



wwPDB EM Validation Summary Report ⓘ

Dec 30, 2024 – 10:45 AM EST

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

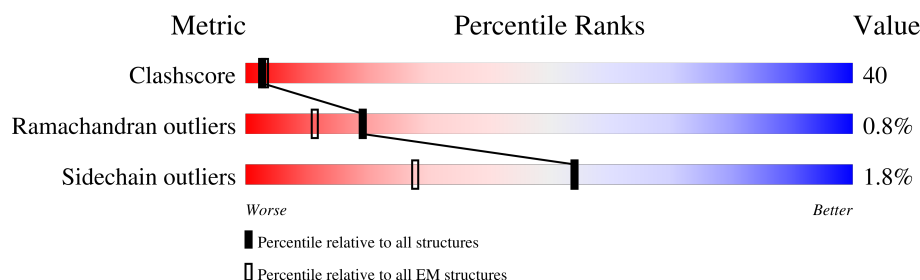
1 Overall quality at a glance

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.



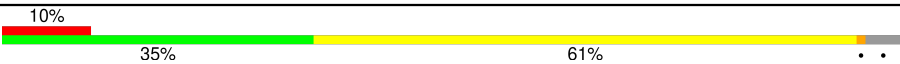
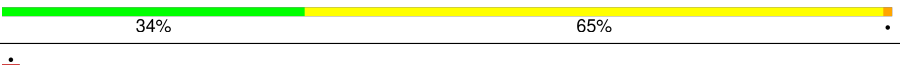
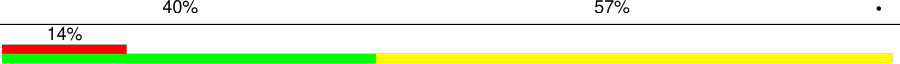
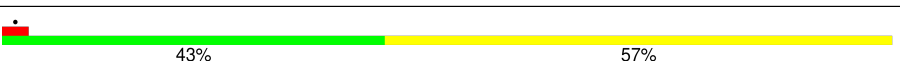
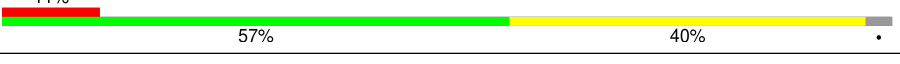





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	Quality of chain
1	A	4620	<div> <div>16%</div> <div>72%</div> <div>23%</div> <div>• •</div> </div>
2	B	4595	<div> <div>13%</div> <div>72%</div> <div>25%</div> <div>• •</div> </div>
3	C	4168	<div> <div>18%</div> <div>77%</div> <div>16%</div> <div>• 5%</div> </div>
4	D	657	<div> <div>8%</div> <div>38%</div> <div>49%</div> <div>• 12%</div> </div>
5	E	670	<div> <div>7%</div> <div>37%</div> <div>45%</div> <div>• 17%</div> </div>
6	F	133	<div> <div>18%</div> <div>47%</div> <div>48%</div> <div>• •</div> </div>
7	G	159	<div> <div>30%</div> <div>51%</div> <div>35%</div> <div>• 7% 5%</div> </div>
8	H	92	<div> <div>37%</div> <div>62%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	110	
10	J	95	
11	K	93	
12	L	111	
13	M	87	
14	N	117	
15	O	132	
16	P	122	
17	Q	202	
18	R	160	

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	A	4701	-	-	X	-
19	ADP	A	4703	-	-	X	-
19	ADP	B	5405	-	-	X	-
19	ADP	C	4305	-	-	X	-
20	ATP	A	4702	-	-	X	-
20	ATP	B	5403	-	-	X	-
21	MG	A	4705	-	-	X	-

2 Entry composition

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	A	4453	Total	C	N	O	S	0	0
			33975	21575	5801	6441	158		

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4519	Total	C	N	O	S	0	0
			34713	22055	5945	6563	150		

- 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	C	3947	Total	C	N	O	S	0	0
			30427	19395	5159	5724	149		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	128	Total	C	N	O	S	0	0
			996	625	176	193	2		

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

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

- Molecule 8 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	91	Total	C	N	O	S	0	0
			750	483	124	139	4		

- Molecule 9 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	106	Total	C	N	O	S	0	0
			827	526	134	161	6		

- Molecule 10 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	95	Total	C	N	O	S	0	0
			807	527	135	140	5		

- Molecule 11 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	90	Total	C	N	O	S	0	0
			754	489	124	137	4		

- Molecule 12 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	111	Total	C	N	O	S	0	0
			855	555	145	152	3		

- Molecule 13 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	87	Total	C	N	O	S	0	0
			735	477	123	130	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	114	Total	C	N	O	S	0	0
			852	542	142	165	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	120	Total	C	N	O	S	0	0
			994	639	173	179	3		

- Molecule 16 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	109	Total	C	N	O	0	0
			541	323	109	109		

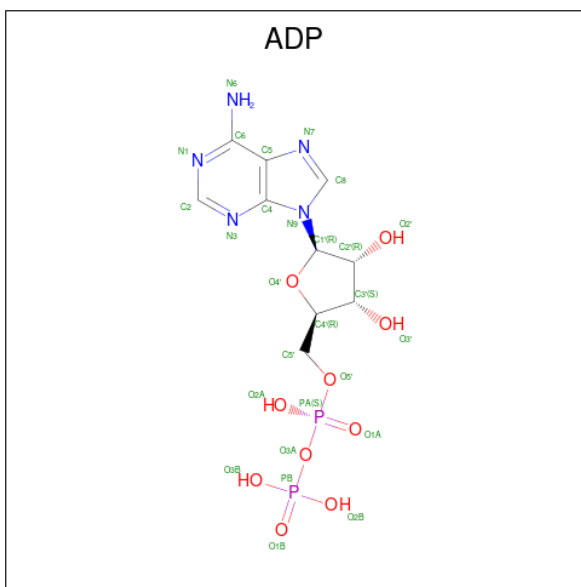
- Molecule 17 is a protein called Dynein light chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	191	Total	C	N	O	0	0
			1001	607	202	192		

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

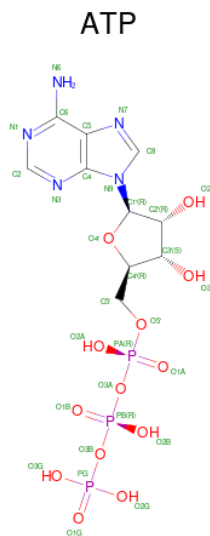
Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	150	Total	C	H	N	O	0	0
			895	439	156	150	150		

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

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



Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 31	C 10	N 5	O 13	P 3	0
20	B	1	Total 31	C 10	N 5	O 13	P 3	0
20	C	1	Total 31	C 10	N 5	O 13	P 3	0

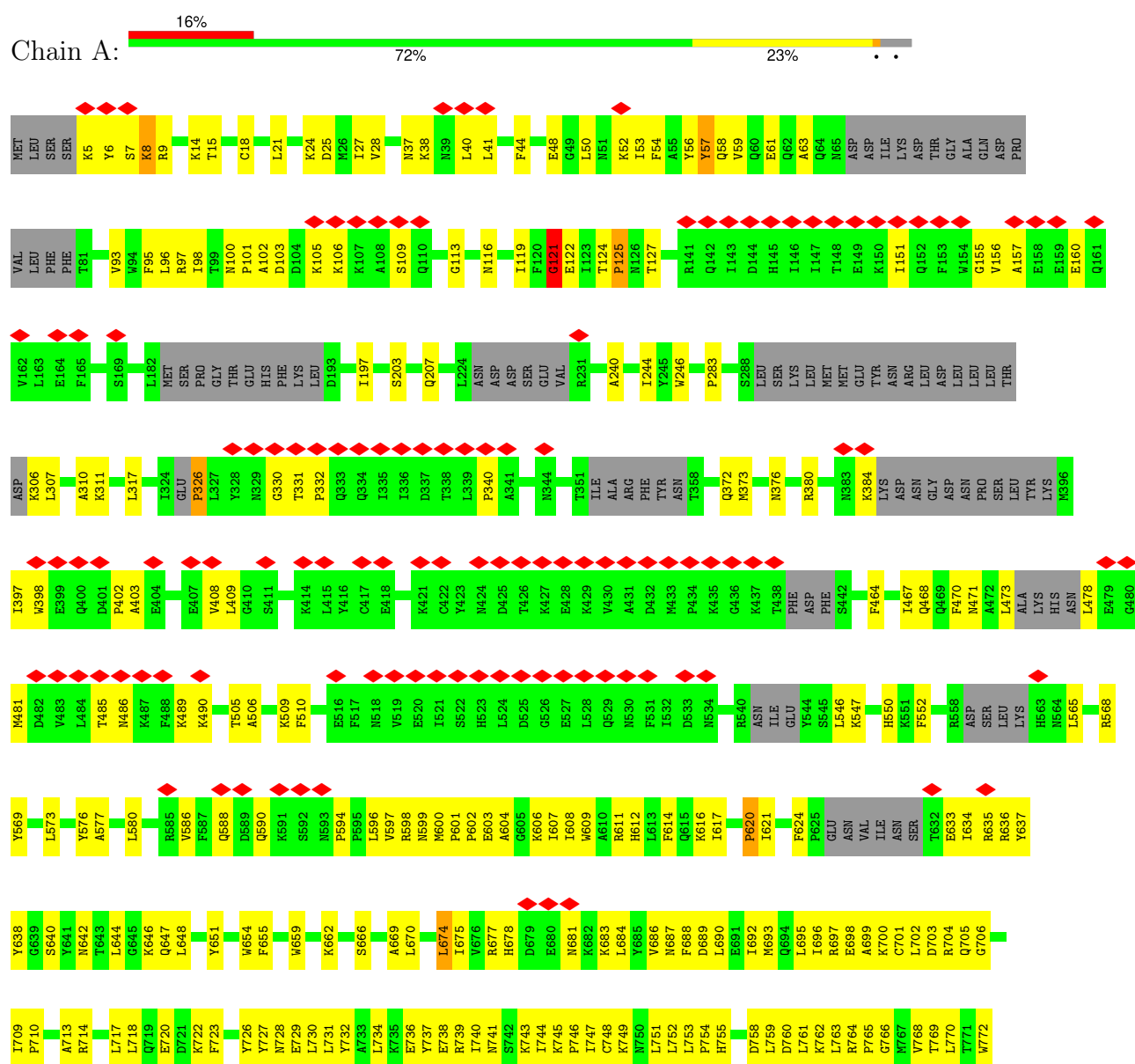
- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

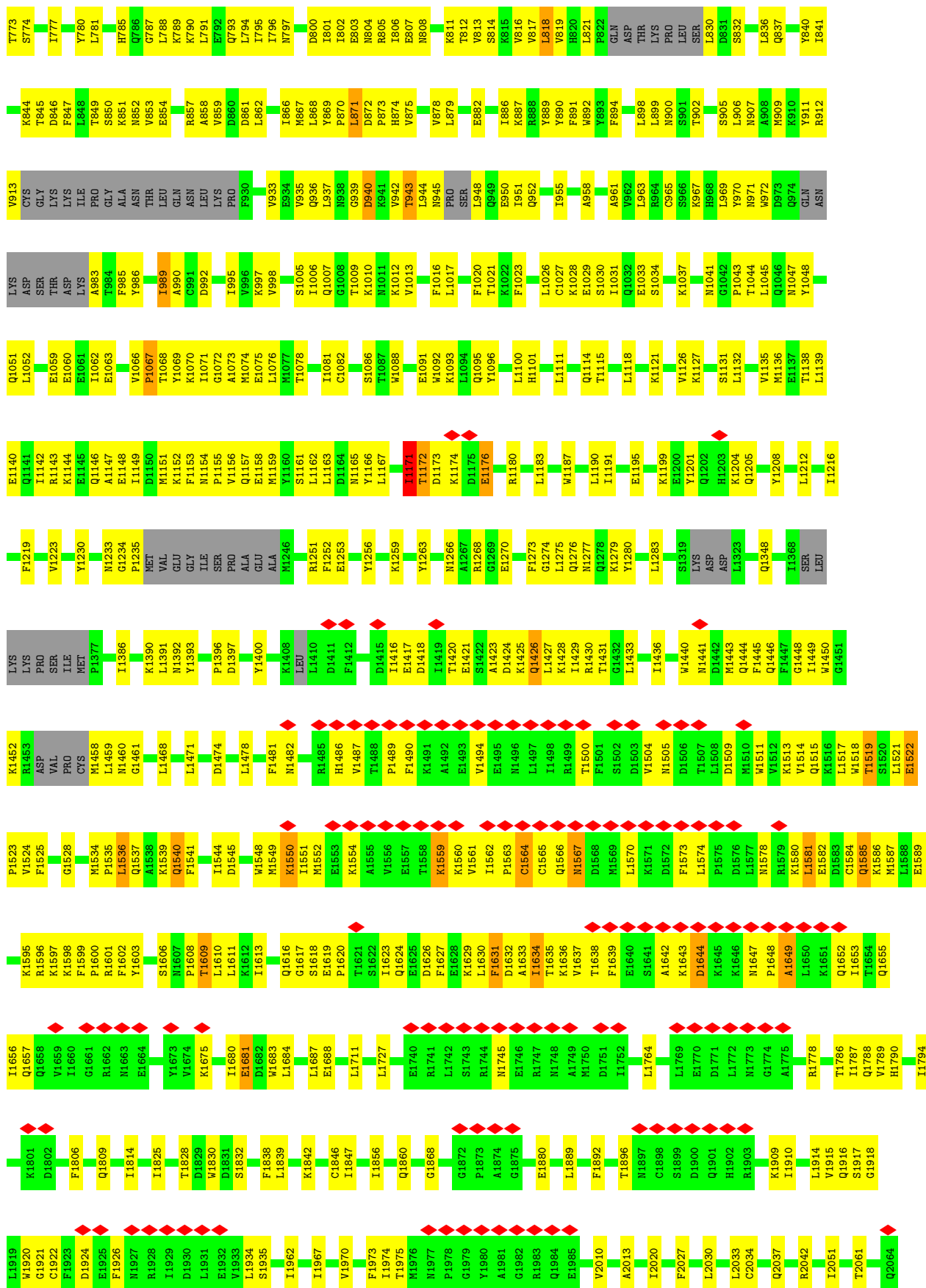
Mol	Chain	Residues	Atoms	AltConf
21	A	3	Total Mg 3 3	0
21	B	3	Total Mg 3 3	0
21	C	3	Total Mg 3 3	0

