



wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 04:12 am GMT

PDB ID : 6ZYW
EMDB ID : EMD-11576
Title : Outer Dynein Arm-Shulin complex - overall structure (Tetrahymena thermophila)
Authors : Mali, G.R.; Abid Ali, F.; Lau, C.K.; Carter, A.P.
Deposited on : 2020-08-03
Resolution : 8.78 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:

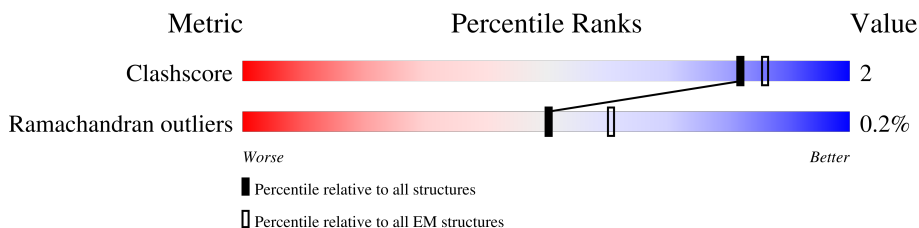
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 8.78 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.





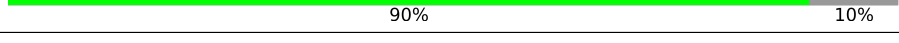
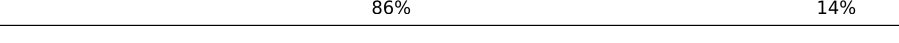
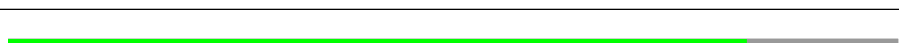
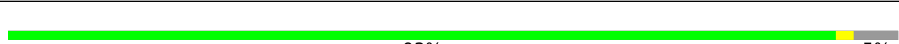

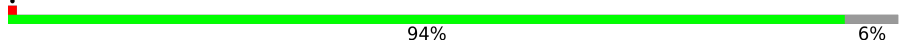
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	4168	
2	B	4595	
3	C	4620	
4	D	667	
4	d	667	
5	E	670	
5	e	670	
6	F	133	
7	G	103	

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Mol	Chain	Length	Quality of chain
8	H	92	 90% 8%
9	I	110	 81% 19%
10	J	93	 90% 10%
11	K	111	 86% 14%
12	L	111	 87% 13%
13	M	87	 99%
14	N	132	 83% 17%
15	O	117	 93% 5%
16	P	110	 90% 6%
17	Y	1200	 94% 6%

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 73897 atoms, of which 0 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-1-alpha heavy chain, flagellar inner arm I1 complex protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	3795	18787	11198	3795	3794	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	4370	20008	12102	3953	3953	0	417

- Molecule 3 is a protein called Dynein heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	4433	19737	11997	3870	3870	0	563

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	321	1588	946	321	321	0	0
4	d	128	637	381	128	128	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	341	1678	996	341	341	0	0
5	e	102	501	297	102	102	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	98	Total	C	N	O	0	0
			486	290	98	98		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	95	Total	C	N	O	0	0
			470	280	95	95		

- Molecule 8 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	85	Total	C	N	O	0	0
			420	250	85	85		

- Molecule 9 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	89	Total	C	N	O	0	0
			439	261	89	89		

- Molecule 10 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	84	Total	C	N	O	0	0
			416	248	84	84		

- Molecule 11 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	95	Total	C	N	O	0	0
			470	280	95	95		

- Molecule 12 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	97	Total	C	N	O	0	0
			479	285	97	97		

- Molecule 13 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	86	426	254	86	86	0	0

- Molecule 14 is a protein called Dynein light chain 2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	N	109	537	319	109	109	0	0

- Molecule 15 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	O	111	550	328	111	111	0	0

- Molecule 16 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	P	103	513	307	103	103	0	0

- Molecule 17 is a protein called Shulin.

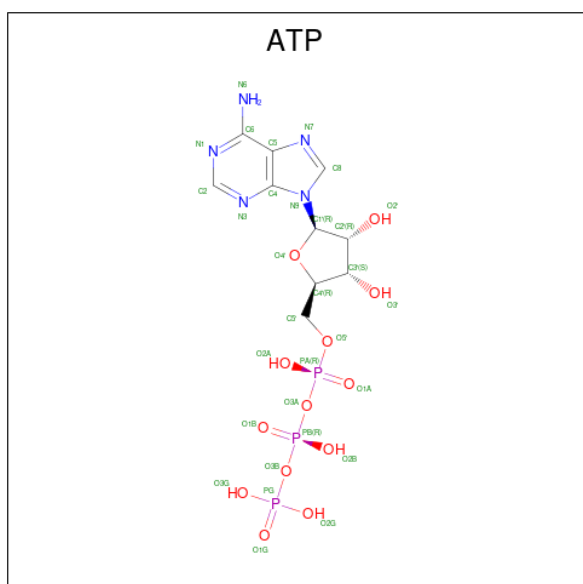
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Y	1133	5611	3345	1133	1133	0	0

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



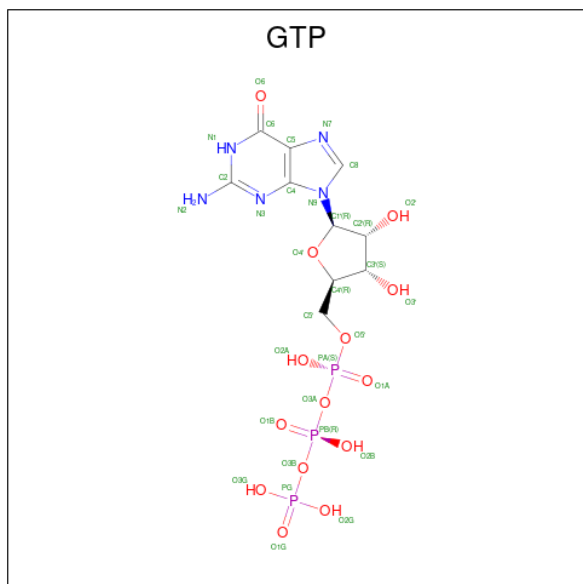
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		
18	C	1	Total	81	30	15	30	6	0
18	C	1	Total	81	30	15	30	6	0
18	C	1	Total	81	30	15	30	6	0

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 20 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

