	T2175	G2178	V2199	K2200				
S2201 ← E2202 ← 12203 ← S2204 ←	D2205 D2206 W2207	I 2208	N2221 R2222 A2223	L2224 K2225 H2226	T2227	V2247	T2255	A2257	G2259	R2261	E2275	N2278	L2298	K2311	R2316	E2318	S2320 D2321	K2322	N2325	K2328 K2329	L2331 12332	N2333	R2335			
F2336 L2339 Q2340 S7341	K2342 E2343	12360 12360 12363	C2367	72373 [2373 [2374	q2375 R2376 T2377	L2378 S2379	E2380 🕈 Q2381	F2386	E2409	L2410 L2411	L2412 A2413	K2414 N2415	A2416 P2417 T2418	12410 P2419 02420	K2421	K2423 E2424	N2425 E2426 T2427	12420 V2428 F2429	D2430	C2443	12476 1 0477	עביו				
N2487 S2488 A2489 L2490	G2496 T2497 A2498	K2499 T2500 D2511	P2512 Q2513 K2514 M2515	K2542	G2544 K2545	K2653	M2564 P2565 F2566	V2567 N2568	R2569	L2576	K2593	1203 1 Q2595	I2608	12621	R2624	K2653	42003 K2655 V7656	F2657 S2658	D2659	T2661	K2663	I.				
L2668 W2676 M2696	R2697 E2698 L2699	12723 L2727 F2728	L2/29 L2745 V2746	V2754	E2764	Q2768 12769	E2770 N2771 E2772	K2776	C2786 V7793	A 2804	L2839 V2840	V 2840	I2855	G 28 63	V 2866	S2871 G2872	<mark>\$2875</mark> L2876	T2877	D2901 L2902 K2903	E2904						
D2905 I2906 K2907 T2921	F2922 L2923 M2924 T2925	L2935 12938 12938	62945	L2951 D2954	E2956 R2956 E2957	V2958 W2959 T 7060	G2961	12963 S2964	ц2965 С2968	K2969	N2972	G2974	12976 • D2977 •	P2978	F2987	R2992	L2999 C3000	L3018	C3022	T3041	F3042 I3043					
F3046 13049	L3059 M3060 H3067	R3083 F3092	Y3095 L3096	Y3099 K3100 T3101	L3102 Y3103 I3104 F3105	K3106	E3110	F3117	G3120 L3121	<u>13124</u> Q3125 F3126	E3120 A3127 T3128	I3129 T3130	I3131 N3132	Q3133 M3134	E3135 I3136	S3137 L3138	K3139 E3140	E3141 • E3142 •	13143	L3145 N3146	E3147 • A3148 •					
T3149 E3150 K3151 T3152	N3153 Q3154 L3155	L3159	D3160 K3161	53163 K3164	K3165 A3166 N3167	Q3168 €X3169	G3170 E3171	E3172 V3173	A3174 A3175 T3175	N3177	03175 03179	C3180 E3181	I3182 Q3183	A3184 E3185	q3186 I3187	S3188 K3189	E3190 K3191	E3192 E3193	A3194 E3195	R3196 E3197	L3198 E3199	A3200	L3202	A3204 L3205	R3206 R3207	A3208
(13209 (13210 (13211) (13212)	D3213 S3214 I3215	E3216 S3217 K3218	D3219 13220 <mark>V3221</mark>	E3222 L3223 K3224	A3225	K3227 K3228	P3229 L3230 D3231	I3232	K3234 Y3235 T2036	M3237	A3239	V3240 L3241 V3242	F3243	K3245 A3246 R3247	L3248 I3249	P3250 13251 03252	E3255	R3256 V3257	F3258 N3259	K3260 K3261	E3262 G3263	K3264 A 3265	V3266 L3267	F3268 L3269		
K3270 E3271 S3272 Y3273 D3274	E3275 S3276 G3277	13278 (33279 13280	G3282 D3283	M3.284 N3.285 F3.286	M3287 K3288 K3288	K3289	E3292	E3294 K3295	D3296	13298 N3299	E3300 E3301	T3302 I3303	E3304 L3305	L3306 E3307	P3308 Y3309	L3310 N3311	ua312 83313 83313	D3315	W3316 F3317	N3318 D3319	T3320 F3321	A3322	K3324	S3326 K3327	A3328 A3329	
A3330 G3331 13332 L3333	K3334 W3335 A3336	<mark>F3337</mark> A3338 I3339	Y3340 E3341 Y3342	H3343 Q3344 K3345	S3346 K3347	13348 V3349	K3350 P3351 K3352	R3353	प3355 ◆ V3356	A3357	A3359 E3360	G3361 R3362	ц3363 ♦ А3364 ●	I3365 + A3366 +	L3367	E3369 L3370	E3371 + K3372 +	A3373	E3375	L3377	13379	13381 (13381	Y3383	K3385	L3387	D3389
V3390 S3421 L3422	E3425 W3429	13436 K3440 R3441	K3 44 2 L3443 V3444 G3445	N3446 V3447 S3448	L34450 83450 13451	R3453 F3453 13454	83455 73456 C3457	V3475	K3478 K3479	T3485	L3488	F3493	13508 L3508	13 <mark>515</mark>	D3532 P3533	ជុន534 ៨3535 ជុន536	G3537 Q3538 M3530	N35540 13541	K3544	L3545						
S3546 I3549 I3550 P3551	E3552	T3557	H3560	E3581	N3582	N3585 E3586 V3587	D3592 D3593	C3627	A3630	L3638	K3641	F3647 T3648	Q3651	L3694	L3 <mark>691</mark>	L3696	I3700 🔶 N3701	S3702	G3704	D3709						