3 Residue-property plots

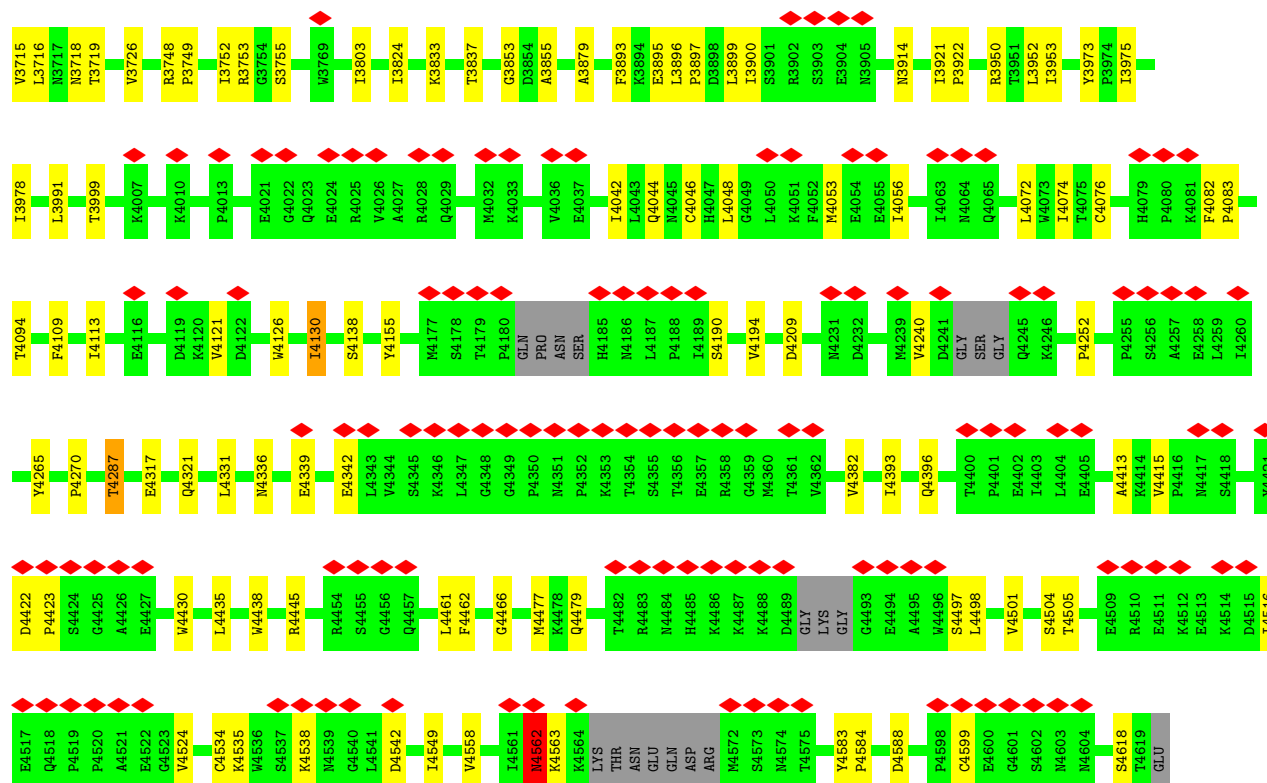
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

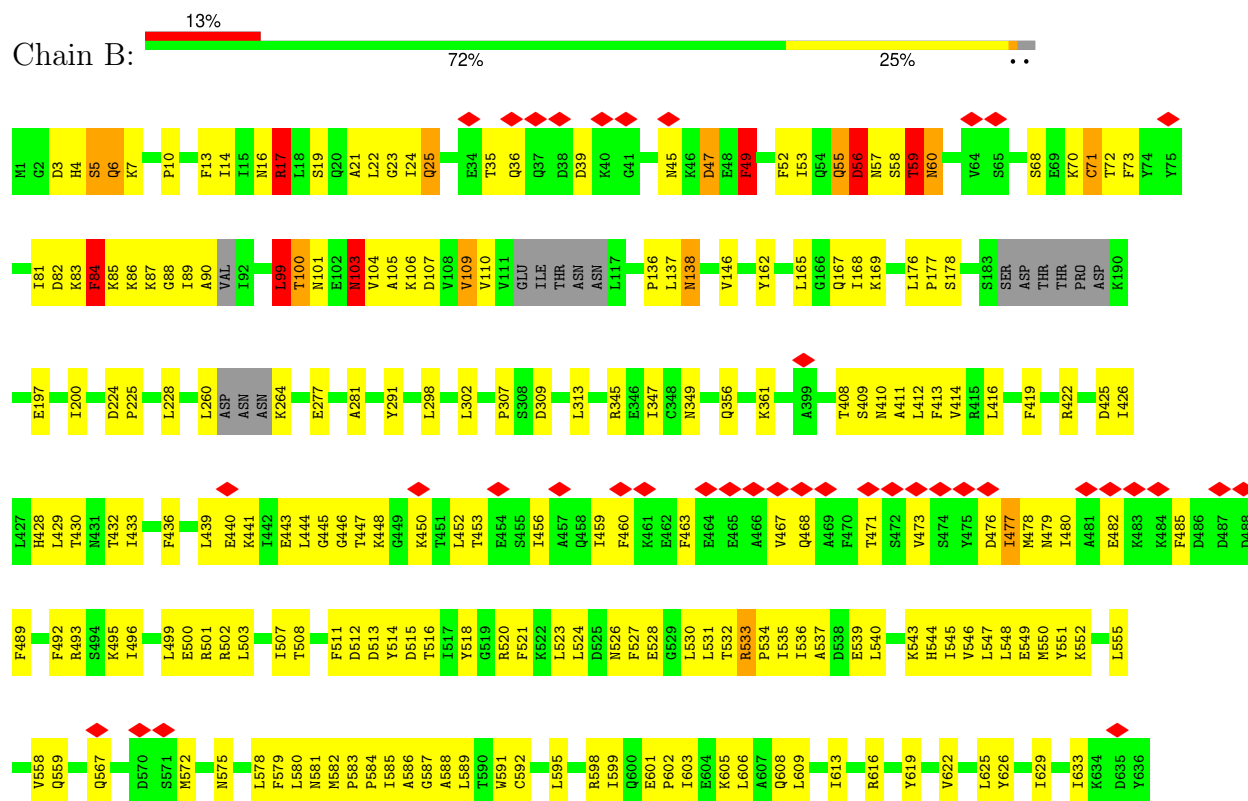






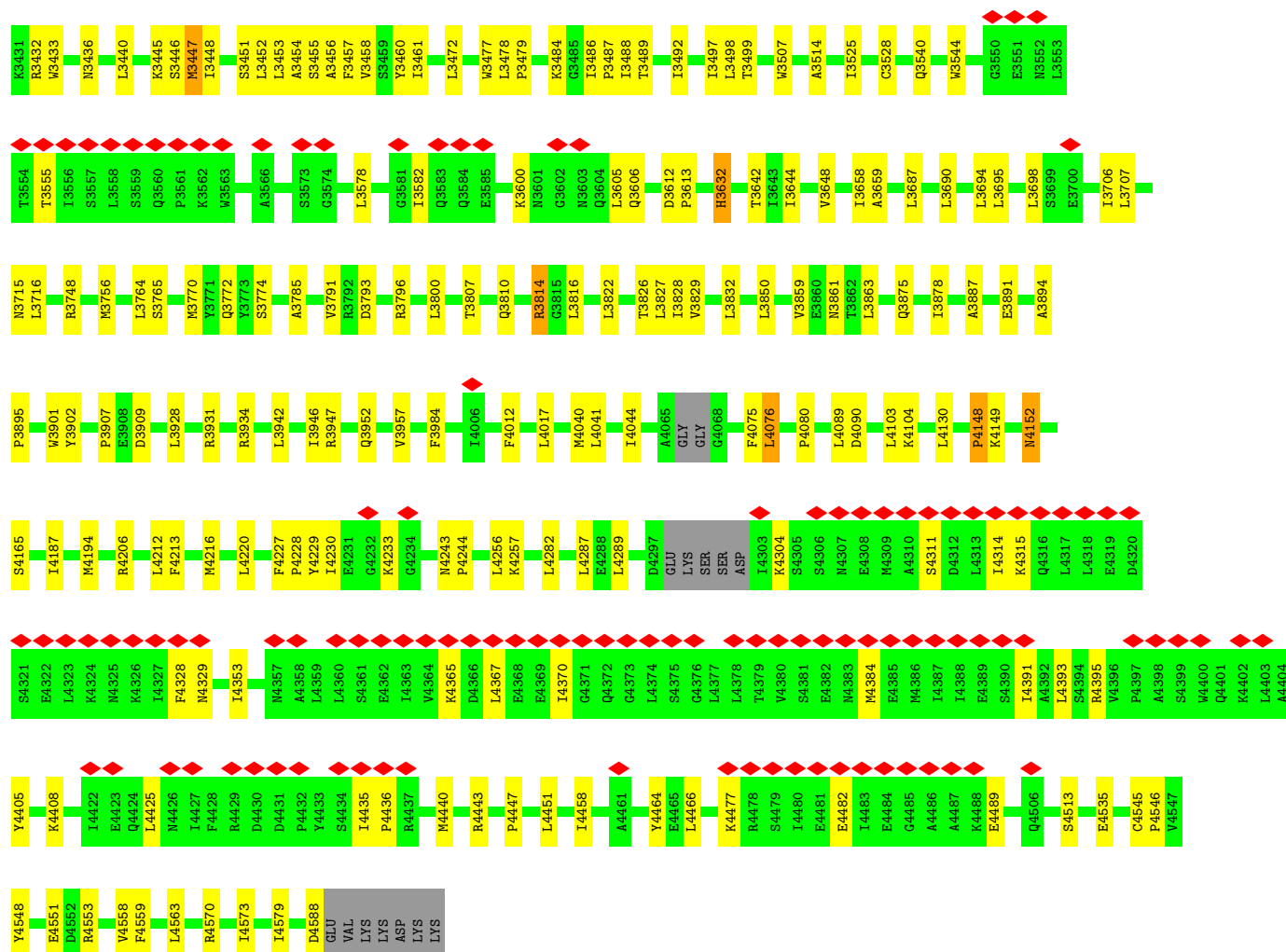


• Molecule 2: Outer arm dynein beta heavy chain

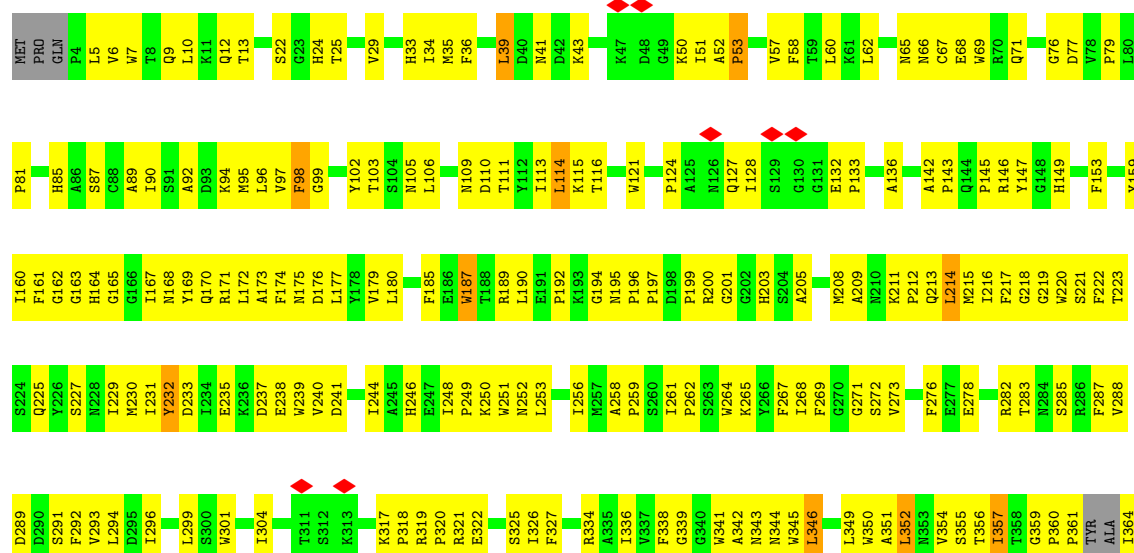
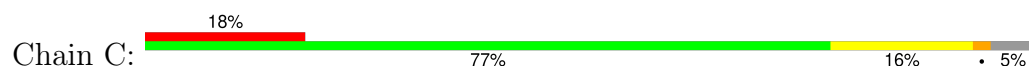