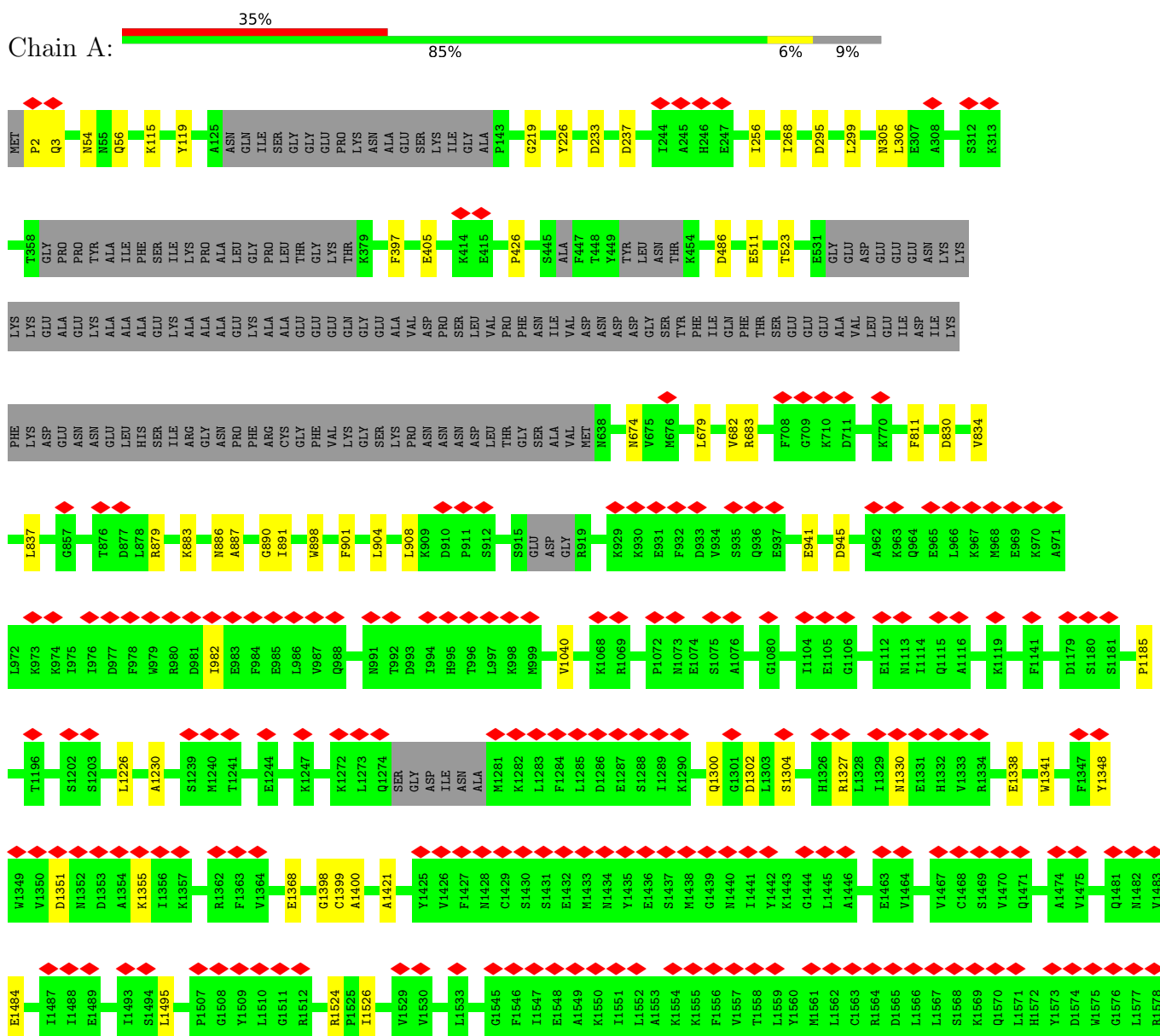


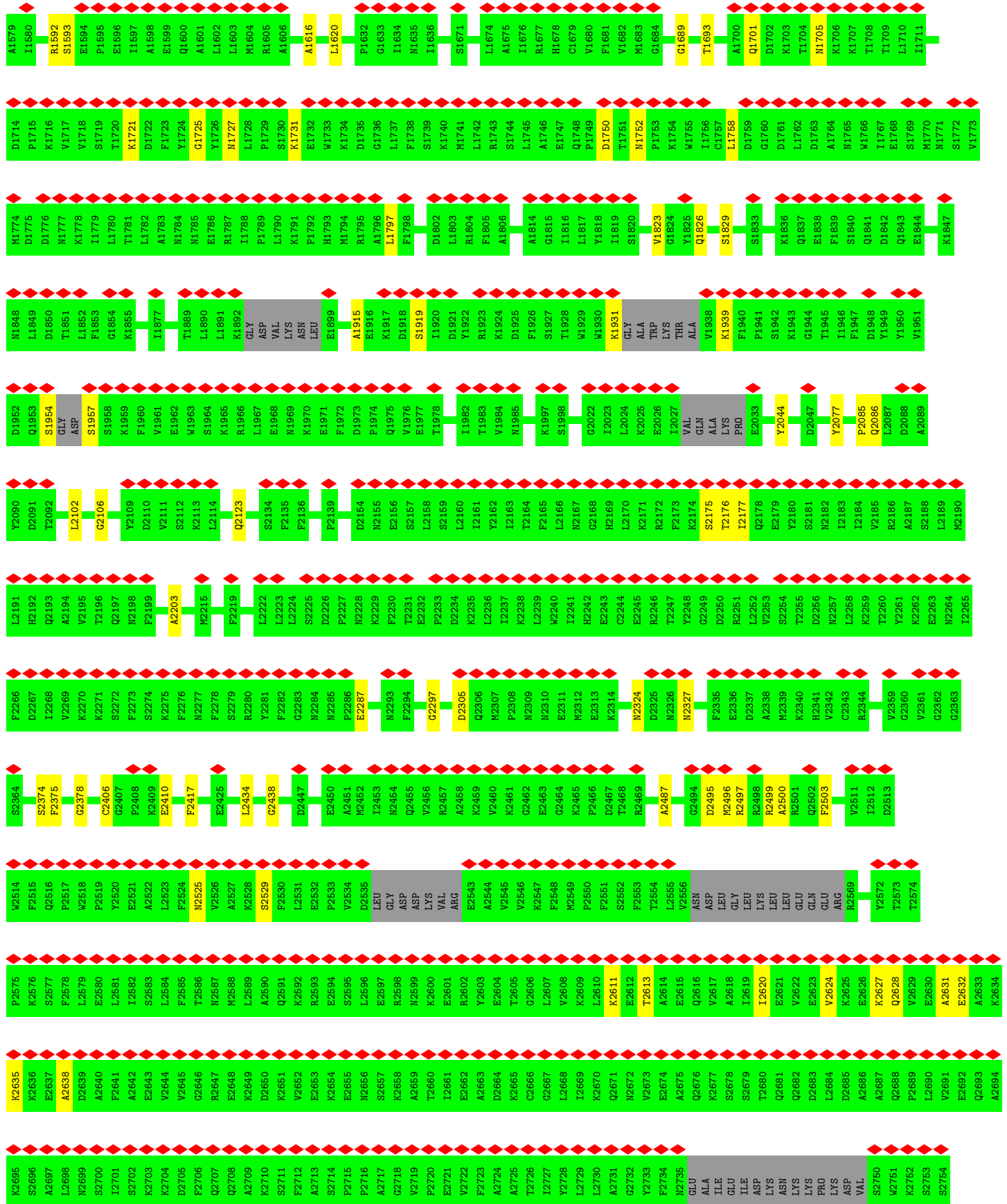
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	Y	1	32	10	5	14	3	0