PROTEIN DATA BANK

<mark>01945</mark> Տ1946	G1947	E1954 F1955	N1956	V1966	N2005	P2006	G2007	A2009	G2010	R2011	R2023	N2038	M2039		G2044	R2049	L2058	1900	L2066	K2070		D2073	A2078	L2083	42084 Q2085	DOOR		T2116 D2117	D2118	12121	D2128	L2129 F2130	P2131 K2132	L2133	D2134	P2135								
P2136	T2150	V2176 R2177	P2185	S2188 C2180	K2190 K2190	C2192	N2203	N2214	H H H H	S2220	D2221	G225	A2226	Y2227	Т2228	T2230	K2231	E2232	W2233 🔶 K2234	N2235	G2236 V2237	V 2231	V2240	K2243	K2247	N2248	E2249	Y2252	K2253 A2254	n2260		17270 4	12267 D2268	P2269	E2270	12272 12272	E2273							
S2274	K2283 V7784	L2285	T2286 L2287	V2288	N2290	D2291 R2292	12293	F2294		R2300 L2301	12302 F2303	E2304	L2308	R2309	N2310 A2311	E2326		M2332 P2333	Y2334 M2335		N2345	K2348	q2349	A7354		E2358 Y2359	P2360	V2361	12363 D2363	D2364	V2365	K2367	S2368	D2383	P2395		L2409 D2410	A2411						
L2412	12414 12414	Q2415 H2416	L2417	K2419	K2421	Q2422	M2423 K2424	E2425	E2426	D242/ E2428	K2429	Q2430	A2431		F2436	L2441	G2445	C 97 CN		C2479	D2485	12486	N2487	N2489	K2490	W2491 N2492	T2493 W2494		P2501	N2502		V2512 A2513	T2514 T2515	H2516	R2519	TOEOG	12920	R2531	•					
A2540	G2543 K2544	T2545 A2546	R2556	E2558	Q2559 V2560	S2569	L2574	0.05.77		K2586	N2588	G2589	R2590	Y2592	12601	UC OC N	P2610	1000	K2614 Y2615	G2616 T9617	Q2618	S2619 P2620	12621 03633	22 02 h	R2625	R2636	E2637 02638	L2639	E2641	F7644		6707T	N2655	V2663	L2665									
R2666 1.2667	Q2668	M2676	K2685 T2686 T2687	S2690	L2696	S2697	T2698	D2700	D2701	K2702	A2707	V2711	90731	A2732	F2741	R2742	T2754	T2755	G2757	Q2758	Y2759 S2760	G2761	G2762	L2767	L2770	1100 C		D2781	12800	12814 40815	E2816	r 2017 L2818	I2819 F2820	128CA	1203 1 T2835									
<mark>գ2836</mark>	12 <mark>839</mark> P2840	L2846	L2862 V2863	L2864	E2870 H2871	V2872	L2879	N2885	G2893		7290 4	12 <mark>9</mark> 11	N2927		q2930 E2931		K2934	K2935 I2936	A2937	K2938	P2939	R2944	L2959	12960 P2961	12962 N2963		L2966	12971	L2974	P2976	K2977	E2978	M2980	D2981	S2982	L2983 V2984	1007A							
S2985	G2986 V2987	R2988 N2989	E2990	K2992	G2993 E2994	G2995	V2996 D2997	V 2998	N2999	N3000	T3002	A3003	L3004	T3005 S3006	¥3007	F3008	K3017	V3018	<mark>83023</mark>	I3031	R3032	N3041	N3042 T3043	D3046		V3059	F3063	13067	130 <mark>74</mark>	S3077	13078 S3079	L3080 N3081	M3082	V3085	13089		A3092	•						
Y3103	T3106	K3109	L3112 E3113 L3114	I3115 D3116	F3117 Y3118	K3119 K3120	L3121	22107	K3125	13129	43130 R3131	<mark>Q3132</mark> I3133		Y3136	G3139 13140		L3143 A3144		цо14/	V3150	L3153	Q3154 E3155	E3156 13167		K3160 M3161	V3162 E3163	V3164	N3166 K3166	F.3 169	E3170	131/1 D3172	I3173	L3174	I3175 E3176										
K3177	V3178 G3179	K3180 E3181	S3182	L3184	A3185 E3186	E3187	E3188	T3190	I3191	A3192	A3194	E3 195	E3196	E3197 V2100	T3199	N3200	V3201	A3202	A3204	E3205	A3206	E3207	13209	33210	K3211	A3213	T3214	E3215	L3217	A3218		L3221	P3222	L3224	R3225	s3226	A3227	A3229	A3230	V3231	D3232	L3234	K3235	K3236
P3237	H3238 V3239	T3240 E3241	M3242 K3243 M3244	L3245	G3246 S3247	P3248	P3249 A3250	G3251	V3252	13253 V3754	T3255	A3256	R3257	V3259	L3260	I3261	L3262	r 3263 N3264	Q3265	G3266	I3267	1.3269	N3270	D3271	P32/2 D3273	E3274	K3275	V3276 W3277	K3278	K3279	V3281	T3282	F3283 M3284	N3285	N3286	P3287	0,3288 0,3280	F3290	13291	D3292	K3293	K3295	S3296	
F3297	D3298 G3299	E3300	13302	P3304	N3305 13306	I3307	E3308	S3310	N3311	K3312	13314	Q3315	D3316	P3317	K3319	K3320	F3321	N3322	K3324	D3325	M3326	A3327	u3329 ♦	s3330	Y3331	A3333	<mark>\$3334</mark>	K3335	C3337	A3338	A3340	V3341	N3342	V3344	T3345	F3346	N3347	13349	F3350	K3351	Q3352	K3354	P3355	L3356
3357	359	360	3362	3364	3365	3367	• • • • • • • • • • • • • • • • • • •	<u> 3370</u>	373	374	1375	1377 1377	3378	3379	3381	382	383	385	386	387	888	283	392	393	<u>395</u>	399	400 401	402 403	404 405	406	1408	3409	3412	3422	2473	3426	428	429 430						