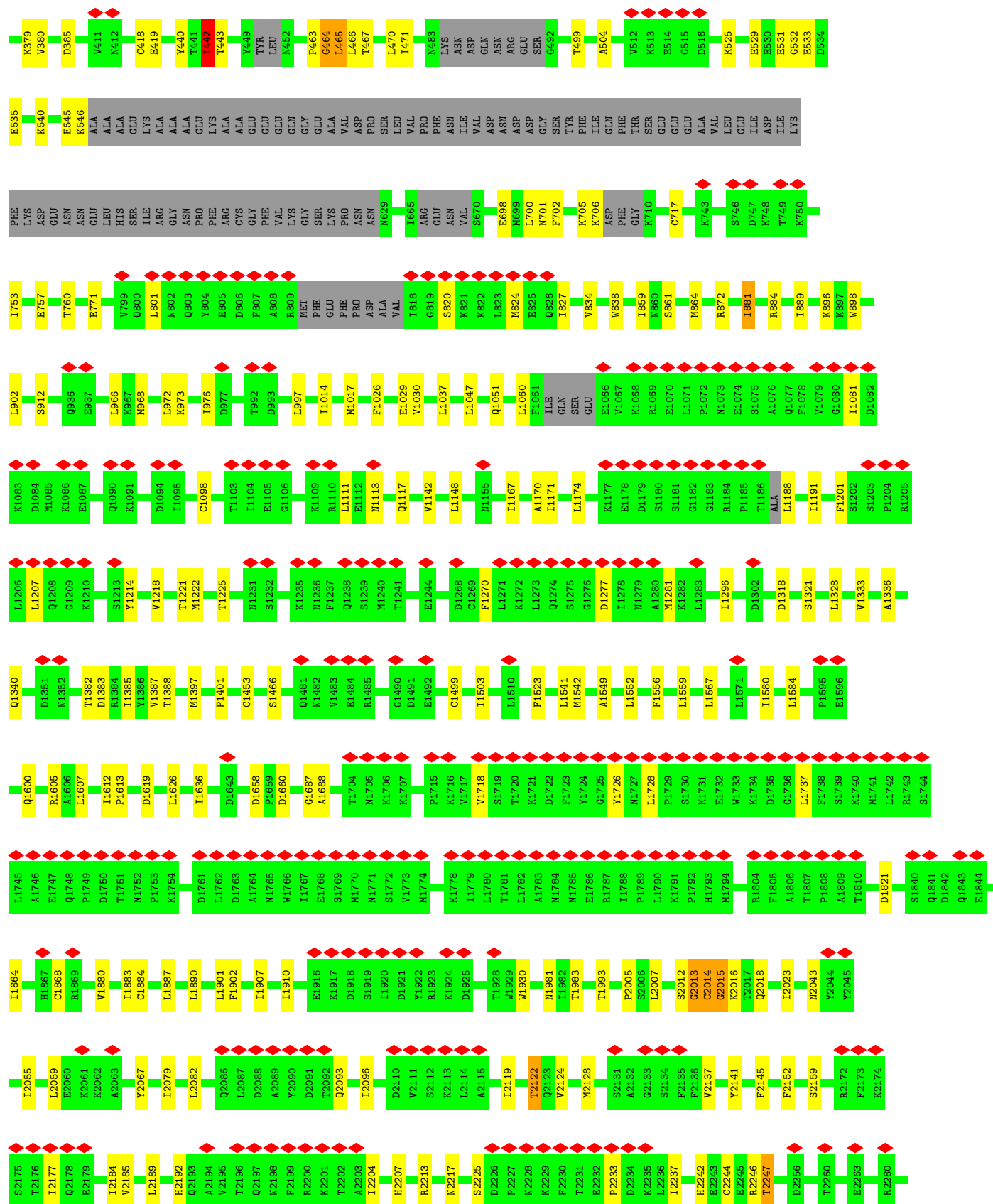


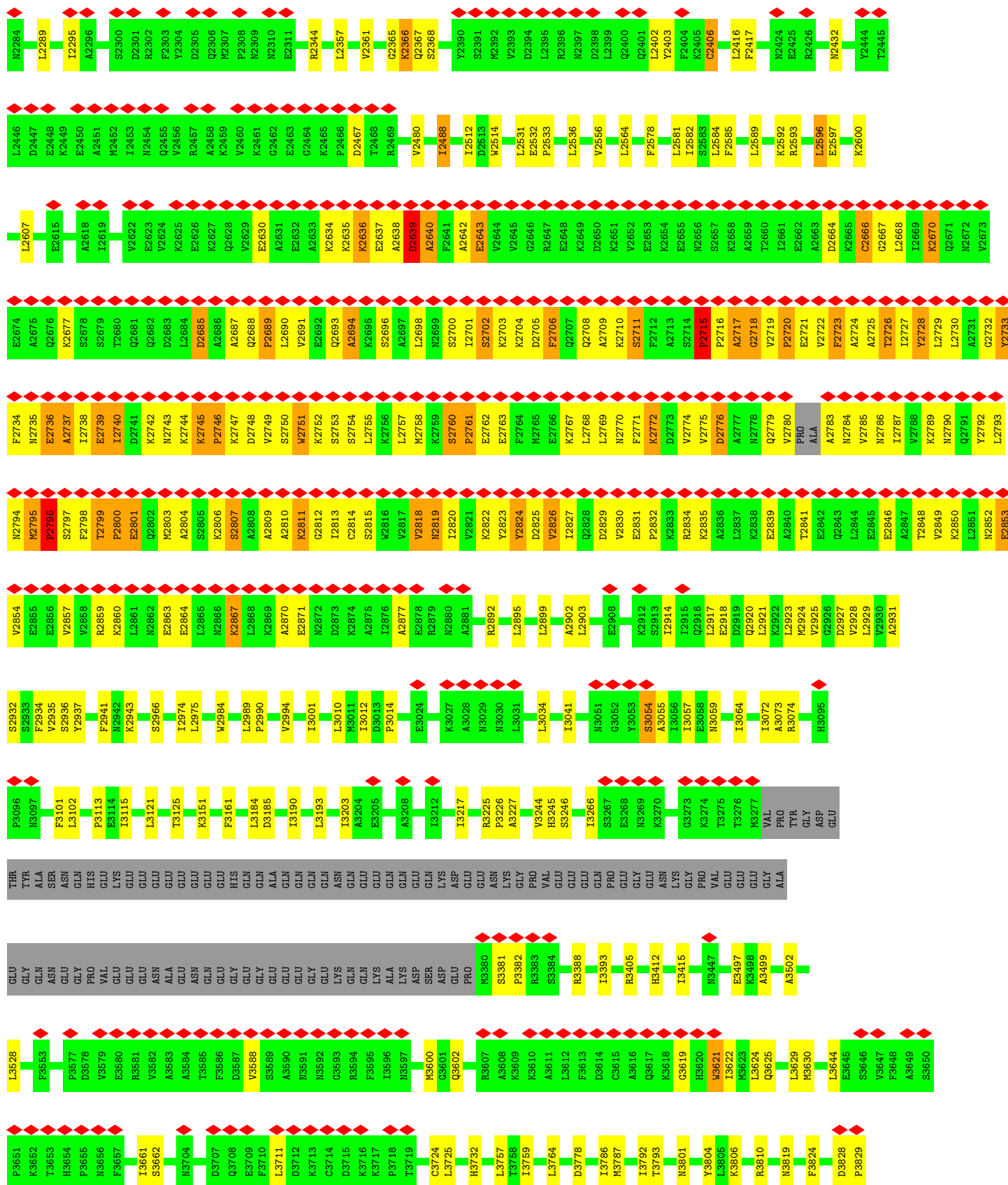
Q1945	S1946	G1947	E1954	F1955	N1956	N1957	V1966	N2005	P2006	G2007	Y2008	A2009	G2010	R2011	R2023	N2038	N2039	L2040	G2044	R2049	L2058	L2065	L2066	K2070	D2073	A2078	L2083	R2084	Q2085	D2095	T2116	D2117	D2118	L2121	D2128	L2129	F2130	P2131	K2132	L2133	D2134	F2135																	
P2136	T2150	V2176	R2177	P2185	S2188	G2189	K2190	T2191	C2192	N2203	N2214	T2219	S2220	D2221	G2225	A2226	Y2227	T2228	K2229	T2230	K2231	E2232	P2233	Y2234	N2235	G2236	V2237	V2240	K2243	K2247	N2248	E2249	Y2252	K2253	A2254	W2260	D2264	I2267	P2268	P2269	E2270	H2271	I2272	E2273															
S2274	K2283	Y2284	T2285	T2286	L2287	Y2288	S2289	S2289	N2290	D2291	L2292	L2293	F2294	L2295	R2300	L2301	L2302	F2303	E2304	L2308	R2309	N2310	A2311	E2326	M2332	P2333	Y2334	M2335	N2345	K2348	Q2349	A2354	E2358	Y2359	P2360	L2361	D2362	D2363	D2364	V2365	A2366	K2367	S2368	D2383	P2395	L2409	D2410	A2411											
L2412	L2413	T2414	Q2415	T2416	L2417	P2418	K2419	L2420	K2421	Q2422	M2423	K2424	E2425	E2426	D2427	E2428	K2429	Q2430	A2431	L2432	F2436	L2441	G2445	N2462	C2479	D2485	T2486	M2487	E2488	N2489	K2490	N2491	N2492	T2493	W2494	L2500	P2501	N2502	D2503	V2512	A2513	T2514	T2515	H2516	R2519	L2526	R2531												
A2540	G2543	K2544	T2545	A2546	R2556	P2557	E2558	Q2559	V2560	S2569	L2574	Q2577	K2586	K2587	N2588	G2589	R2590	N2591	Y2592	I2601	M2609	P2610	K2614	Y2615	T2617	Q2618	S2619	P2620	I2621	Q2622	R2625	R2636	E2637	Q2638	L2639	E2640	E2641	F2644	L2649	N2655	V2663	D2664	L2665																
R2666	L2667	Q2668	N2676	K2685	T2686	L2687	S2690	L2696	S2697	T2698	L2699	D2700	D2701	K2702	A2707	V2711	S2731	A2732	F2741	R2742	T2754	T2755	P2756	G2757	Q2758	Y2759	S2760	Q2761	Q2762	L2767	L2770	K2776	D2781	L2800	T2814	A2815	E2816	P2817	L2818	L2819	F2820	Y2834	T2835																
Q2836	I2839	P2840	L2846	L2862	V2863	L2864	E2870	H2871	V2872	L2879	N2885	G2893	T2904	I2911	N2927	Q2930	E2931	K2934	K2935	L2936	A2937	K2938	P2939	R2944	L2959	I2960	I2962	N2963	L2966	I2971	L2974	P2975	P2976	K2977	E2978	D2979	M2980	D2981	S2982	L2983	V2984																		
S2985	G2986	V2987	R2988	N2989	E2990	A2991	K2992	G2993	E2994	G2995	V2996	D2997	N2998	N2999	N3000	L3001	T3002	A3003	L3004	T3005	S3006	Y3007	F3008	K3017	V3018	S3023	I3031	K3032	N3041	N3042	T3043	D3046	V3059	F3063	I3067	L3074	S3077	T3078	S3079	L3080	N3081	M3082	V3085	I3089	A3092														
Y3103	T3106	K3109	L3112	E3113	L3114	L3115	F3117	G3118	K3119	K3120	L3121	L3122	K3125	T3129	Q3130	R3131	Q3132	I3133	Y3136	G3139	L3140	L3143	A3144	Q3147	V3150	L3153	Q3154	E3155	E3156	L3157	K3160	M3161	V3162	E3163	V3164	N3165	K3166	E3169	E3170	T3171	D3172	L3173	L3174	L3175	E3176														
K3177	V3178	G3179	K3180	E3181	S3182	A3183	L3184	A3185	E3186	E3187	E3188	K3189	T3190	I3191	A3192	N3193	A3194	E3195	E3196	E3197	K3198	T3199	N3200	V3201	F3263	N3264	Q3265	G3266	I3267	T3268	L3269	N3270	D3271	P3272	K3211	E3212	A3213	T3214	E3215	A3216	L3217	A3218	E3219	A3220	L3221	P3222	A3223	L3224	A3225	P3226	Q3287	A3289	F3290	I3291	D3292	K3293	V3294	K3295	S3296
P3237	H3238	G3239	T3240	E3241	M3242	K3243	N3244	L3245	G3246	S3247	P3248	P3249	A3250	G3251	V3252	I3253	L3254	T3255	A3256	R3257	V3258	P3259	L3260	L3261	F3263	N3264	E3265	G3266	I3267	T3268	L3269	N3270	D3271	P3272	K3211	E3212	A3213	T3214	E3215	A3216	L3217	A3218	E3219	A3220	L3221	P3222	A3223	L3224	A3225	P3226	Q3287	A3289	F3290	I3291	D3292	K3293	V3294	K3295	S3296
F3297	D3298	G3299	E3300	N3301	I3302	E3303	P3304	N3305	I3306	I3307	E3308	Q3309	S3310	N3311	K3312	I3313	I3314	Q3315	D3316	P3317	S3318	K3319	K3320	F3321	N3322	E3323	K3324	D3325	M3326	A3327	G3328	Q3329	S3330	Y3331	A3332	A3333	S3334	K3335	L3336	C3337	A3338	W3339	A3340	V3341	N3342	I3343	V3344	T3345	F3346	N3347	K3348	I3349	F3350	K3351	Q3352	V3353	K3354	P3355	L3356
Q3357	D3358	A3359	Q3360	K3361	Q3362	A3363	N3364	E3365	I3366	L3367	E3368	F3369	K3370	E3373	L3374	A3375	I3376	V3377	K3378	K3379	R3380	V3381	E3382	E3383	L3384	N3385	A3386	K3387	V3388	N3389	K3392	R3393	I3394	L3395	E3399	K3400	K3401	K3402	K3403	L3404	Y3405	E3406	Q3407	A3408	C3412	L3422	V3423	L3426	A3427	G3428	E3429	N3430							

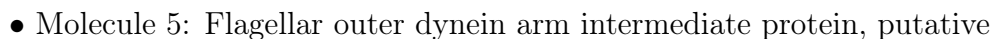


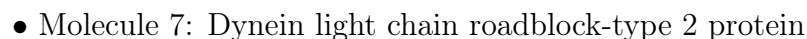
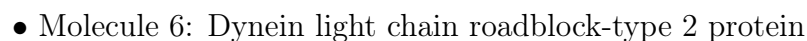
• Molecule 3: Dynein-1-alpha heavy chain, flagellar inner arm I1 complex protein, putative