3 Residue-property plots

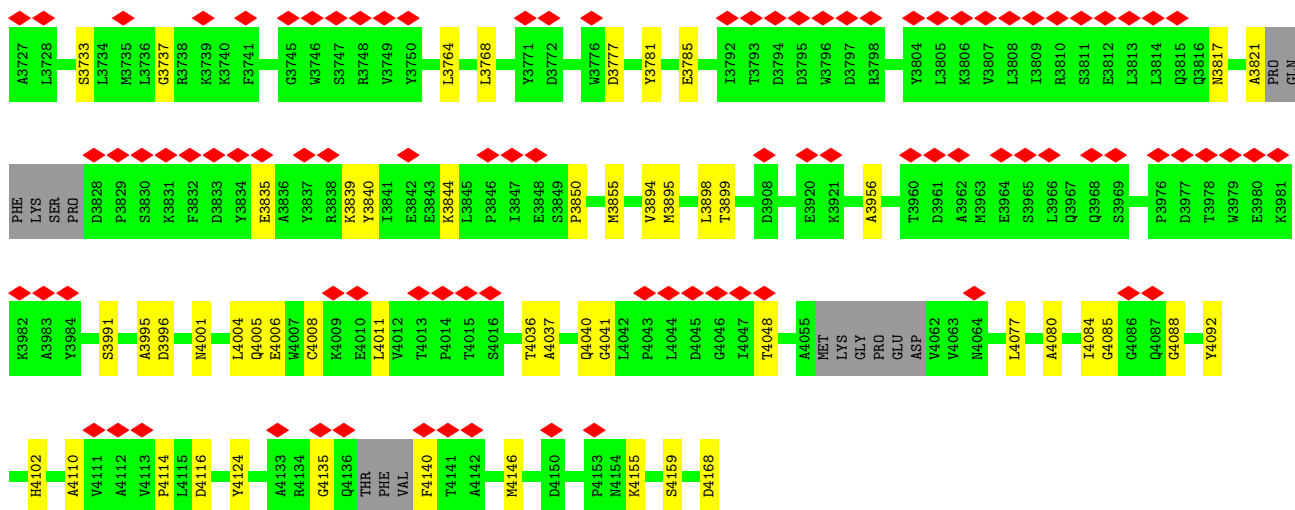
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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-1-alpha heavy chain, flagellar inner arm I1 complex protein, putative

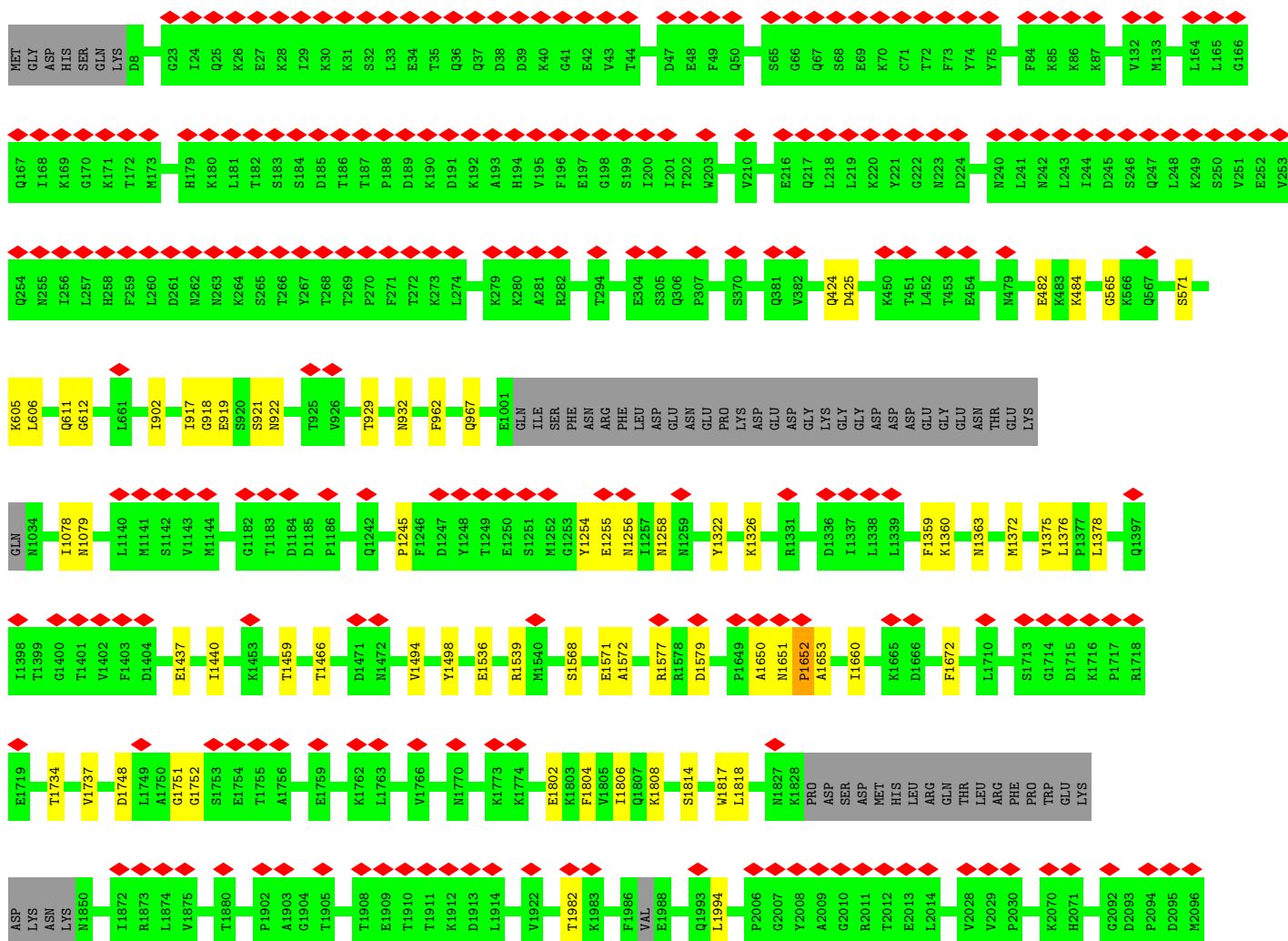
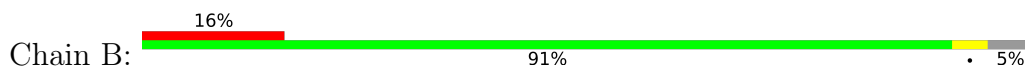