N2284	L2289	12295	A2296	82300	D2301	F2303	Y2304	D2305	M2307	P2308	N2310	E2311	R2344	L2357		V2301	G2365 K2366	02367	S2368	Y2390	S2391	V2393	D2394	L2395	R2396	D2398	L2399	q2401	L2402 V2403	F2404	C2406 C2406	L2416	F2417	N2424	E2425 B2426		N2432	Y2444	T2445					
L2446	D2447 E2448	K2449	E2450	M2452	I2453	n 2454	V2456	A2458	K2459	V2460	G2462	E2463	G2464	K2465 P2466	D2467	T2468	R2469	V2480	I2488	T2512	D2513	₽T CZ M	L2531 Encon	E2532 P2533	L2536	V2556			F2578	L2581 12582	S2583 L2584	F2585	L2589	K2592	R2593	L2596 E2607		N2600						
L2607	1 E C C C C C C C C C C C C C C C C C C	CTOZE	A2618	I2619	V2622	E2623 V2624	K2625	E2626 K2627	Q2628	V2629	E2630	E2632	A2633	K2634	K2635 K7636	E2637	A2638	D2639	F2641	A2642	E2643	V2644	02646 G2646	R2647	E2648	D2650	K2651	V2652	K2654	E2655	N26550	K2658	A2659	I2661	E2662	A2663	K2665	C2666	G2667	I2669	K2670	u2671 N2672	V2673	
E2674	A2675	K2677	S2678	52679 T2680	Q2681	Q2682	L2684	D2685	A2686	Q2688	P2689	L2690	E2692	<mark>q2693</mark>	A2694	K2695	A2697	L2698	N2699	S2700	S2702	K2703	K2704	D2705 F2706	q2707	q2708	K2710	S2711	F2712	S2714	P2715	A2717	G2718	V2719	E2721	V2722	F2723	A2725	T2726	12727 V7778	L2729	L2730	G2732	V7733
F2734	N2735 E2736	A2737	12738	E2739 I2740	D2741	K2742	K2744	K2745	P2746 K2747	D2748	V2749	S2750	K2752	S2753	S2754	L2755		M2758	K2759	S2760	E2762	E2763	F2764	M2765 E 2766	K2767	L2768	N2770	F2771	K2772	V2774	V2775	A2777	N2778	02779 17780	PRO	ALA A2783	N2784	V2785	N2/86	V2788	K2789	q2791	Y2792	L2793
N2794	M2795	<mark>\$2797</mark>	F2798	P2800	E2801	Q2802	A2804	S2805	K2806 S2807	A2808	A2809	A2810	62812	12813	C2814	S2815	V2817	V2818	N2819	12820 V2821	K2822	Y2823	Y2824	D2825 V2826	12827	12828 Theorem	V2830	E2831	P2832	R2834	K2835	A2836 L2837	K2838	E2839	T2841	E2842	Q2843 L2844	E2845	E2846	A2847	V2849	K2850		E DOE D