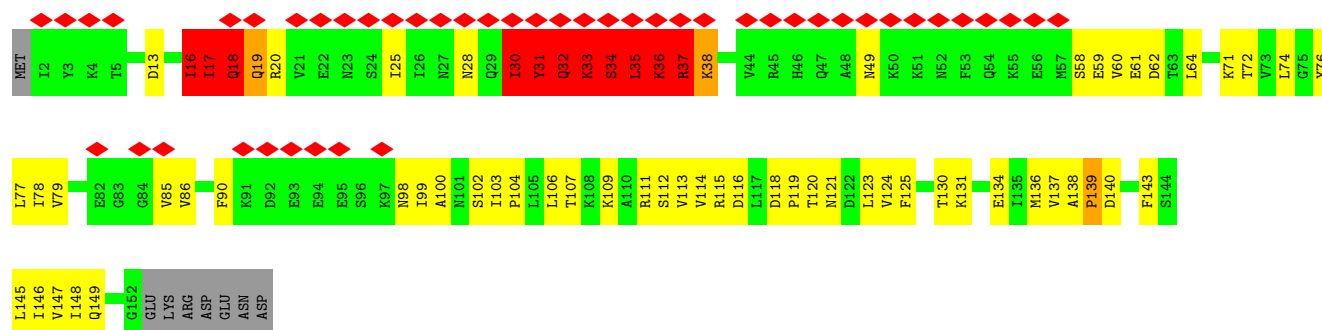




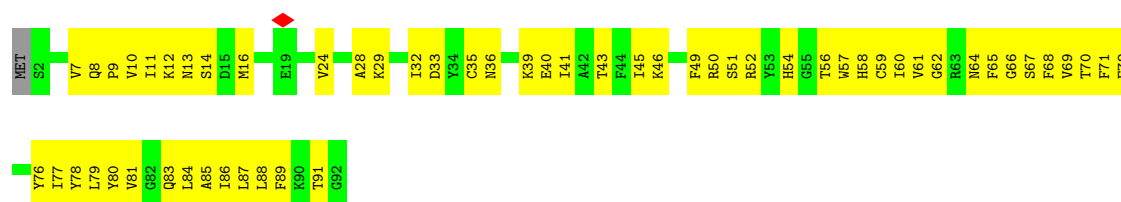




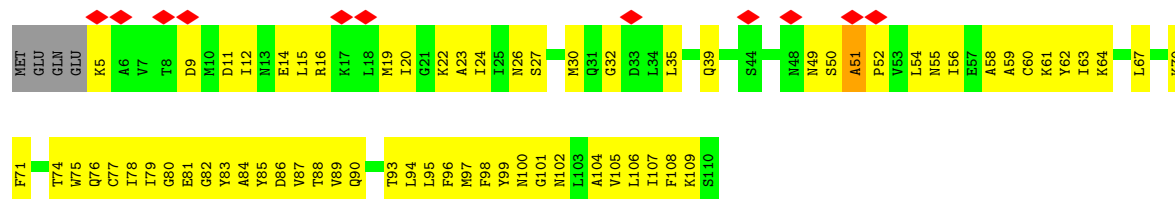




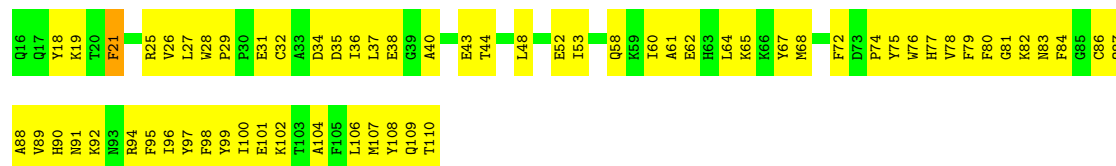
• Molecule 8: Dynein light chain



• Molecule 9: Dynein light chain

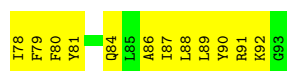


• Molecule 10: Dynein light chain

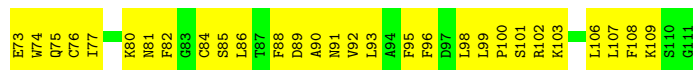


• Molecule 11: Dynein light chain





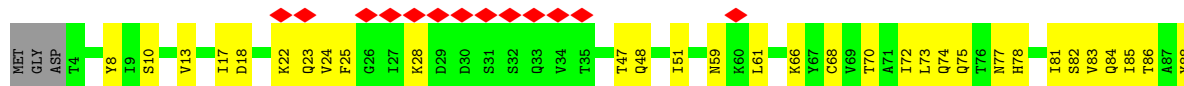
• Molecule 12: Dynein light chain



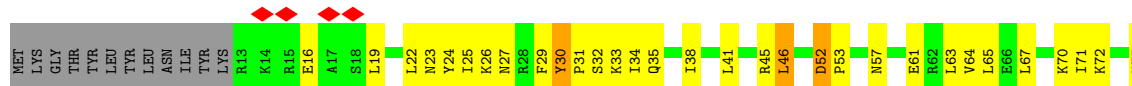
• Molecule 13: Dynein light chain



• Molecule 14: Dynein light chain tctex-type 1 protein

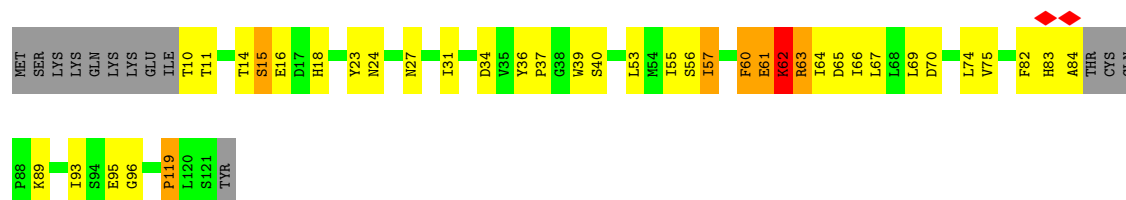


• Molecule 15: Dynein light chain 2A

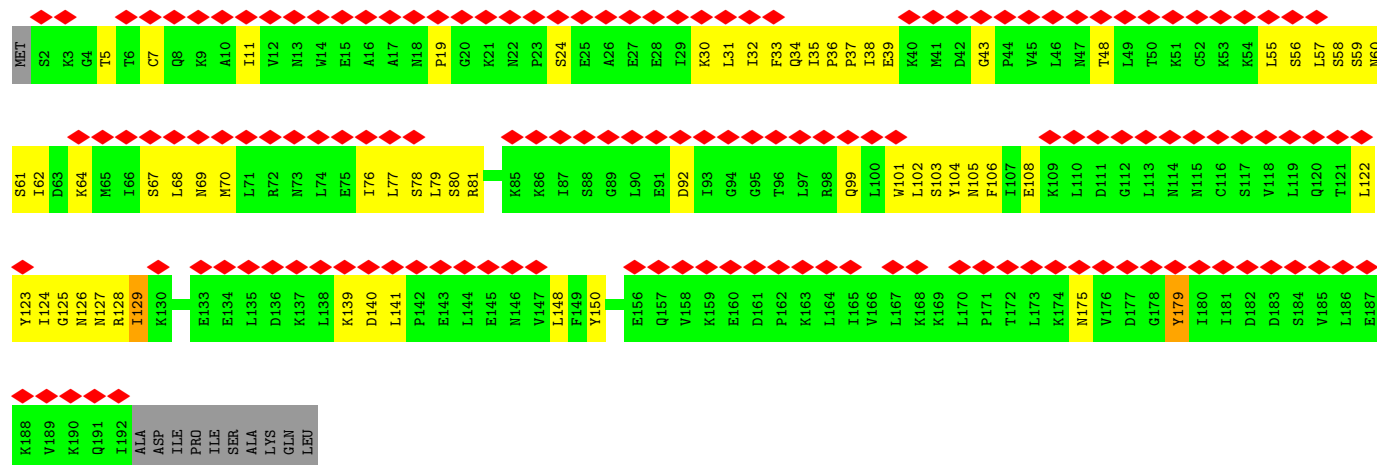


• Molecule 16: Thioredoxin

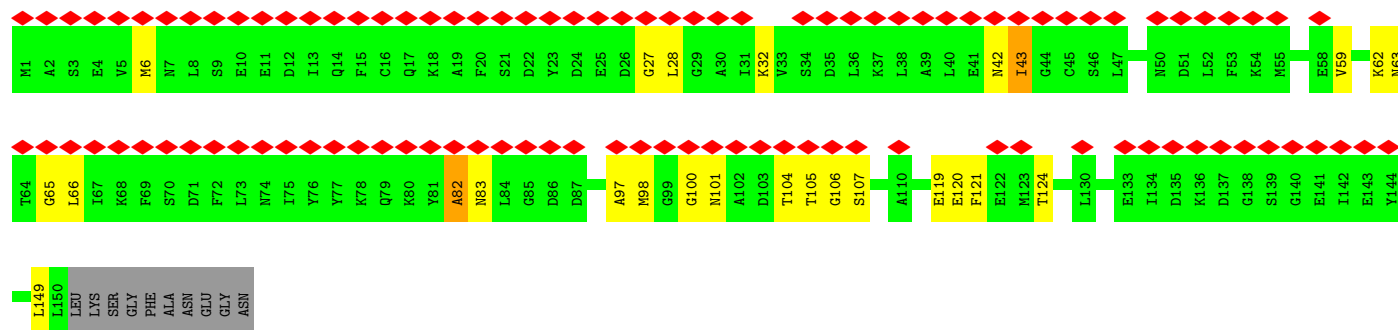
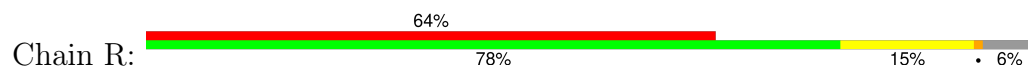




• Molecule 17: Dynein light chain 1



• Molecule 18: Dynein light chain 4A



4 Experimental information

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 (\AA)	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 (\AA)	8.49, 8.49, 8.49	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.72	7/34544 (0.0%)	0.81	24/46728 (0.1%)
2	B	0.72	7/35318 (0.0%)	0.82	37/47792 (0.1%)
3	C	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	E	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	H	0.63	0/767	0.61	0/1031
9	I	0.66	0/838	0.59	0/1131
10	J	0.61	0/832	0.65	0/1119
11	K	0.62	0/776	0.60	0/1038
12	L	0.61	0/872	0.61	0/1176
13	M	0.62	0/752	0.61	0/1006
14	N	0.66	0/864	0.67	0/1175
15	O	0.64	0/1012	0.64	0/1358
16	P	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	A	0	4
2	B	0	11
3	C	0	2
4	D	0	1
7	G	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	P	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)	Ideal(Å)
1	A	1067	PRO	N-CD	51.23	2.19	1.47
2	B	59	THR	C-N	-39.10	0.44	1.34
16	P	62	LYS	C-N	-30.49	0.64	1.34
16	P	15	SER	C-N	20.55	1.81	1.34
1	A	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(°)	Ideal(°)
1	A	1171	ILE	CA-C-N	-49.33	8.66	117.20
1	A	1171	ILE	C-N-CA	-46.87	4.53	121.70
2	B	59	THR	O-C-N	-39.36	59.73	122.70
2	B	49	PHE	O-C-N	-27.91	78.05	122.70
3	C	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	A	1171	ILE	Mainchain,Peptide
1	A	121	GLY	Mainchain
1	A	1649	ALA	Mainchain
2	B	25	GLN	Peptide
2	B	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	A	33975	0	32349	2867	0

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

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4391/4620 (95%)	4177 (95%)	189 (4%)	25 (1%)	22	60
2	B	4491/4595 (98%)	4255 (95%)	199 (4%)	37 (1%)	16	55
3	C	3923/4168 (94%)	3692 (94%)	208 (5%)	23 (1%)	22	60
4	D	569/657 (87%)	546 (96%)	16 (3%)	7 (1%)	11	44
5	E	551/670 (82%)	531 (96%)	18 (3%)	2 (0%)	30	68
6	F	126/133 (95%)	120 (95%)	6 (5%)	0	100	100
7	G	147/159 (92%)	134 (91%)	7 (5%)	6 (4%)	2	18
8	H	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
9	I	104/110 (94%)	100 (96%)	3 (3%)	1 (1%)	13	49
10	J	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
11	K	88/93 (95%)	85 (97%)	3 (3%)	0	100	100
12	L	109/111 (98%)	104 (95%)	4 (4%)	1 (1%)	14	52
13	M	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
14	N	112/117 (96%)	105 (94%)	7 (6%)	0	100	100
15	O	118/132 (89%)	112 (95%)	4 (3%)	2 (2%)	7	37
16	P	103/122 (84%)	90 (87%)	7 (7%)	6 (6%)	1	14
17	Q	189/202 (94%)	173 (92%)	13 (7%)	3 (2%)	8	38
18	R	148/160 (92%)	121 (82%)	19 (13%)	8 (5%)	1	15
All	All	15436/16323 (95%)	14606 (95%)	709 (5%)	121 (1%)	19	55

5 of 121 Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	A	1171	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3430/4197 (82%)	3358 (98%)	72 (2%)	48	66
2	B	3520/4145 (85%)	3441 (98%)	79 (2%)	47	65
3	C	3139/3691 (85%)	3089 (98%)	50 (2%)	58	73
4	D	511/600 (85%)	507 (99%)	4 (1%)	79	85
5	E	488/597 (82%)	484 (99%)	4 (1%)	79	85
6	F	105/109 (96%)	104 (99%)	1 (1%)	73	82
7	G	86/149 (58%)	86 (100%)	0	100	100
8	H	82/83 (99%)	82 (100%)	0	100	100
9	I	91/95 (96%)	91 (100%)	0	100	100
10	J	82/82 (100%)	81 (99%)	1 (1%)	67	78
11	K	80/82 (98%)	80 (100%)	0	100	100
12	L	90/99 (91%)	90 (100%)	0	100	100
13	M	78/78 (100%)	78 (100%)	0	100	100
14	N	84/104 (81%)	84 (100%)	0	100	100
15	O	108/119 (91%)	106 (98%)	2 (2%)	52	69
17	Q	11/186 (6%)	11 (100%)	0	100	100
All	All	11985/14416 (83%)	11772 (98%)	213 (2%)	54	71

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

Mol	Chain	Res	Type
2	B	3032	ARG
2	B	4408	LYS
3	C	4050	GLN
2	B	3222	PRO

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Mol	Chain	Res	Type
2	B	3793	ASP

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

Mol	Chain	Res	Type
3	C	9	GLN
3	C	2483	ASN
12	L	28	GLN
3	C	126	ASN
3	C	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 oligosaccharides 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	ATP	B	5403	21	28,33,33	0.74	0	34,52,52	0.78	1 (2%)
20	ATP	A	4702	21	28,33,33	0.88	0	34,52,52	1.12	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	ADP	B	5406	21	24,29,29	0.73	0	29,45,45	0.76	1 (3%)
20	ATP	C	4302	21	28,33,33	0.68	0	34,52,52	0.90	2 (5%)
19	ADP	C	4306	21	24,29,29	0.72	0	29,45,45	1.04	2 (6%)
19	ADP	C	4305	3,21	24,29,29	0.77	1 (4%)	29,45,45	1.24	3 (10%)
19	ADP	A	4701	21	24,29,29	0.84	0	29,45,45	1.37	4 (13%)
19	ADP	B	5405	21	24,29,29	0.71	0	29,45,45	0.83	1 (3%)
19	ADP	A	4703	21	24,29,29	0.87	1 (4%)	29,45,45	1.22	3 (10%)

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
20	ATP	B	5403	21	-	1/18/38/38	0/3/3/3
20	ATP	A	4702	21	-	3/18/38/38	0/3/3/3
19	ADP	B	5406	21	-	1/12/32/32	0/3/3/3
20	ATP	C	4302	21	-	1/18/38/38	0/3/3/3
19	ADP	C	4306	21	-	4/12/32/32	0/3/3/3
19	ADP	C	4305	3,21	-	5/12/32/32	0/3/3/3
19	ADP	A	4701	21	-	8/12/32/32	0/3/3/3
19	ADP	B	5405	21	-	1/12/32/32	0/3/3/3
19	ADP	A	4703	21	-	6/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	4703	ADP	O4'-C1'	2.06	1.43	1.40
19	C	4305	ADP	C8-N7	-2.06	1.30	1.34

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	4305	ADP	C4'-O4'-C1'	-4.34	105.95	109.92
20	A	4702	ATP	N3-C2-N1	-3.76	123.57	128.67
19	C	4306	ADP	C4'-O4'-C1'	-3.70	106.53	109.92
19	A	4701	ADP	C4'-O4'-C1'	3.49	113.12	109.92
19	A	4701	ADP	N3-C2-N1	-3.47	123.96	128.67

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

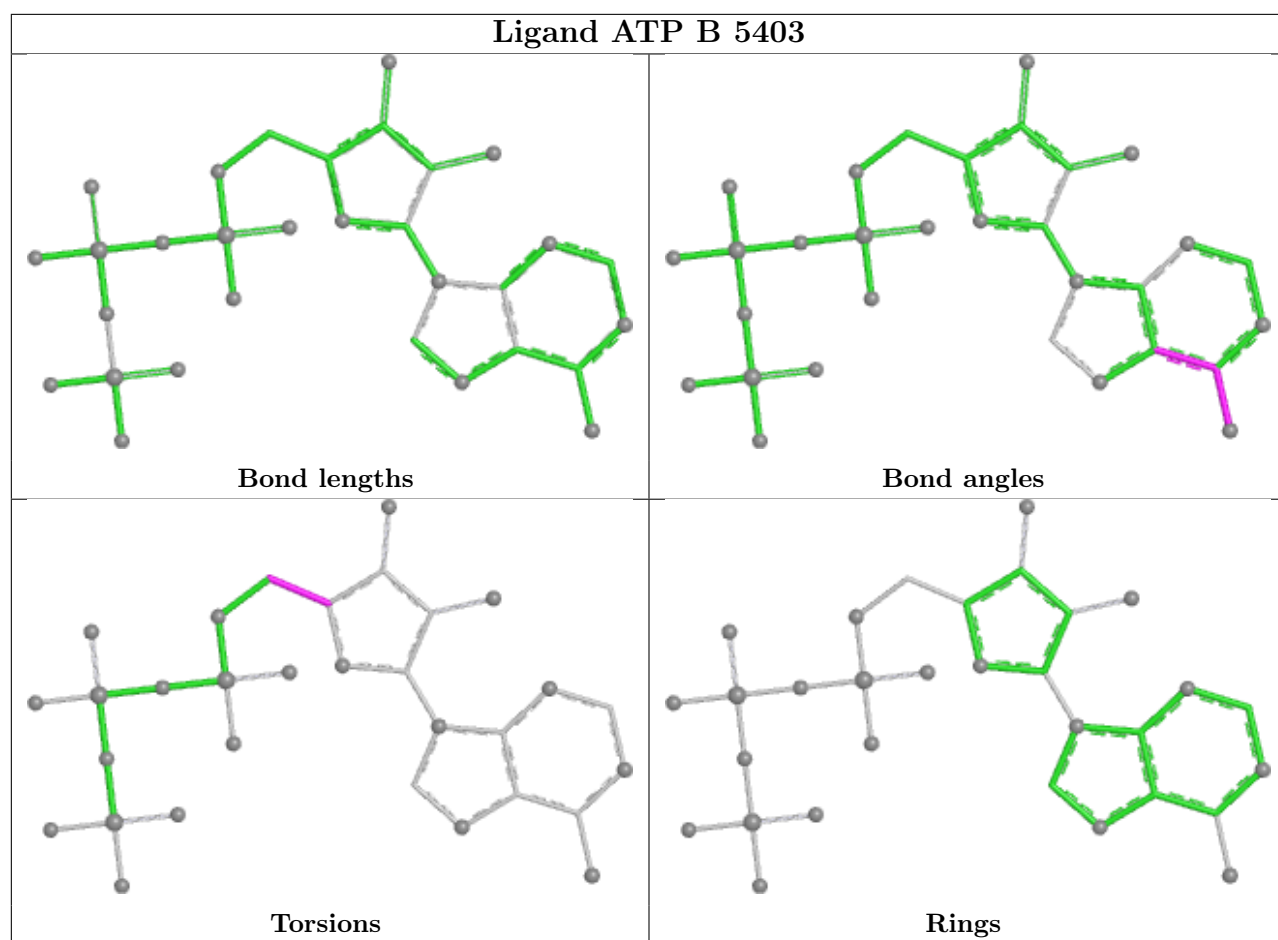
Mol	Chain	Res	Type	Atoms
19	A	4701	ADP	PB-O3A-PA-O5'
19	A	4701	ADP	C5'-O5'-PA-O1A
19	A	4701	ADP	C5'-O5'-PA-O2A
19	A	4701	ADP	C5'-O5'-PA-O3A
19	A	4703	ADP	PB-O3A-PA-O5'