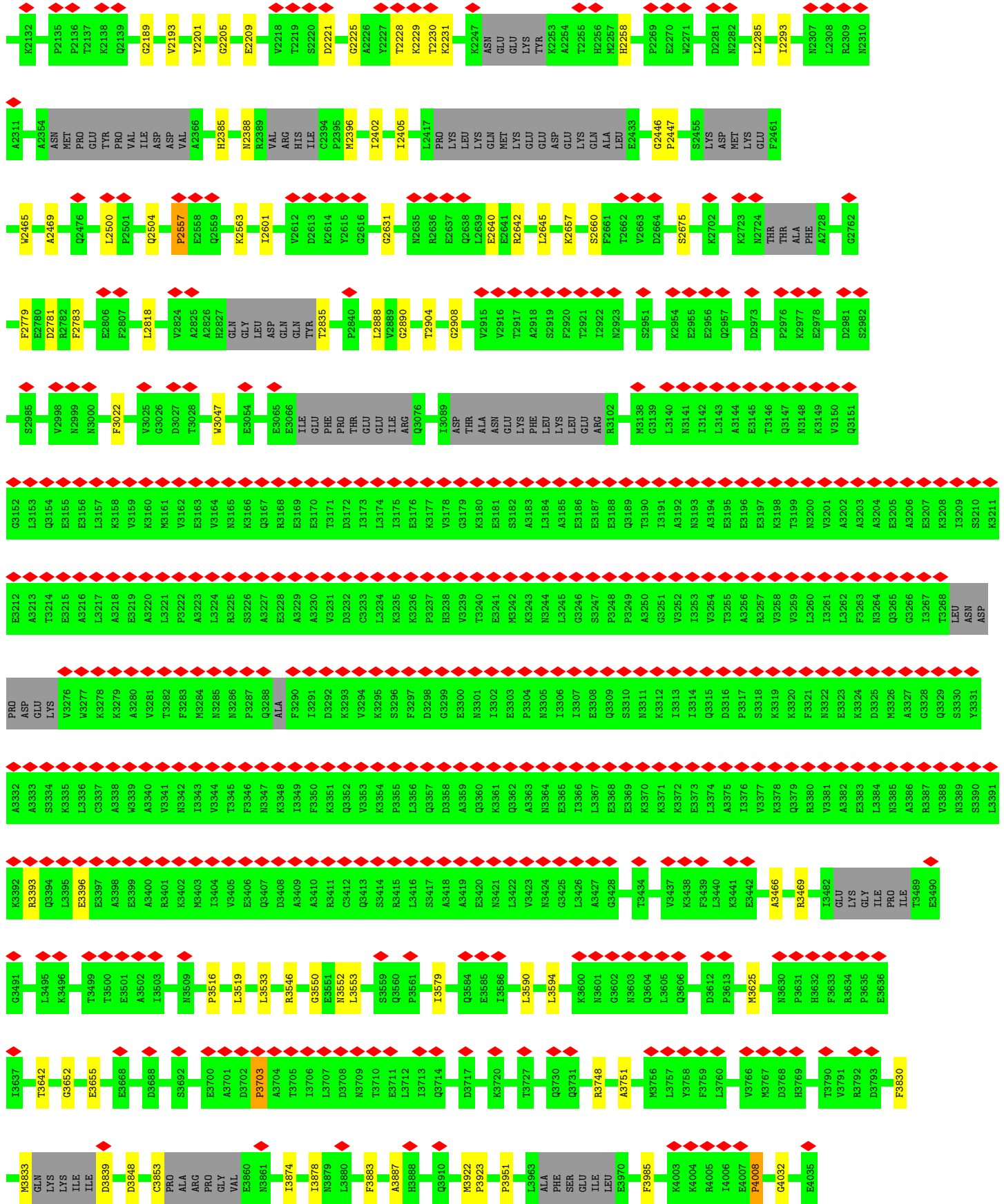


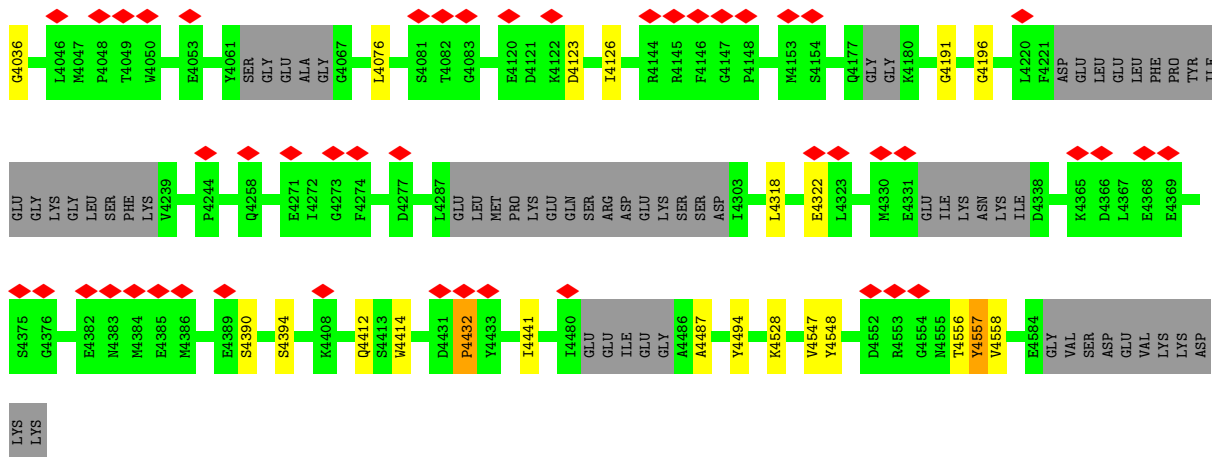
L2755	L2756	L2757	L2758	L2759	L2760	L2761	GLU	E2763	F2764	H2765	E2766	K2767	L2768	L2769	L2770	F2771	LYS	ASP	VAL	VAL	D2776	A2777	K2778	Q2779	V2780	F2781	A2782	A2783	L2784	V2785	H2786	L2787	L2788	L2789	H2790	I2791	L2792	L2793	L2794	H2795	F2796	S2797	F2798	L2799	F2800	E2801	Q2802	H2803	A2804	S2805	K2806	S2807	A2808	A2809	A2810	K2811	G2812	L2813	C2814	S2815	W2816	V2817	V2818	N2819	L2820	V2821	K2822	Y2823	Y2824	D2825	V2826	L2827	Q2828	D2829	V2830	E2831	P2832	K2833	R2834	K2835	A2836	L2837	K2838	E2839	A2840	T2841	E2842	Q2843	L2844	E2845	E2846	T2847	V2848	K2850	L2851	E2853	E2855	E2856	V2857	V2858	R2859	K2860	L2861	E2862	E2863	E2864	L2865	N2866	L2867	L2868	K2869	A2870	E2871	N2872	L2873	K2874	A2875	I2876	A2877	E2878	K2879	N2880	A2881	A2882	S2883	L2884	E2885	A2886	E2887	R2888	C2889	A2890	R2891	R2892	L2893	M2894	L2895	A2896	Q2897	R2898	L2899	V2900	T2901	A2902	L2903	S2904	S2905	E2906	N2907	E2908	R2909	W2910	G2911	K2912	S2913	L2914	I2915	Q2916	L2917	E2918	R2919	Q2920	L2921	K2922	L2923	M2924	V2925	Q2926	N2927	V2928	L2929	V2930	A2931	S2932	S2933	F2934	V2935	S2936	Y2937	P2940	K2943	M2947	L2948	H2949	L2950	M2951	Q2952	M2953	F2954	M2955	K2956	F2957	M2958	K2959	GLU	HIS	THR	ILE	PRO	MET	S2966	P2967	D2968	P2969	M2970	P2971	L2972	I2973	L2974	L2975	T2976	D2977	E2978	E3050	S2979	T2980	I2981	A2982	L2983	W2984	M2985	R2986	Q2987	K2988	L2989	P2990	S2991	D2992	S2993	V2994	S2995	L2996	E2997	M2998	G2999	T3000	I3001	L3002	T3003	N3004	L3010	M3011	I3012	D3013	F3014	Q3015	L3016	Q3017	T3020	W3021	I3022	R3023	E3024	K3025	E3026	K3027	N3029	N3030	K3039	N3040	I3041	N3042	R3043	D3044	L3045	E3046	L3047	S3048	I3049	E3050	N3051	G3052	M3060	N3061	E3062	R3063	M3064	I3067	I3077	K3078	