V2854	E2855 E 2856	V2857	V2858	K2859 K2860	L2861	N2862	E2864	L2865	N2866 K2867	L2868	K2869	A2870	N2872	D2873	K2874	A2875	A2877	E2878	R2879 N7980	A2881	R2892		L2895	L2 <mark>899</mark>	A2902	L2903	E2908	K2912	S2913 12914	12915	42916 L2917	E2918 D2919	<mark>q2920</mark> L2921	K2922 1 2623	M2924	V2925 G2926	D2927 V2928	L2929	V2930 A2931					
S2932 S2933	F2934 V2935	S2936	Y 2937	F2941 N2942	K2943	<mark>S2966</mark>	I2974	F.2975	W2984	L2989	P2990	V2994	13001	L3010	M3011 13012	D3013	P3014	E3024	10064	A3028	N3029	N3030	L3031	L3034	I3041	N3051	G3052	Y3053	53054 A3055	I3056 I3057	E3058 N3059	13064	13072	A3073	R3074	H3095								
P3096	N3097	F3101 L3102	10 10 10 10 10	E3114	I3115	L3121	T3125	K3151	F3161	L3184	D3185	13190	L3193		13203 A3204	E3205	43208		13212	13217	R3225	P3226 A3227	7770	V3 <mark>244</mark> H3245	33246	13266	53267 1000	E3 200 N3 269	K3270	G3273	K3274	132/5 T3276	M3277	VAL PRO	TYR GLY	ASP								
THR	ALA SER	ASN	GLN	GLU	GLU GLU	0115 0115	GLU	GLU	GLU	GLN	GLN	GLN	GLN	GLN	CLUD	GLU	GLN	01D	LYS	ASP		LYS LYS	GLY BPD		GLU GLU	GLU	PRO	GLY GLY	2 GLU ASN	2 CTY	Z ϕ PRO VAL	dTI GLU	d C C C C C C C C C C C C C C C C C C C	ALA	N									
GLV GLV	GLN GSN	GLU GLU	GLY PRO	VAL	GLU GLU	ASN	GLU	GLN GLN	GLU GLU	GLU	GLU GLU	GLU GLU	GLY	CTU CTU		TAS	ALA	ASP	ASP	GLU	M338t	8338	P338	K338	R338		1339.	R340	H341	I341	N344	E349	K349		Noon Noon					•				
L3526	F3553	₱3577	D3578		R3581	V3582 A3503	A3584	T3585	F3586		S3589	A3590	N3591	G3593	R3594	F3595	13597 N3597	UU SEM	M3600 G3601	43602	R3607	A3608	K360S	A3611	L3612	F3613 D3614	C3615	A3616	43617 K3618	G3619	H3620 W3621	I3622 M3603	L3624	4362t	L3629 M3630	1 261	E3645	S3646	V3644 F3648	A3645	S3650			
P3651	K3652 T3653	H3654	P3655	N3656 F3657	13661	S3662	N3704	70700	0.15U	E3709	F3710	D3712	K3713	C3714	D3715 K3716	K3717	P3718	1.3/ 19	C3724		H3732	L3757 T3758	I3759	L3764	D.3778		13786 M3787	13792	T3793	N3801	Y3804	L3805 K3806	R3810	N3819	VC0C4	r 3824	D3828	F3829						