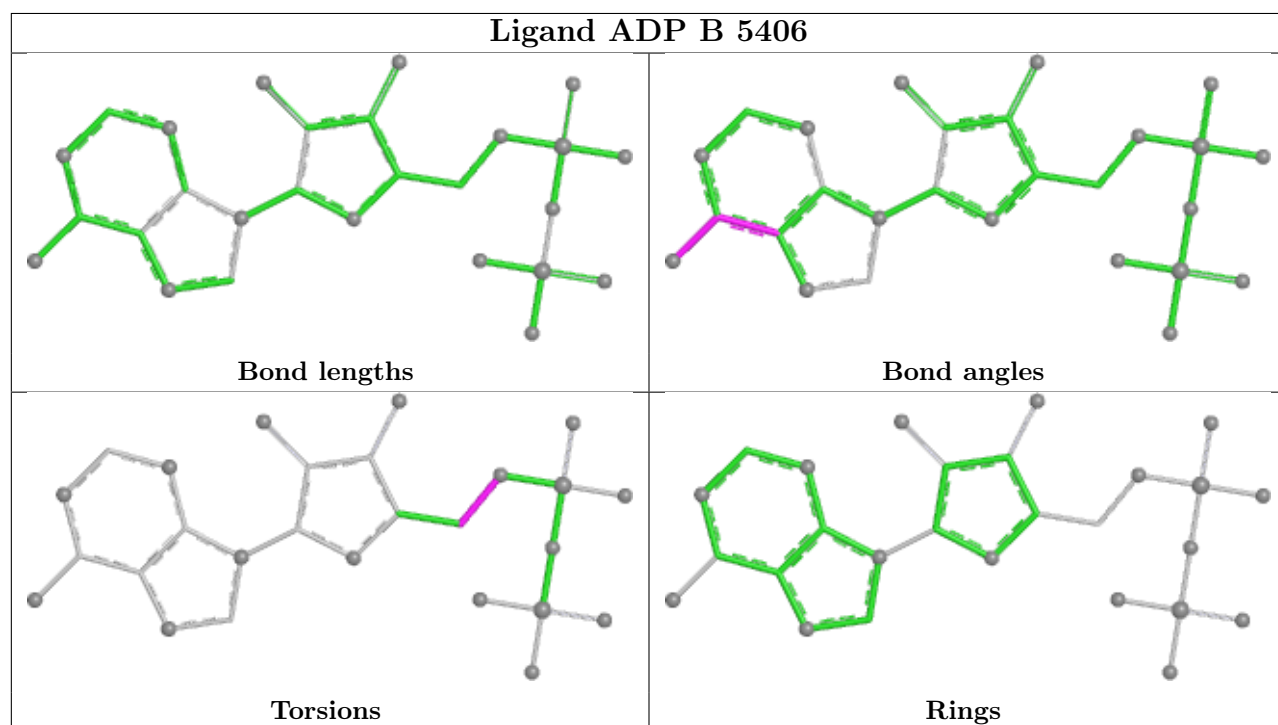
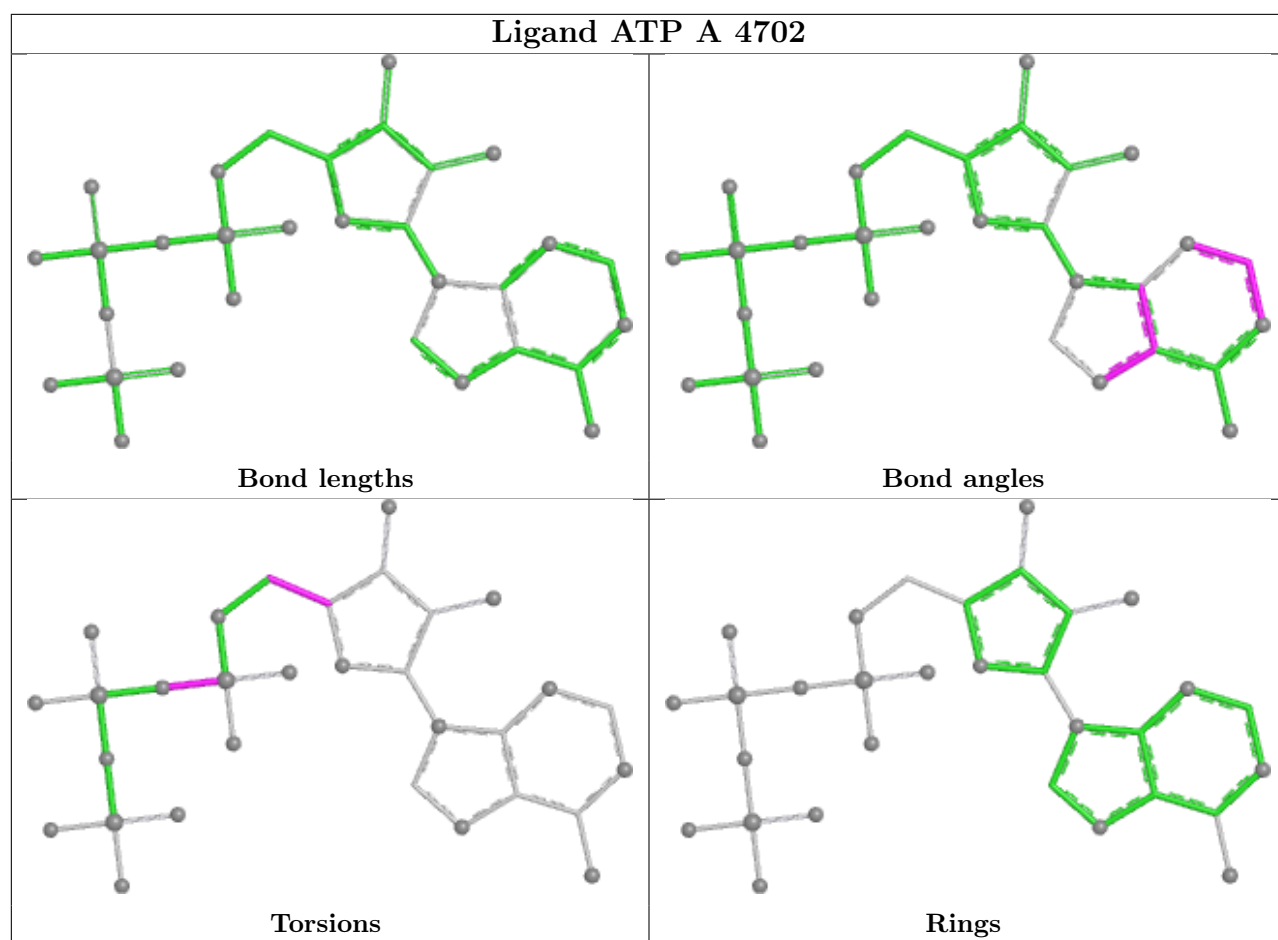
There are no ring outliers.

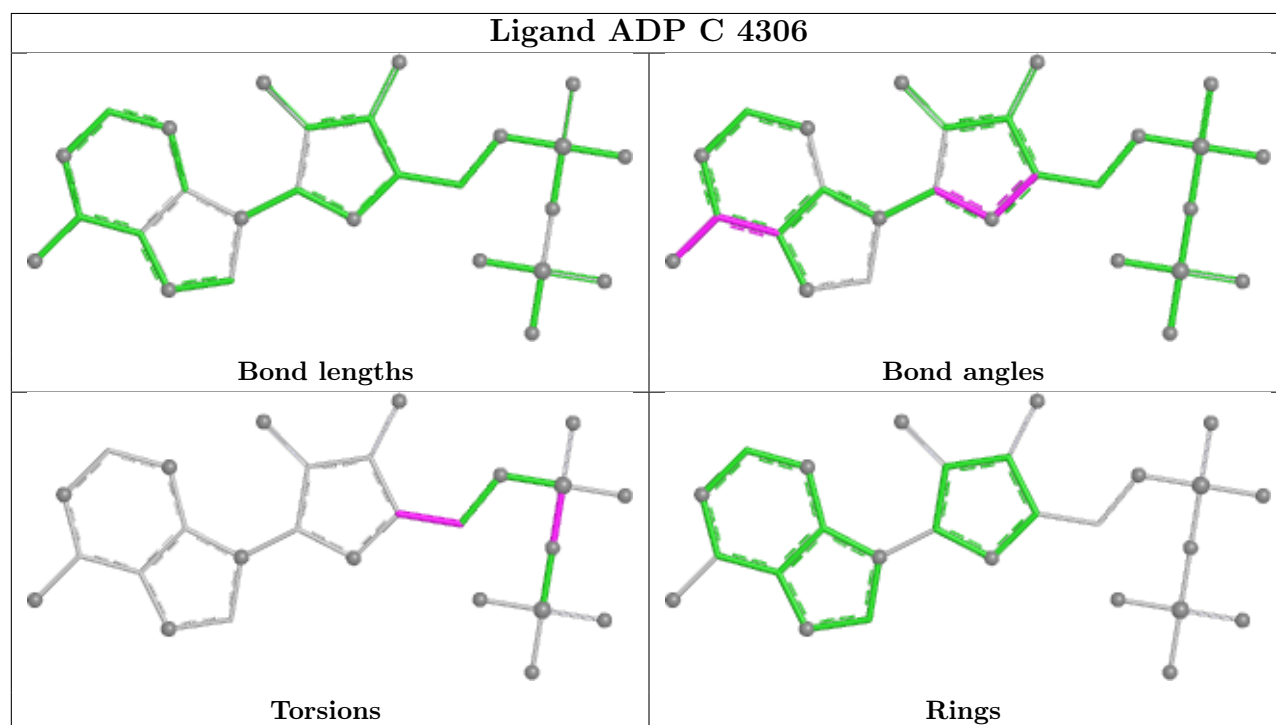
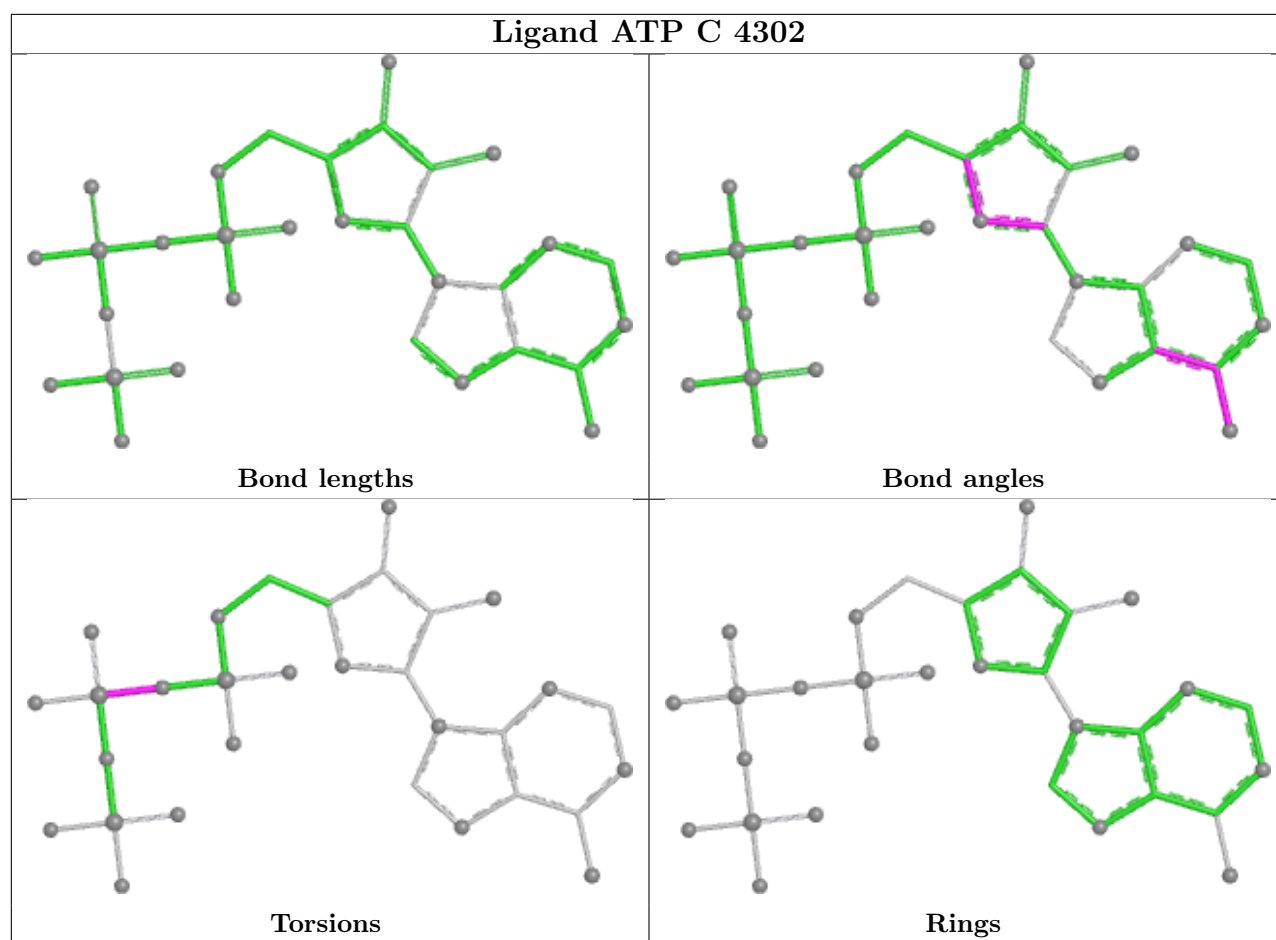
9 monomers are involved in 140 short contacts:

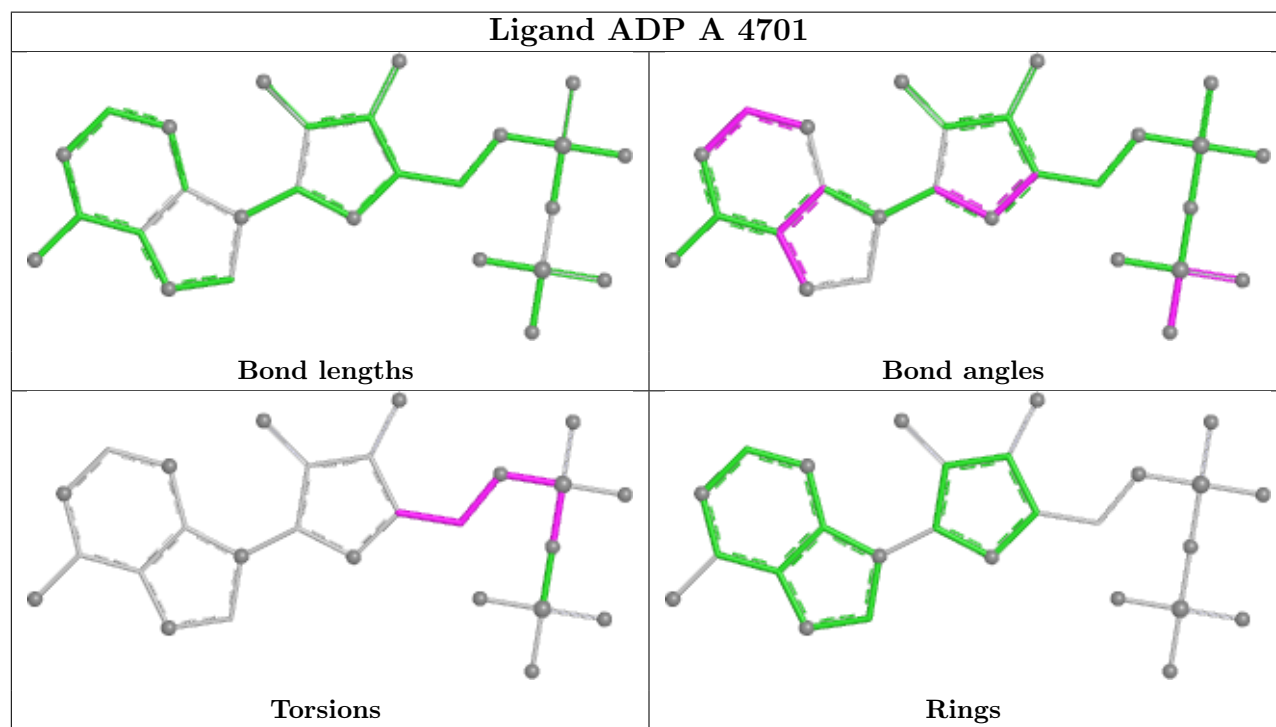
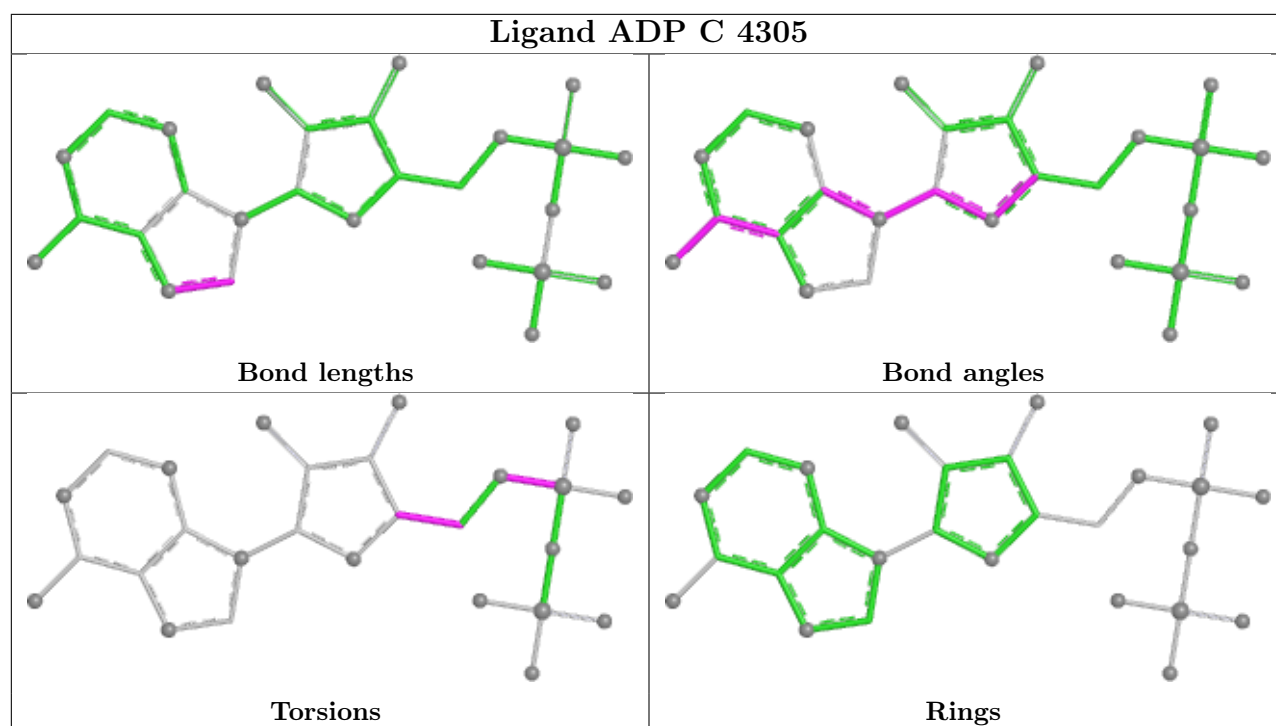
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	5403	ATP	44	0
20	A	4702	ATP	10	0
19	B	5406	ADP	3	0
20	C	4302	ATP	1	0
19	C	4306	ADP	8	0
19	C	4305	ADP	25	0
19	A	4701	ADP	12	0
19	B	5405	ADP	16	0
19	A	4703	ADP	21	0

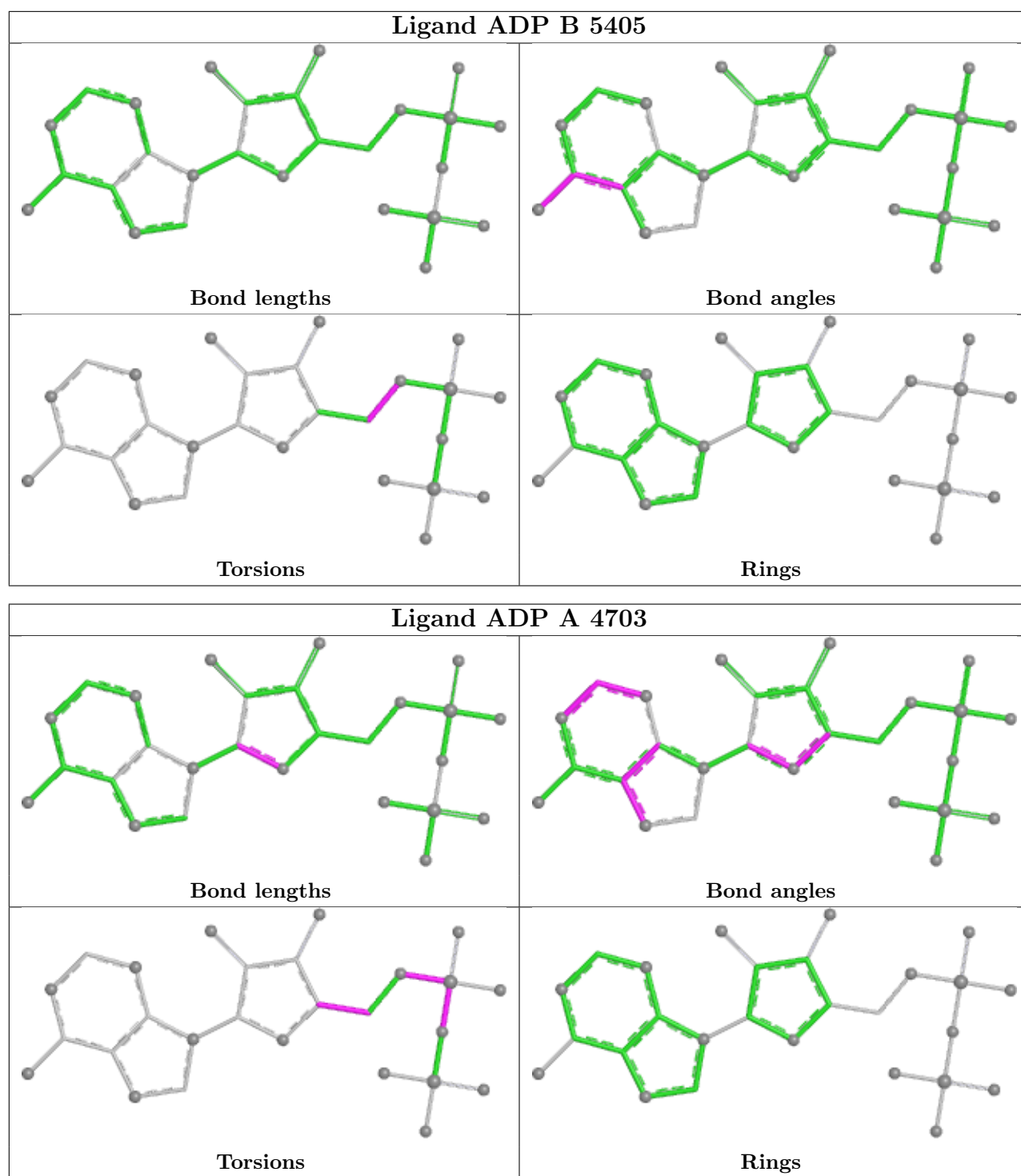
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	10
1	A	9
16	P	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	A	3250:PRO	C	3251:ILE	N	5.80
1	A	3251:ILE	C	3252:GLN	N	4.89
1	A	24:LYS	C	25:ASP	N	3.36
1	B	79:PRO	C	80:PRO	N	3.22
1	D	216:HIS	C	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.

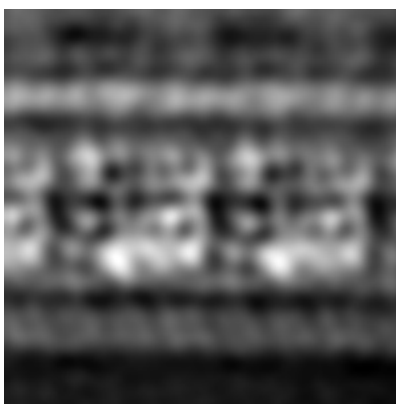
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

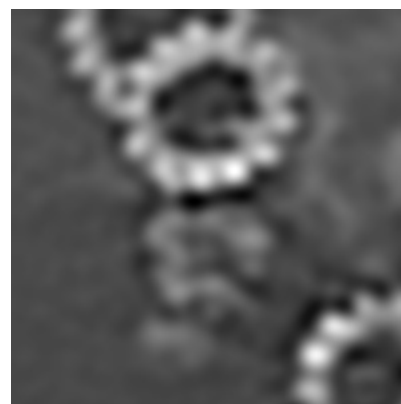
6.1.1 Primary map



X



Y

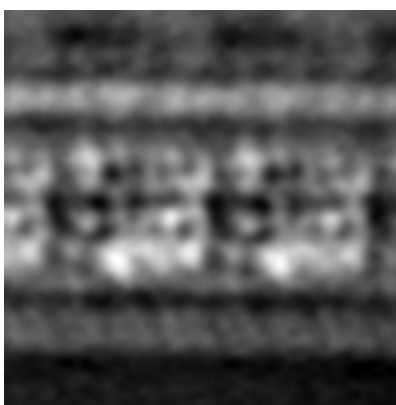


Z

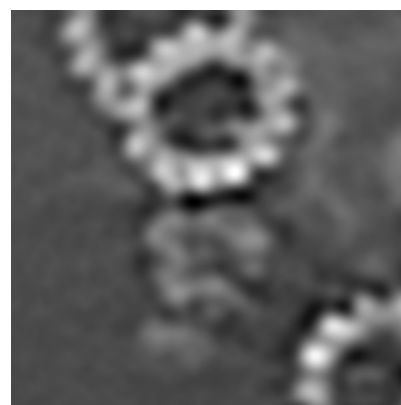
6.1.2 Raw map



X



Y



Z

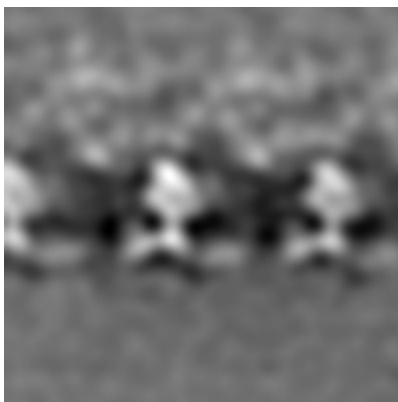
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 37

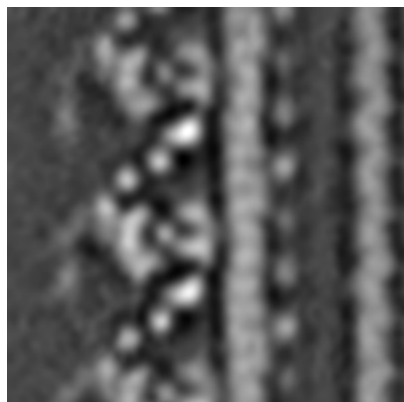


Y Index: 37

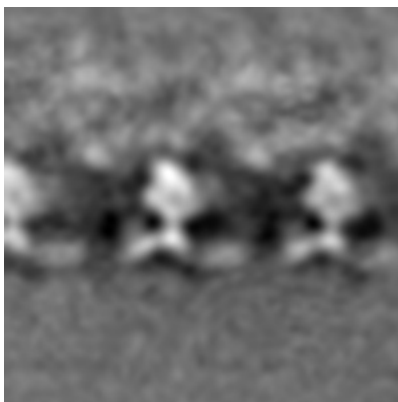


Z Index: 37

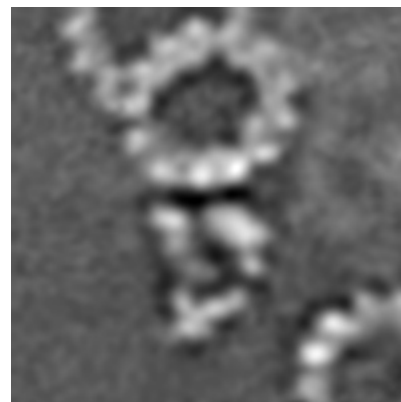
6.2.2 Raw map



X Index: 37



Y Index: 37



Z Index: 37

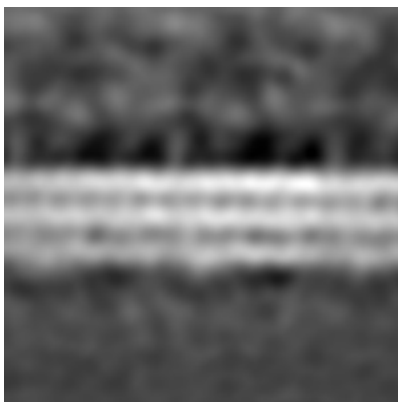
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 41



Y Index: 43

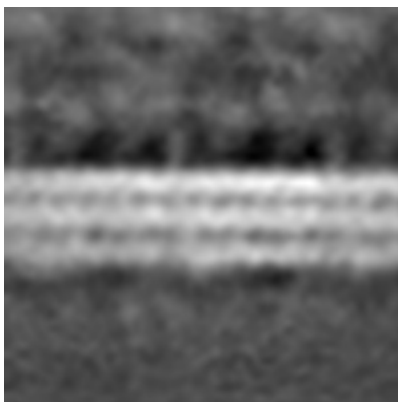


Z Index: 21

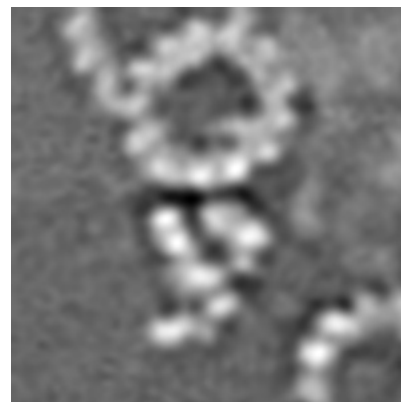
6.3.2 Raw map



X Index: 41



Y Index: 43

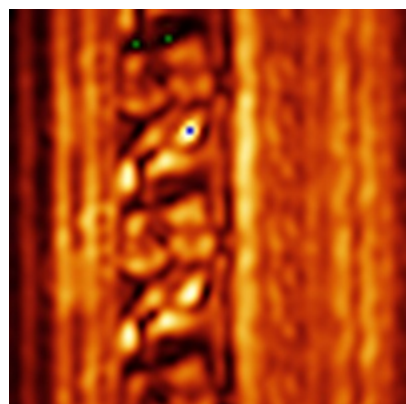


Z Index: 35

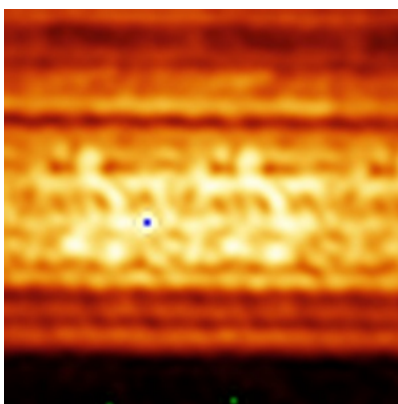
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