R3079	G3080	K3081	N3082	K3083	I3084	I3085	K3086	F3087	A3088	G3089	K3090	D3091	L3092	L3093	L3094	H3095	T3104	K3105	L3106	S3107	N3108	F3109	H3110	Y3111	F3112	F3113	E3114	I3115	Q3116	A3117	E3118	A3119	A3120	L3121	L3122	N3123	F3124	L3135	V3139	V3140	A3141	R3142	E3143	R3144	F3145	D3146	L3147	A3148	K3149	M3150	K3151	I3152	E3153	L3154	L3155	T3156	Q3157	Q3158	N3159	D3160	F3161	K3162	I3163	K3164	L3165	K3166	D3167	L3168	E3169	D3170	E3171	L3172	L3173	Y3174	K3175	L3176	A3177	N3178	A3179	G3180	K3181	D3182	I3183	L3184	D3185	L3186	I3187	L3188	I3189	I3190	E3191	N3192	L3193	E3194	Y3195	K3196	L3197	K3198	L3199	S3200	V3201	E3202	I3203	A3204	K3206	V3207	A3208	A3209	A3210	K3211	I3212	L3213	L3214	E3214	A3215	I3217	N3218	E3219	T3220	E3222	N3223	Y3224	R3225	S3242	K3243	V3244	H3245	S3246	F3247	Y3248	K3249	L3250	S3251	L3252	E3253	F3254	S3255	F3256	L3257	V3258	I3259	N3260	R3261	D3264	A3265	L3266	S3267	E3268	N3269	LYS	ILE	GLU	TYR	GLY	THR	ALA	GLU	THR	VAL	GLN	ASN	PRO	VAL	L3426	R3427	S3428	E3429	E3430	L3431	M3432	S3433	D3437	H3438	I3441	G3442	LYS	VAL	ASP	ASP	VAL	V3619	H3620	W3621	V3627	H3628	L3629	Q3631	S3632	W3633	L3634	Y3635	L3644	GLU	SER	VAL	P3549	F3550	F3551	M3552	I3552	L3553	F3554	F3555	F3556	Q3557	E3558	L3559	F3559	S3560	K3561	T3562	F3563	P3564	F3570	P3571	G3572	L3573	D3574	P3575	A3583	A3584	F3585	F3586	D3587	S3588	A3589	A3590	N3591	N3592	K3593	R3594	Q3602	G3603	C3615	G3619	D3710	W3621	D3712	V3627	H3628	C3714	L3629	Q3631	S3632	W3633	L3634	Y3635	L3644	GLU	SER	VAL	F3703	N3704	K3705	F3706	D3707	Q3708	E3709	F3710	L3711	K3713	C3714	D3715	K3716	K3717	P3718	W3633	L3634	E3720	F3721	K3722	S3723	C3724	L3725	F3726
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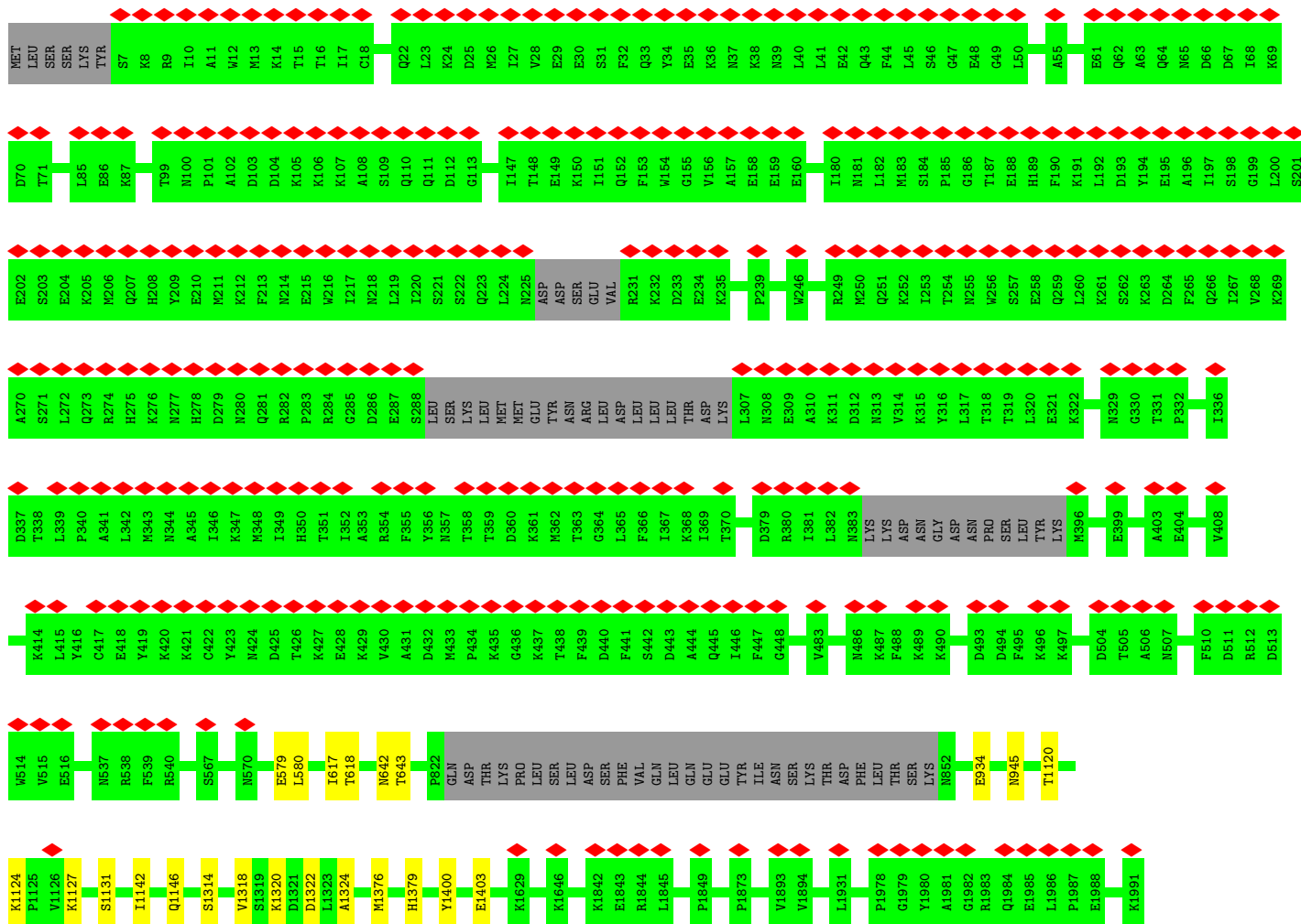
• Molecule 2: Outer arm dynein beta heavy chain