• Molecule 5: Flagellar outer dynein arm intermediate protein, putative



















• Molecule 17: Dynein light chain 1







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	2131	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	80.0	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.222	Depositor
Minimum map value	-0.797	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.196	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	628.26, 628.26, 628.26	wwPDB
Map dimensions	74, 74, 74	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	8.49, 8.49, 8.49	Depositor



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, ATP, MG

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).

Mal	Chain	В	ond lengths	I	Bond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.72	7/34544~(0.0%)	0.81	24/46728~(0.1%)
2	В	0.72	7/35318~(0.0%)	0.82	37/47792~(0.1%)
3	С	0.88	63/31033~(0.2%)	0.89	52/42007~(0.1%)
4	D	0.63	1/4789~(0.0%)	0.74	6/6477~(0.1%)
5	Ε	0.61	0/4540	0.64	0/6136
6	F	0.57	0/1008	0.58	0/1355
7	G	0.63	0/1030	0.98	11/1403~(0.8%)
8	Н	0.63	0/767	0.61	0/1031
9	Ι	0.66	0/838	0.59	0/1131
10	J	0.61	0/832	0.65	0/1119
11	Κ	0.62	0/776	0.60	0/1038
12	L	0.61	0/872	0.61	0/1176
13	М	0.62	0/752	0.61	0/1006
14	Ν	0.66	0/864	0.67	0/1175
15	0	0.64	0/1012	0.64	0/1358
16	Р	1.92	3/538~(0.6%)	1.60	15/746~(2.0%)
17	Q	0.34	0/1004	0.59	1/1385~(0.1%)
18	R	0.83	1/738~(0.1%)	0.95	2/1025~(0.2%)
All	All	0.76	82/121255~(0.1%)	0.82	148/164088~(0.1%)