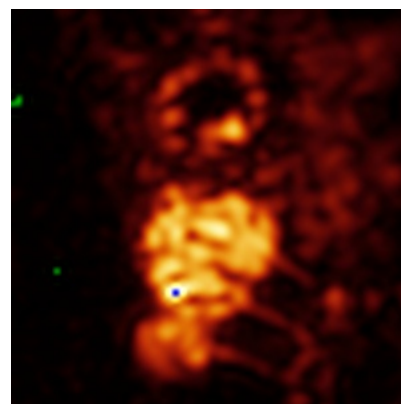
6.4.1 Primary map



X

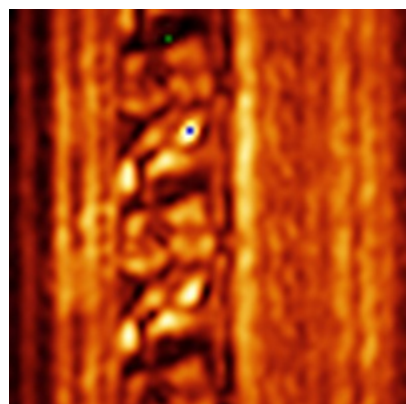


Y

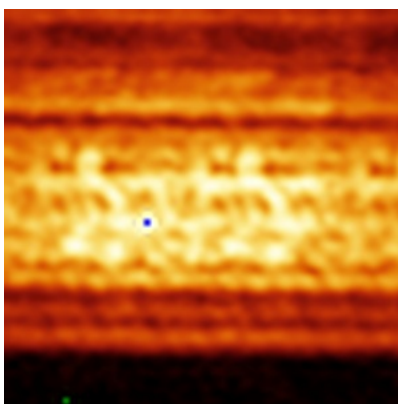


Z

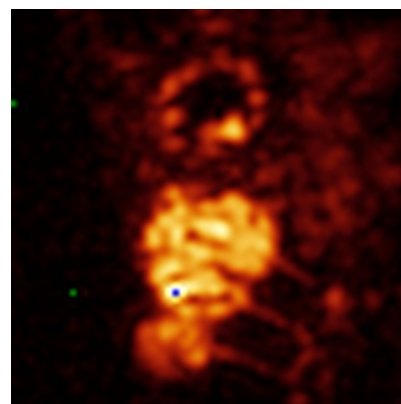
6.4.2 Raw map



X



Y

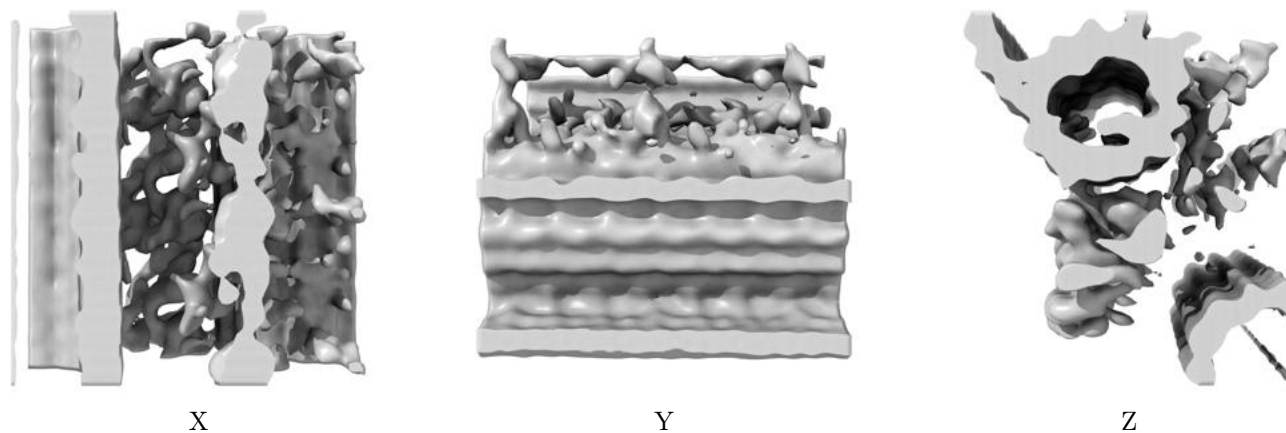


Z

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.

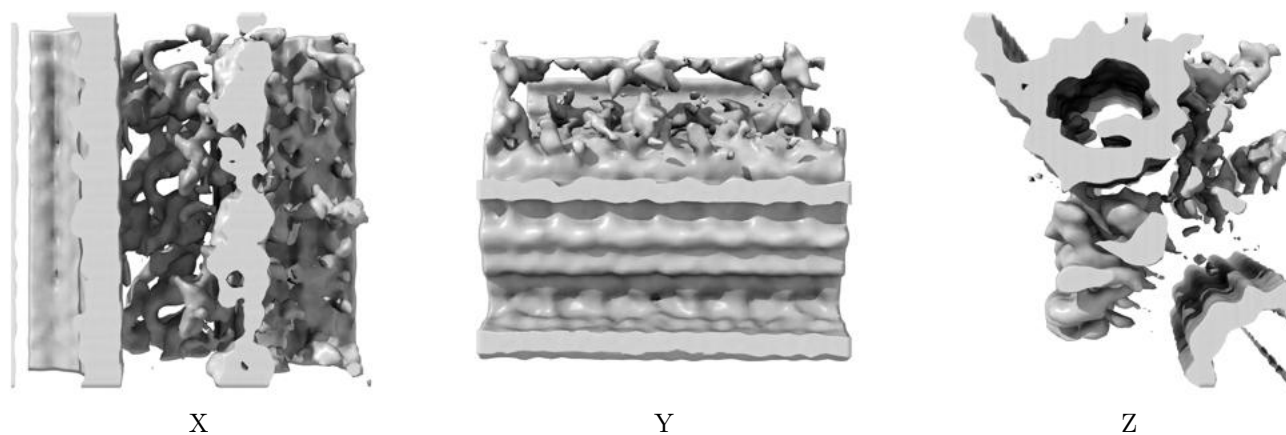
6.5 Orthogonal surface views [i](#)

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.

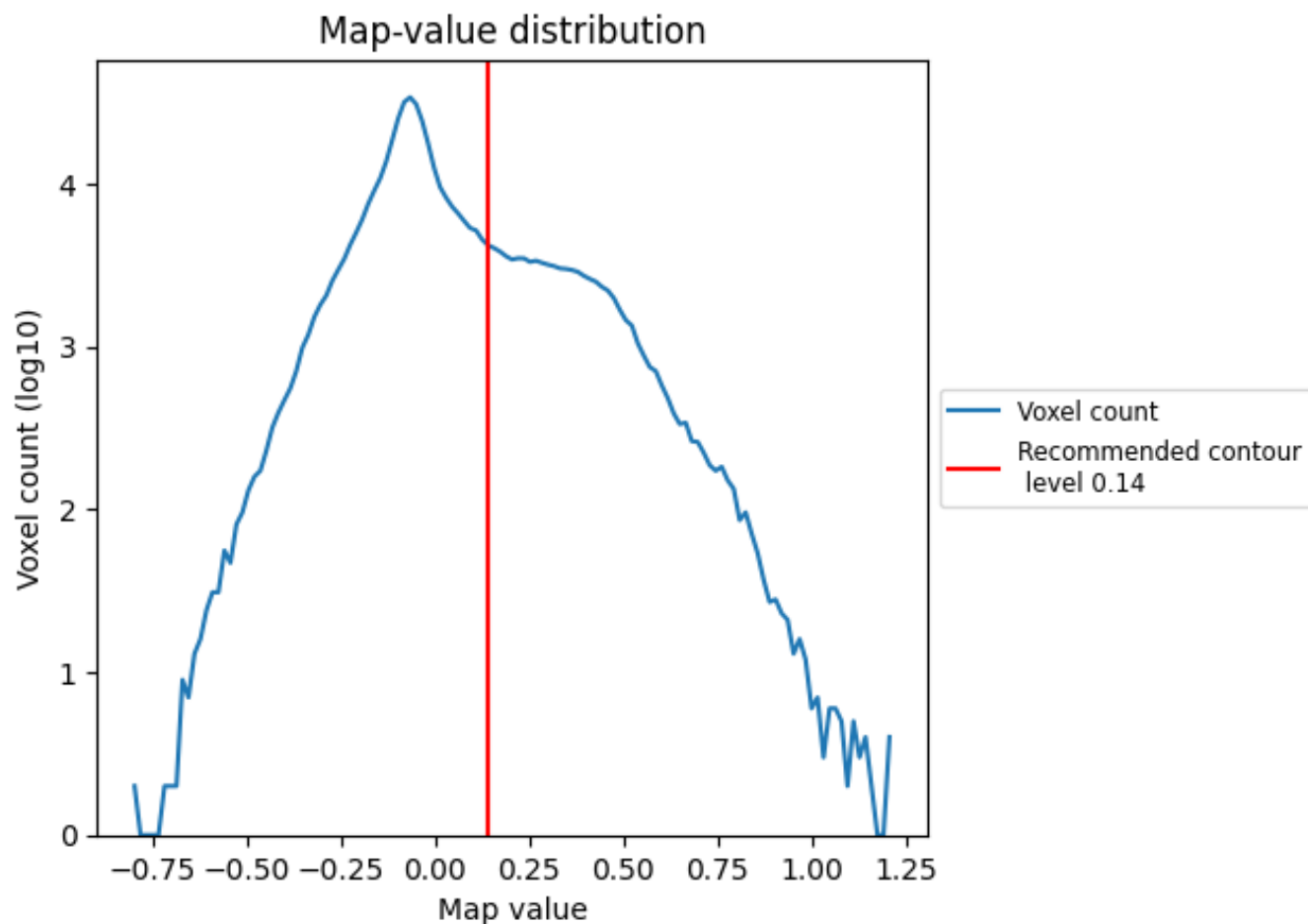
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

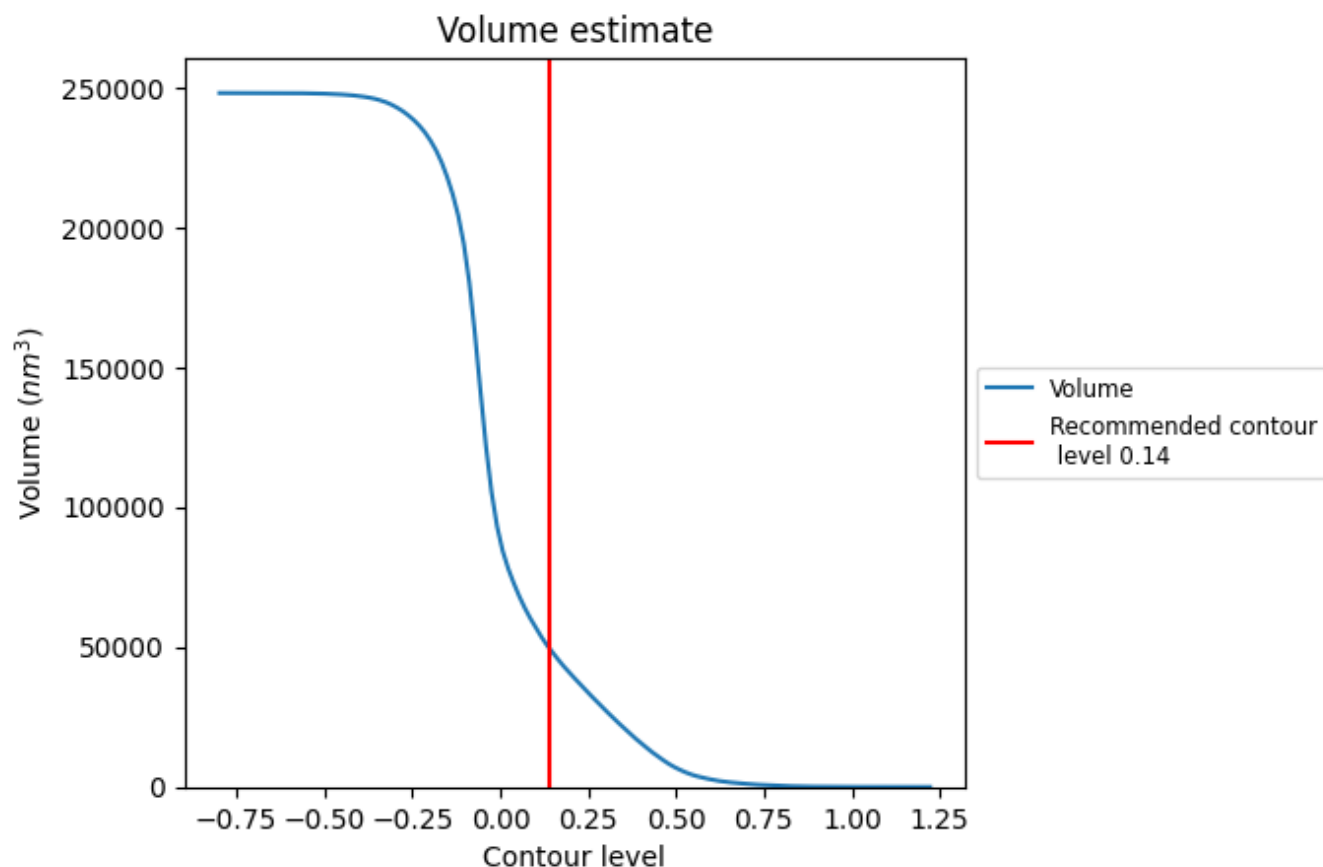
This section contains the results of statistical analysis of the map.

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.