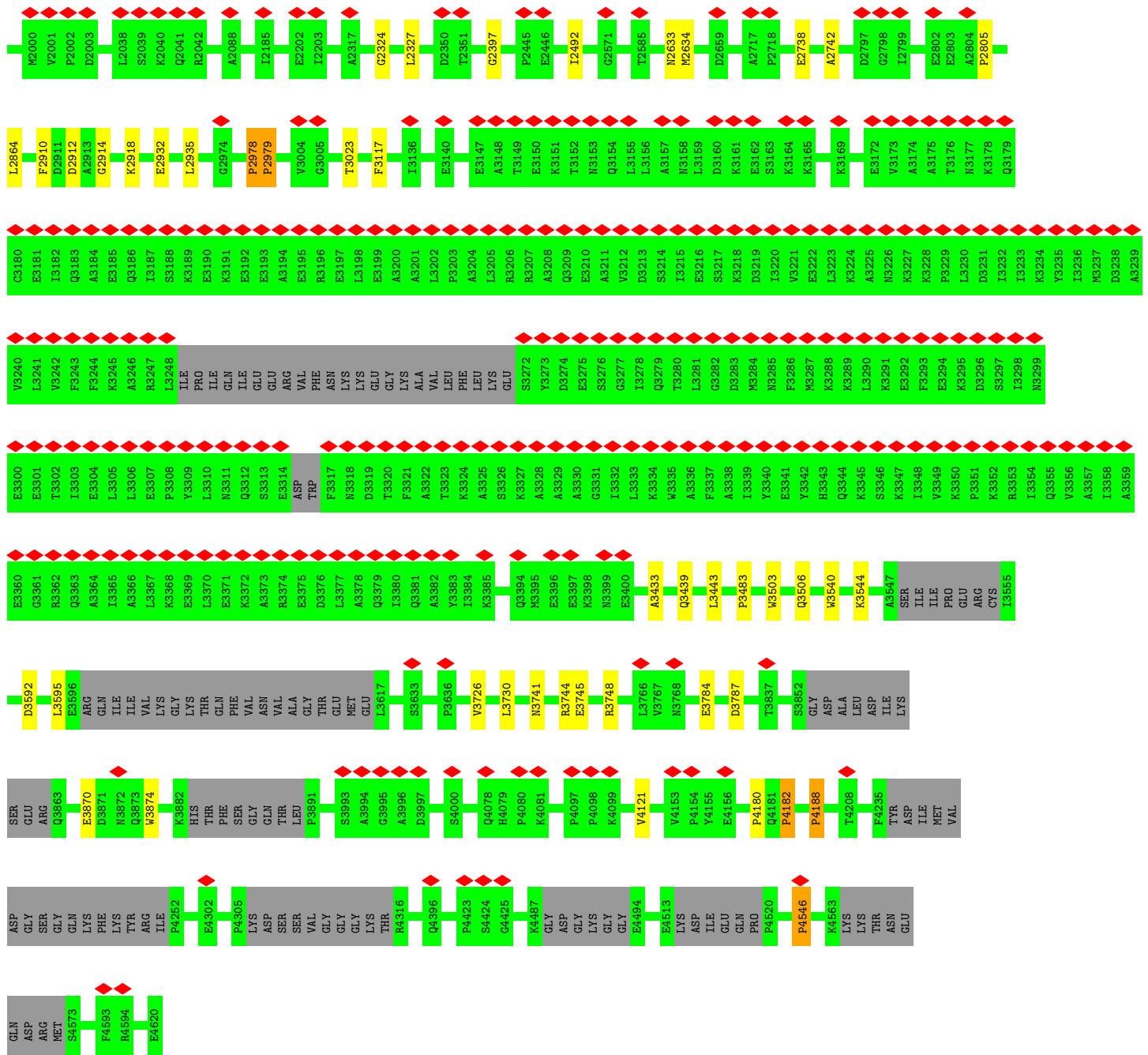




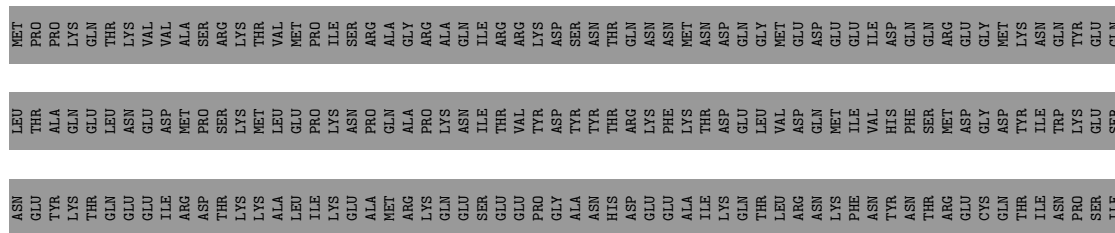


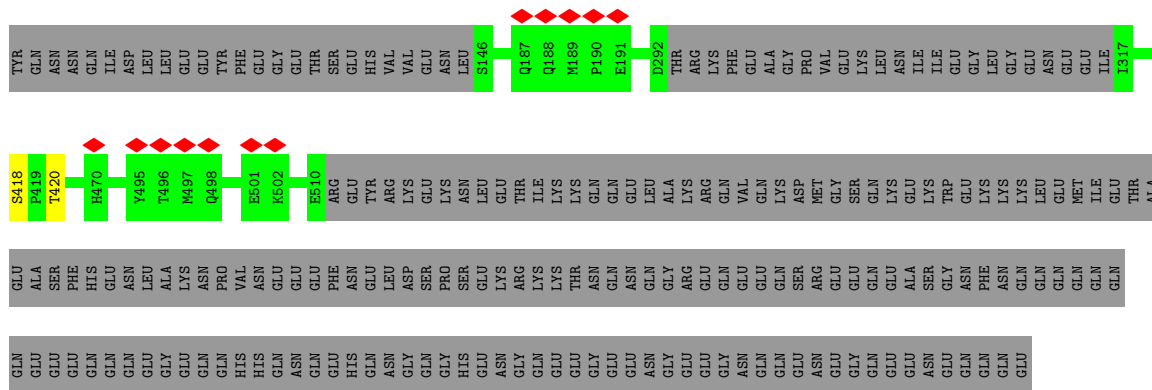
• Molecule 3: Dynein heavy chain, outer arm protein