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	А	0	4
2	В	0	11
3	С	0	2
4	D	0	1
7	G	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	Р	0	2
All	All	0	32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	1067	PRO	N-CD	51.23	2.19	1.47
2	В	59	THR	C-N	-39.10	0.44	1.34
16	Р	62	LYS	C-N	-30.49	0.64	1.34
16	Р	15	SER	C-N	20.55	1.81	1.34
1	А	1649	ALA	C-N	-17.39	0.94	1.34

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	1171	ILE	CA-C-N	-49.33	8.66	117.20
1	А	1171	ILE	C-N-CA	-46.87	4.53	121.70
2	В	59	THR	O-C-N	-39.36	59.73	122.70
2	В	49	PHE	O-C-N	-27.91	78.05	122.70
3	С	467	THR	N-CA-CB	23.78	155.48	110.30

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	1171	ILE	Mainchain,Peptide
1	А	121	GLY	Mainchain
1	А	1649	ALA	Mainchain
2	В	25	GLN	Peptide
2	В	49	PHE	Mainchain

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	А	33975	0	32349	2867	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	34713	0	33234	2520	0
3	С	30427	0	29349	1401	0
4	D	4680	0	4509	1322	0
5	Е	4440	0	4304	1005	0
6	F	996	0	1019	262	0
7	G	1024	0	883	185	0
8	Н	750	0	734	218	0
9	Ι	827	0	826	292	0
10	J	807	0	772	261	0
11	Κ	754	0	715	127	0
12	L	855	0	854	214	0
13	М	735	0	735	235	0
14	Ν	852	0	796	199	0
15	0	994	0	1017	307	0
16	Р	541	0	217	55	0
17	Q	1001	0	490	284	0
18	R	739	156	339	37	0
19	А	54	0	23	33	0
19	В	54	0	24	19	0
19	С	54	0	22	33	0
20	А	31	0	12	10	0
20	В	31	0	12	44	0
20	С	31	0	12	1	0
21	А	3	0	0	2	0
21	В	3	0	0	0	0
21	С	3	0	0	0	0
All	All	119374	156	113247	9374	0

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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 40.

The worst 5 of 9374 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)
10:J:86:CYS:SG	11:K:61:VAL:HG22	1.24	1.74
2:B:1474:MET:SD	2:B:1515:VAL:HG11	1.32	1.66
1:A:935:VAL:HG22	1:A:944:LEU:CD2	1.23	1.65
1:A:3232:ILE:HG12	1:A:3316:TRP:CZ3	1.14	1.65
2:B:582:MET:HE1	2:B:587:GLY:CA	1.26	1.65

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 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	P	erce	entiles
1	А	4391/4620~(95%)	4177 (95%)	189 (4%)	25~(1%)		25	66
2	В	4491/4595~(98%)	4255~(95%)	199 (4%)	37 (1%)		19	60
3	С	3923/4168~(94%)	3692 (94%)	208 (5%)	23 (1%)		25	66
4	D	569/657~(87%)	546 (96%)	16 (3%)	7 (1%)		13	50
5	Е	551/670~(82%)	531 (96%)	18 (3%)	2(0%)		34	72
6	F	126/133~(95%)	120 (95%)	6 (5%)	0		100	100
7	G	147/159~(92%)	134 (91%)	7 (5%)	6 (4%)		3	23
8	Н	89/92~(97%)	88 (99%)	1 (1%)	0	-	100	100
9	Ι	104/110~(94%)	100 (96%)	3 (3%)	1 (1%)		15	55
10	J	93/95~(98%)	90~(97%)	3 (3%)	0	-	100	100
11	K	88/93~(95%)	85~(97%)	3 (3%)	0	1	100	100
12	L	109/111~(98%)	104 (95%)	4 (4%)	1 (1%)		17	57
13	М	85/87~(98%)	83~(98%)	2 (2%)	0	1	100	100
14	Ν	112/117~(96%)	105 (94%)	7 (6%)	0	-	100	100
15	Ο	118/132~(89%)	112 (95%)	4 (3%)	2(2%)		9	42
16	Р	103/122~(84%)	90 (87%)	7 (7%)	6 (6%)		1	18
17	Q	189/202~(94%)	173 (92%)	13 (7%)	3 (2%)		9	44
18	R	148/160~(92%)	121 (82%)	19 (13%)	8 (5%)		2	19
All	All	15436/16323~(95%)	14606 (95%)	709 (5%)	121 (1%)		24	60