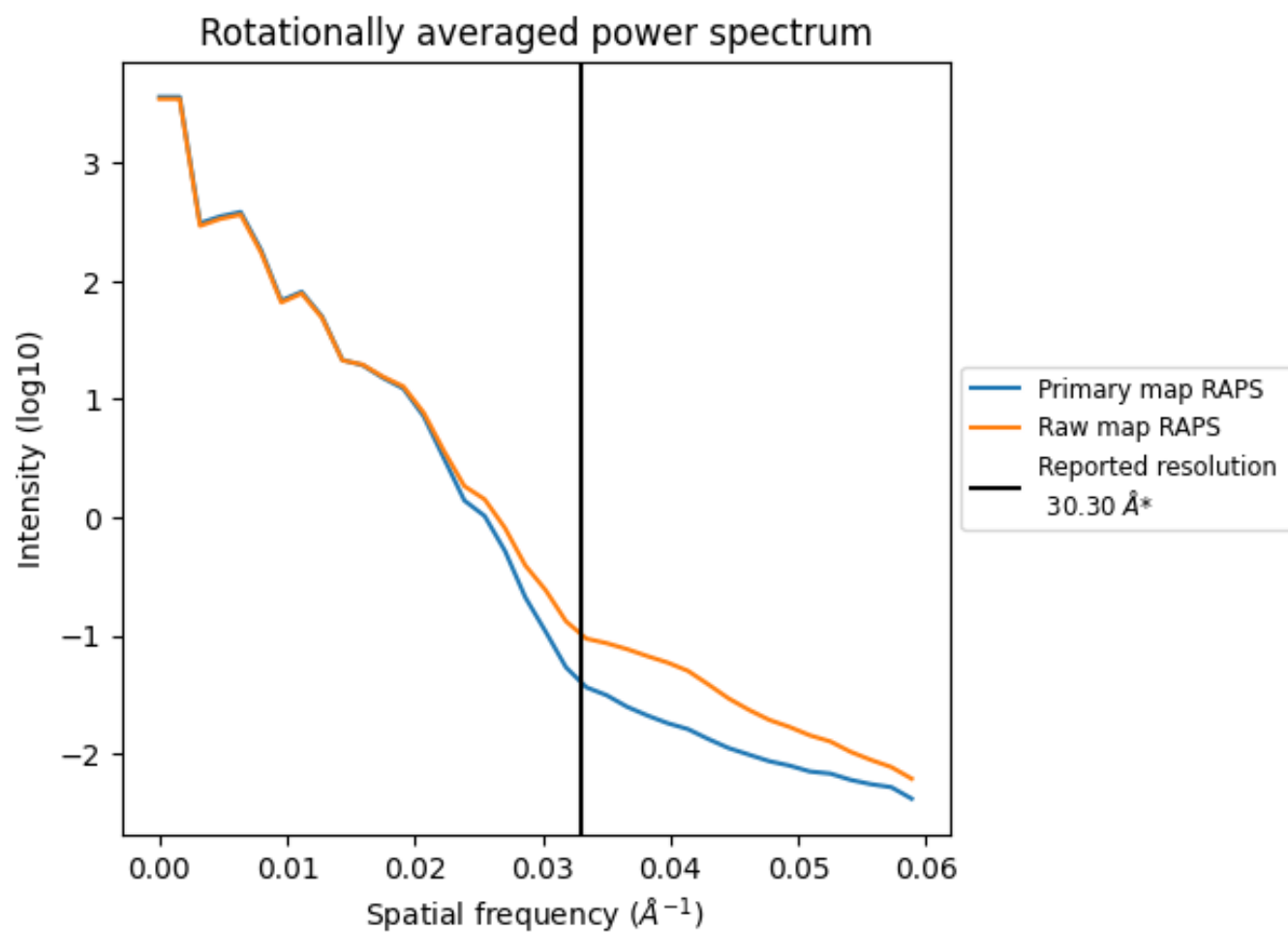
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 49562 nm³; 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 ⓘ

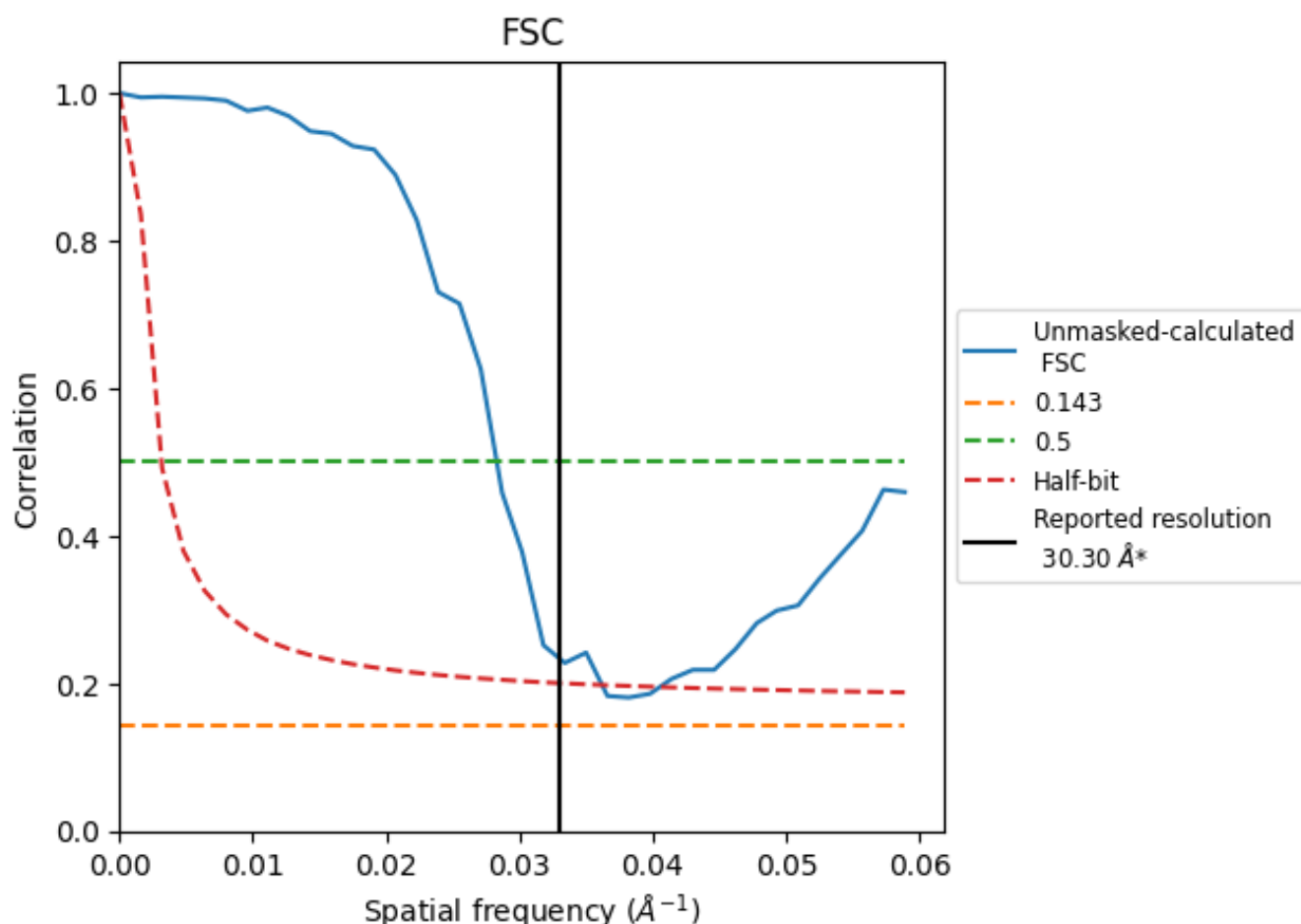


*Reported resolution corresponds to spatial frequency of 0.033 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [i](#)

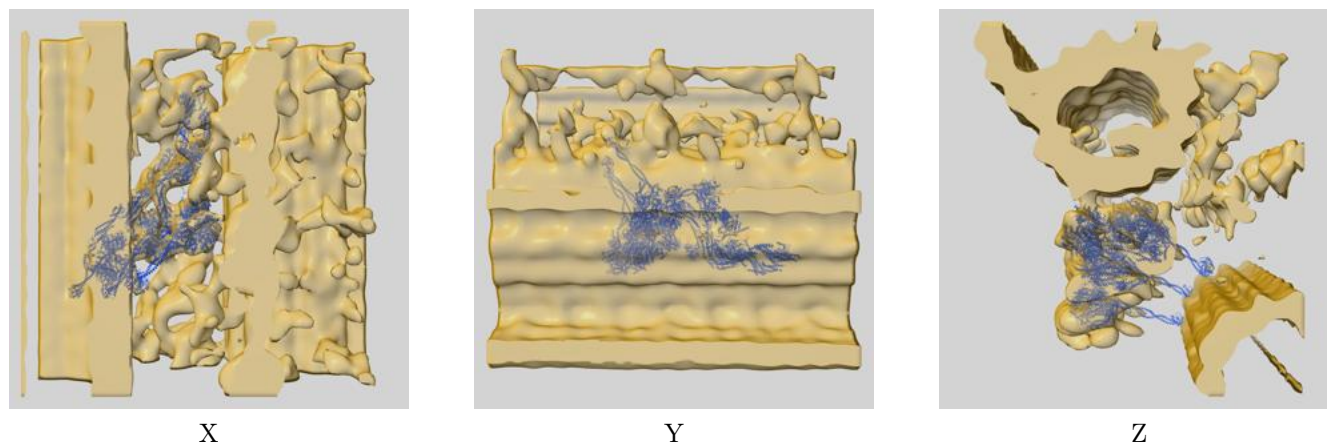
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	30.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	-	35.34	27.62

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

9 Map-model fit [i](#)

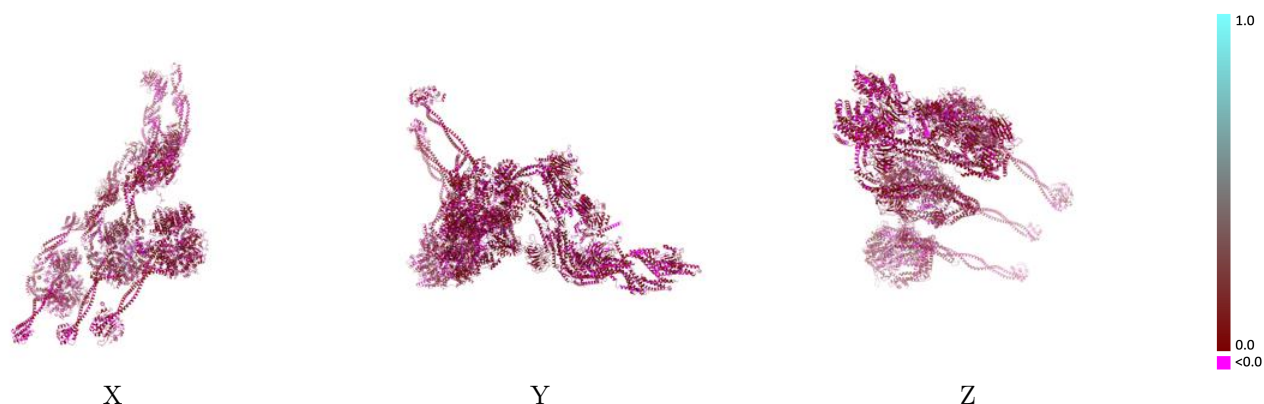
This section contains information regarding the fit between EMDB map EMD-16312 and PDB model 8BX8. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



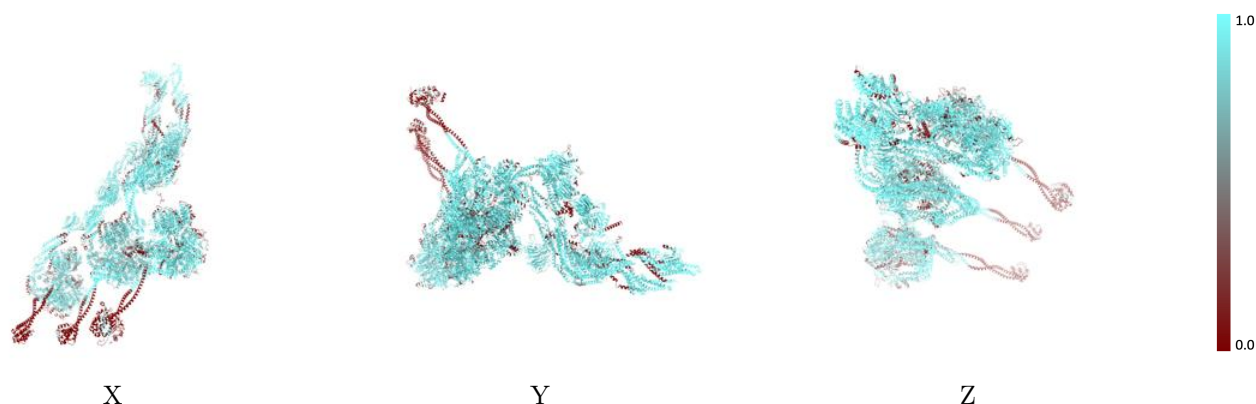
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



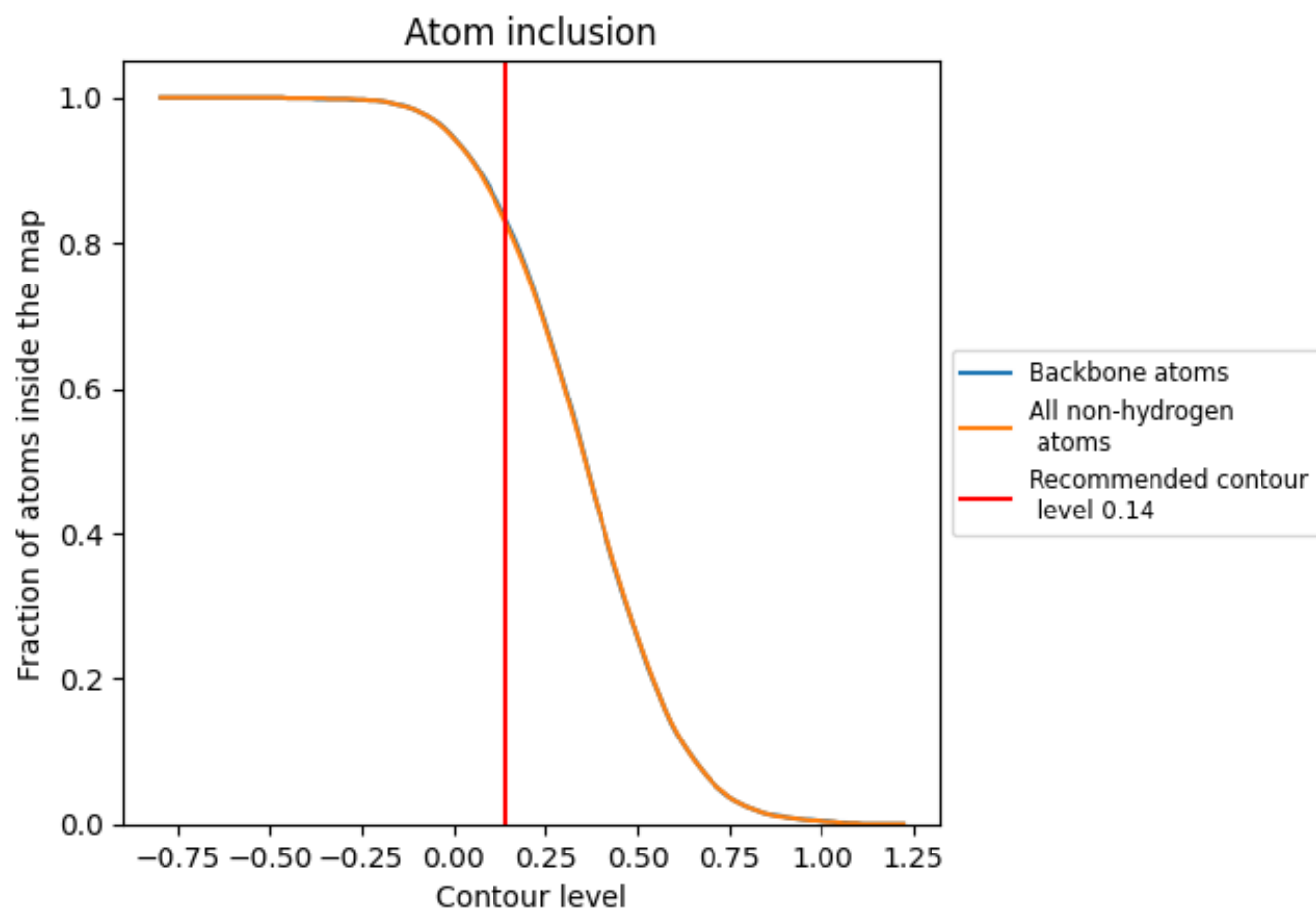
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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.

9.5 Map-model fit summary

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
A	 0.8230	 0.0460
B	 0.8570	 0.0460
C	 0.7930	 0.0370
D	 0.9090	 0.0390
E	 0.9000	 0.0400
F	 0.8060	 0.0430
G	 0.7350	 0.0120
H	 0.9840	 0.0390
I	 0.8590	 0.0400
J	 0.9870	 0.0630
K	 0.9720	 0.0530
L	 0.8830	 0.0290
M	 0.9310	 0.0400
N	 0.8960	 0.0440
O	 0.9600	 0.0410
P	 0.9850	 0.0630
Q	 0.2450	 0.0610
R	 0.3110	 -0.0180