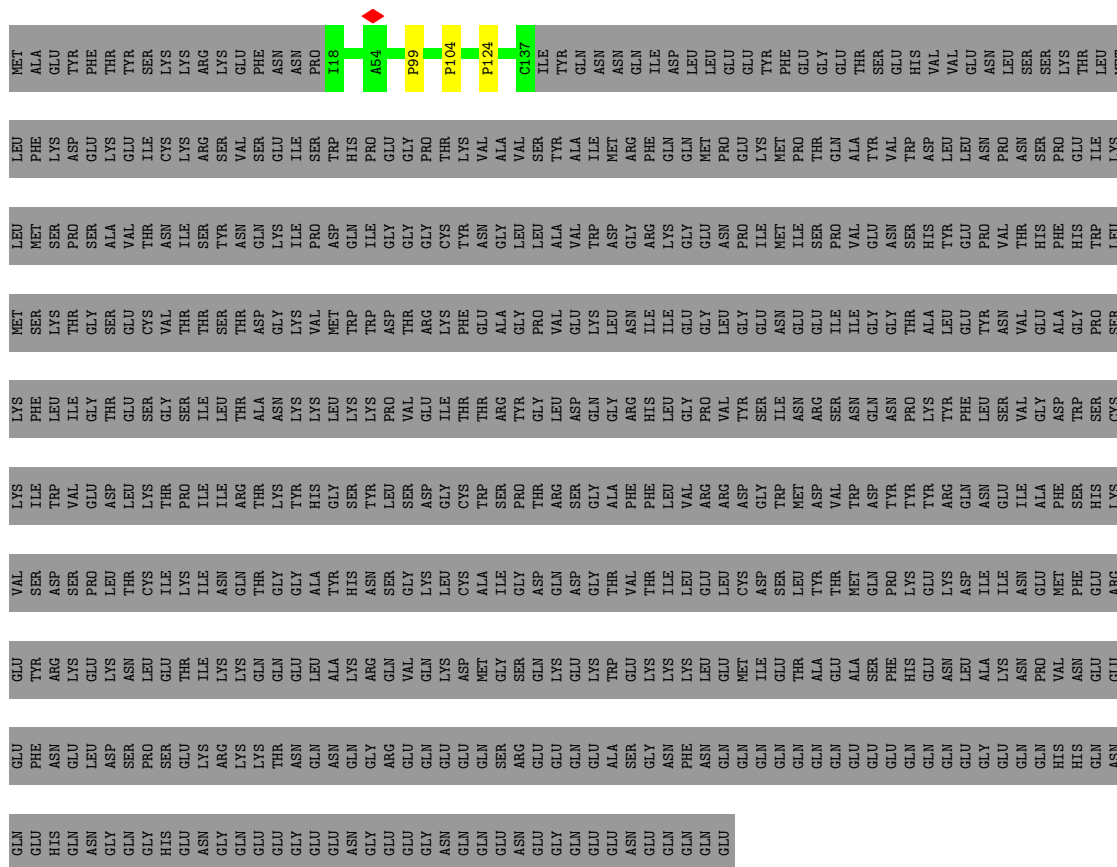
● Molecule 4: Dynein intermediate chain 2





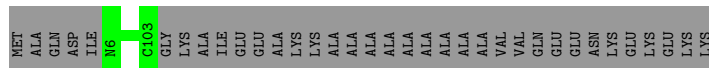
- Molecule 5: Flagellar outer dynein arm intermediate protein, putative

Chain e: 15% 85%




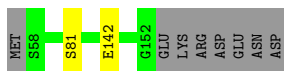
- Molecule 6: Dynein light chain roadblock-type 2 protein

Chain F: 74% 26%




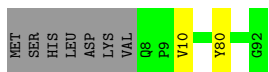
- Molecule 7: Dynein light chain roadblock-type 2 protein

Chain G:  90% 8%




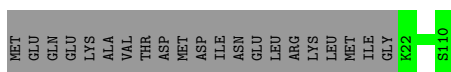
- Molecule 8: Dynein light chain

Chain H:  90% 8%




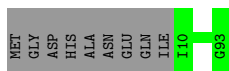
- Molecule 9: Dynein light chain

Chain I:  81% 19%



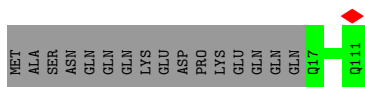
- Molecule 10: Dynein light chain

Chain J:  90% 10%




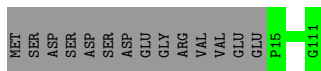
- Molecule 11: Dynein light chain

Chain K:  86% 14%



- Molecule 12: Dynein light chain

Chain L:  87% 13%

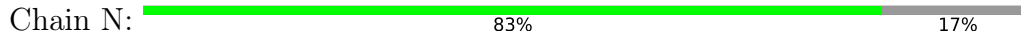


- Molecule 13: Dynein light chain

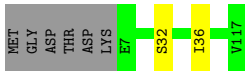
Chain M:  99%



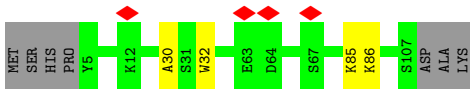
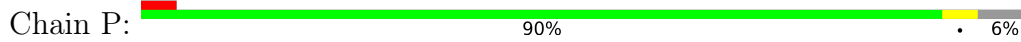
- Molecule 14: Dynein light chain 2A



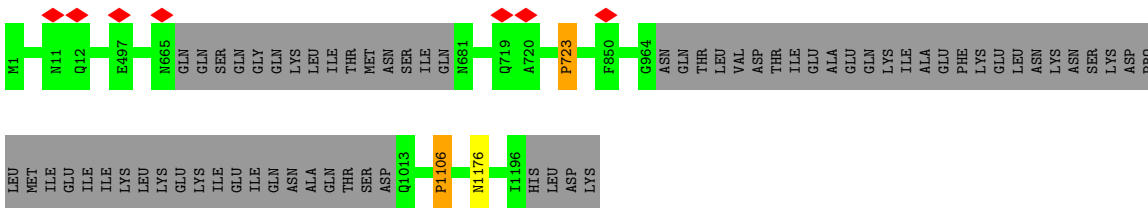
● Molecule 15: Dynein light chain tctex-type 1 protein