5 of 121 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	101	PRO
1	А	125	PRO
1	А	127	THR
1	А	151	ILE

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Mol	Chain	\mathbf{Res}	Type
1	А	1171	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	\mathbf{ntiles}
1	А	3430/4197~(82%)	3358~(98%)	72 (2%)	53	72
2	В	3520/4145~(85%)	3441 (98%)	79 (2%)	52	71
3	С	3139/3691~(85%)	3089~(98%)	50 (2%)	62	79
4	D	511/600~(85%)	507~(99%)	4 (1%)	81	89
5	Ε	488/597~(82%)	484 (99%)	4 (1%)	81	89
6	F	105/109~(96%)	104 (99%)	1 (1%)	76	86
7	G	86/149~(58%)	86 (100%)	0	100	100
8	Η	82/83~(99%)	82 (100%)	0	100	100
9	Ι	91/95~(96%)	91 (100%)	0	100	100
10	J	82/82~(100%)	81 (99%)	1 (1%)	71	83
11	Κ	80/82~(98%)	80 (100%)	0	100	100
12	L	90/99~(91%)	90 (100%)	0	100	100
13	М	78/78~(100%)	78 (100%)	0	100	100
14	Ν	84/104~(81%)	84 (100%)	0	100	100
15	0	108/119~(91%)	106 (98%)	2(2%)	57	75
17	Q	11/186~(6%)	11 (100%)	0	100	100
All	All	11985/14416 (83%)	11772 (98%)	213 (2%)	61	77

5 of 213 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	3032	ARG
2	В	4408	LYS
3	С	4050	GLN
2	В	3222	PRO

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Mol	Chain	Res	Type
2	В	3793	ASP

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 211 such side chains are listed below:

Mol	Chain	Res	Type
3	С	9	GLN
3	С	2483	ASN
12	L	28	GLN
3	С	126	ASN
3	С	1300	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 for Mogul analysis.

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).

Mal	Turne	Chain	Dec	I inly Bond lengths			Bond angles			
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
19	ADP	А	4701	21	24,29,29	0.95	1 (4%)	29,45,45	1.44	5 (17%)
19	ADP	В	5405	21	24,29,29	0.65	0	29,45,45	0.93	2 (6%)



Mal	Tuno	Chain	Dec	Tink	Bo	Bond lengths			Bond angles		
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
19	ADP	С	4306	21	24,29,29	0.66	0	29,45,45	0.86	2 (6%)	
20	ATP	С	4302	21	26,33,33	0.69	0	31,52,52	0.89	2 (6%)	
19	ADP	В	5406	21	24,29,29	0.66	0	29,45,45	0.75	1 (3%)	
20	ATP	В	5403	21	26,33,33	0.66	0	31,52,52	0.83	1 (3%)	
19	ADP	С	4305	3,21	24,29,29	0.70	1 (4%)	29,45,45	1.03	2 (6%)	
19	ADP	А	4703	21	24,29,29	0.94	1 (4%)	29,45,45	1.47	4 (13%)	
20	ATP	А	4702	21	26,33,33	0.93	1 (3%)	31,52,52	1.40	4 (12%)	

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
19	ADP	А	4701	21	-	7/12/32/32	0/3/3/3
19	ADP	В	5405	21	-	1/12/32/32	0/3/3/3
19	ADP	С	4306	21	-	4/12/32/32	0/3/3/3
20	ATP	С	4302	21	-	1/18/38/38	0/3/3/3
19	ADP	В	5406	21	-	2/12/32/32	0/3/3/3
20	ATP	В	5403	21	-	1/18/38/38	0/3/3/3
19	ADP	С	4305	3,21	-	5/12/32/32	0/3/3/3
19	ADP	А	4703	21	-	6/12/32/32	0/3/3/3
20	ATP	А	4702	21	-	3/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	А	4703	ADP	C5-C4	2.32	1.47	1.40
19	А	4701	ADP	C5-C4	2.29	1.47	1.40
20	А	4702	ATP	C5-C4	2.11	1.46	1.40
19	С	4305	ADP	C8-N7	-2.11	1.30	1.34

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
20	А	4702	ATP	PB-O3B-PG	-3.71	120.09	132.83
19	А	4703	ADP	PA-O3A-PB	-3.55	120.64	132.83
19	А	4701	ADP	C3'-C2'-C1'	3.52	106.28	100.98
19	А	4703	ADP	C3'-C2'-C1'	3.47	106.19	100.98

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
20	А	4702	ATP	N3-C2-N1	-3.27	123.57	128.68

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	А	4701	ADP	PB-O3A-PA-O5'
19	А	4701	ADP	C5'-O5'-PA-O1A
19	А	4701	ADP	C5'-O5'-PA-O2A
19	А	4703	ADP	PB-O3A-PA-O5'
19	А	4703	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

9 monomers are inv	olved in 140	short contacts:
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	А	4701	ADP	12	0
19	В	5405	ADP	16	0
19	С	4306	ADP	8	0
20	С	4302	ATP	1	0
19	В	5406	ADP	3	0
20	В	5403	ATP	44	0
19	С	4305	ADP	25	0
19	А	4703	ADP	21	0
20	А	4702	ATP	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





















5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	В	10
1	А	9
16	Р	4
4	D	2
7	G	1
18	R	1

The worst 5 of 27 chain breaks are listed below:



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	А	3250:PRO	С	3251:ILE	N	5.80
1	А	3251:ILE	С	3252:GLN	N	4.89
1	А	24:LYS	С	25:ASP	N	3.36
1	В	79:PRO	С	80:PRO	N	3.22
1	D	216:HIS	С	217:GLN	N	2.93



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-16312. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



The images above show the map projected in three orthogonal directions.



6.2 Central slices (i)

6.2.1 Primary map



X Index: 37



Y Index: 37



Z Index: 37

6.2.2 Raw map



X Index: 37

Y Index: 37

Z Index: 37

The images above show central slices of the map in three orthogonal directions.



6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 41



Y Index: 43



Z Index: 21

6.3.2 Raw map



X Index: 41

Y Index: 43

Z Index: 35

The images above show the largest variance slices of the map in three orthogonal directions.



6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



7.2 Volume estimate (i)



The volume at the recommended contour level is 49562 $\rm nm^3;$ this corresponds to an approximate mass of 44771 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.033 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.033 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\mathbf{Bosolution ostimato}(\mathbf{\hat{A}})$	Estim	Estimation criterion (FSC cut-off)				
Resolution estimate (A)	0.143	0.5	Half-bit			
Reported by author	30.30	-	-			
Author-provided FSC curve	-	-	-			
Unmasked-calculated*	-	35.34	27.62			

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-16312 and PDB model 8BX8. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).



9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.8300	0.0430	
А	0.8230	0.0470	
В	0.8570	0.0480	
С	0.7930	0.0360	
D	0.9090	0.0380	
E	0.9000	0.0390	
F	0.8060	0.0450	
G	0.7350	0.0200	
Н	0.9840	0.0390	
Ι	0.8590	0.0400	
J	0.9870	0.0630	
К	0.9720	0.0530	
L	0.8830	0.0290	
М	0.9310	0.0400	
N	0.8960	0.0440	
0	0.9600	0.0410	
Р	0.9850	0.0670	
Q	0.2450	0.0610	
R	0.3110	-0.0180	