● Molecule 16: Thioredoxin



● Molecule 17: Shulin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131142	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.010	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0008	Depositor
Map size (Å)	499.5, 499.5, 499.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	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, GTP, ATP

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	0.34	0/18743	0.69	1/26057 (0.0%)
2	B	0.39	0/19561	0.65	6/27233 (0.0%)
3	C	0.31	0/19162	0.56	8/26702 (0.0%)
4	D	0.36	0/1584	0.84	0/2201
4	d	0.31	0/634	0.61	0/881
5	E	0.36	0/1676	0.78	0/2327
5	e	0.44	0/498	0.76	3/687 (0.4%)
6	F	0.46	0/485	0.86	0/675
7	G	0.37	0/469	0.73	0/652
8	H	0.42	0/419	0.84	0/582
9	I	0.40	0/438	0.86	0/608
10	J	0.31	0/415	0.57	0/577
11	K	0.28	0/469	0.56	0/652
12	L	0.28	0/478	0.57	0/664
13	M	0.29	0/425	0.55	0/591
14	N	0.28	0/536	0.57	0/744
15	O	0.24	0/549	0.50	0/764
16	P	0.78	0/512	0.92	0/714
17	Y	0.29	1/5608 (0.0%)	0.55	2/7814 (0.0%)
All	All	0.35	1/72661 (0.0%)	0.64	20/101125 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	1176	ASN	C-N	6.01	1.47	1.34

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4432	PRO	N-CA-CB	8.75	113.80	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	4182	PRO	N-CA-CB	6.65	111.28	103.30
3	C	4188	PRO	N-CA-CB	6.65	111.28	103.30
17	Y	1106	PRO	N-CA-CB	6.55	111.16	103.30
3	C	2978	PRO	N-CA-CB	6.33	110.89	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	18787	0	8282	131	0
2	B	20008	0	8566	89	0
3	C	19737	0	8300	29	0
4	D	1588	0	693	3	0
4	d	637	0	261	0	0
5	E	1678	0	724	1	0
5	e	501	0	215	0	0
6	F	486	0	218	0	0
7	G	470	0	203	1	0
8	H	420	0	185	1	0
9	I	439	0	202	0	0
10	J	416	0	184	0	0
11	K	470	0	215	0	0
12	L	479	0	209	0	0
13	M	426	0	189	0	0
14	N	537	0	231	0	0
15	O	550	0	247	1	0
16	P	513	0	213	2	0
17	Y	5611	0	2410	0	0
18	C	81	0	36	0	0
19	C	31	0	12	0	0
20	Y	32	0	12	0	0
All	All	73897	0	31807	258	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 2.

The worst 5 of 258 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)
2:B:917:ILE:O	2:B:921:SER:CB	2.17	0.92
3:C:617:ILE:C	3:C:618:THR:CA	2.46	0.84
2:B:4318:LEU:O	2:B:4322:GLU:N	2.12	0.83
3:C:642:ASN:CA	3:C:643:THR:N	2.43	0.81
2:B:2229:LYS:O	2:B:2230:THR:N	2.13	0.81

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	Percentiles	
1	A	3707/4168 (89%)	3206 (86%)	493 (13%)	8 (0%)	47	81
2	B	3893/4595 (85%)	3484 (90%)	398 (10%)	11 (0%)	41	77
3	C	3846/4620 (83%)	3509 (91%)	330 (9%)	7 (0%)	47	81
4	D	313/667 (47%)	268 (86%)	45 (14%)	0	100	100
4	d	122/667 (18%)	112 (92%)	10 (8%)	0	100	100
5	E	337/670 (50%)	287 (85%)	50 (15%)	0	100	100
5	e	96/670 (14%)	86 (90%)	10 (10%)	0	100	100
6	F	96/133 (72%)	79 (82%)	17 (18%)	0	100	100
7	G	93/103 (90%)	81 (87%)	12 (13%)	0	100	100
8	H	83/92 (90%)	76 (92%)	7 (8%)	0	100	100
9	I	87/110 (79%)	79 (91%)	8 (9%)	0	100	100
10	J	82/93 (88%)	77 (94%)	5 (6%)	0	100	100
11	K	93/111 (84%)	83 (89%)	10 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	95/111 (86%)	90 (95%)	5 (5%)	0	100	100
13	M	84/87 (97%)	77 (92%)	7 (8%)	0	100	100
14	N	107/132 (81%)	100 (94%)	7 (6%)	0	100	100
15	O	109/117 (93%)	99 (91%)	10 (9%)	0	100	100
16	P	101/110 (92%)	97 (96%)	4 (4%)	0	100	100
17	Y	1127/1200 (94%)	1071 (95%)	54 (5%)	2 (0%)	47	81
All	All	14471/18456 (78%)	12961 (90%)	1482 (10%)	28 (0%)	50	81

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1823	VAL
2	B	1651	ASN
2	B	1652	PRO
2	B	2557	PRO
2	B	3703	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

5 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
18	ADP	C	4704	-	24,29,29	0.92	1 (4%)	29,45,45	1.49	4 (13%)
19	ATP	C	4702	-	26,33,33	0.87	1 (3%)	31,52,52	1.68	5 (16%)
20	GTP	Y	1301	-	26,34,34	1.21	2 (7%)	32,54,54	1.65	6 (18%)
18	ADP	C	4701	-	24,29,29	0.96	1 (4%)	29,45,45	1.49	3 (10%)
18	ADP	C	4703	-	24,29,29	0.93	1 (4%)	29,45,45	1.54	4 (13%)

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
18	ADP	C	4704	-	-	3/12/32/32	0/3/3/3
19	ATP	C	4702	-	-	4/18/38/38	0/3/3/3
20	GTP	Y	1301	-	-	6/18/38/38	0/3/3/3
18	ADP	C	4701	-	-	1/12/32/32	0/3/3/3
18	ADP	C	4703	-	-	4/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Y	1301	GTP	C5-C6	-4.38	1.38	1.47
18	C	4704	ADP	C5-C4	2.25	1.46	1.40
18	C	4701	ADP	C5-C4	2.18	1.46	1.40
20	Y	1301	GTP	C2-N3	2.17	1.38	1.33
18	C	4703	ADP	C5-C4	2.13	1.46	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	4702	ATP	PA-O3A-PB	-5.12	115.25	132.83
18	C	4701	ADP	PA-O3A-PB	-4.56	117.17	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
18	C	4704	ADP	PA-O3A-PB	-4.21	118.36	132.83
19	C	4702	ATP	PB-O3B-PG	-4.13	118.64	132.83
18	C	4703	ADP	PA-O3A-PB	-4.13	118.66	132.83

There are no chirality outliers.

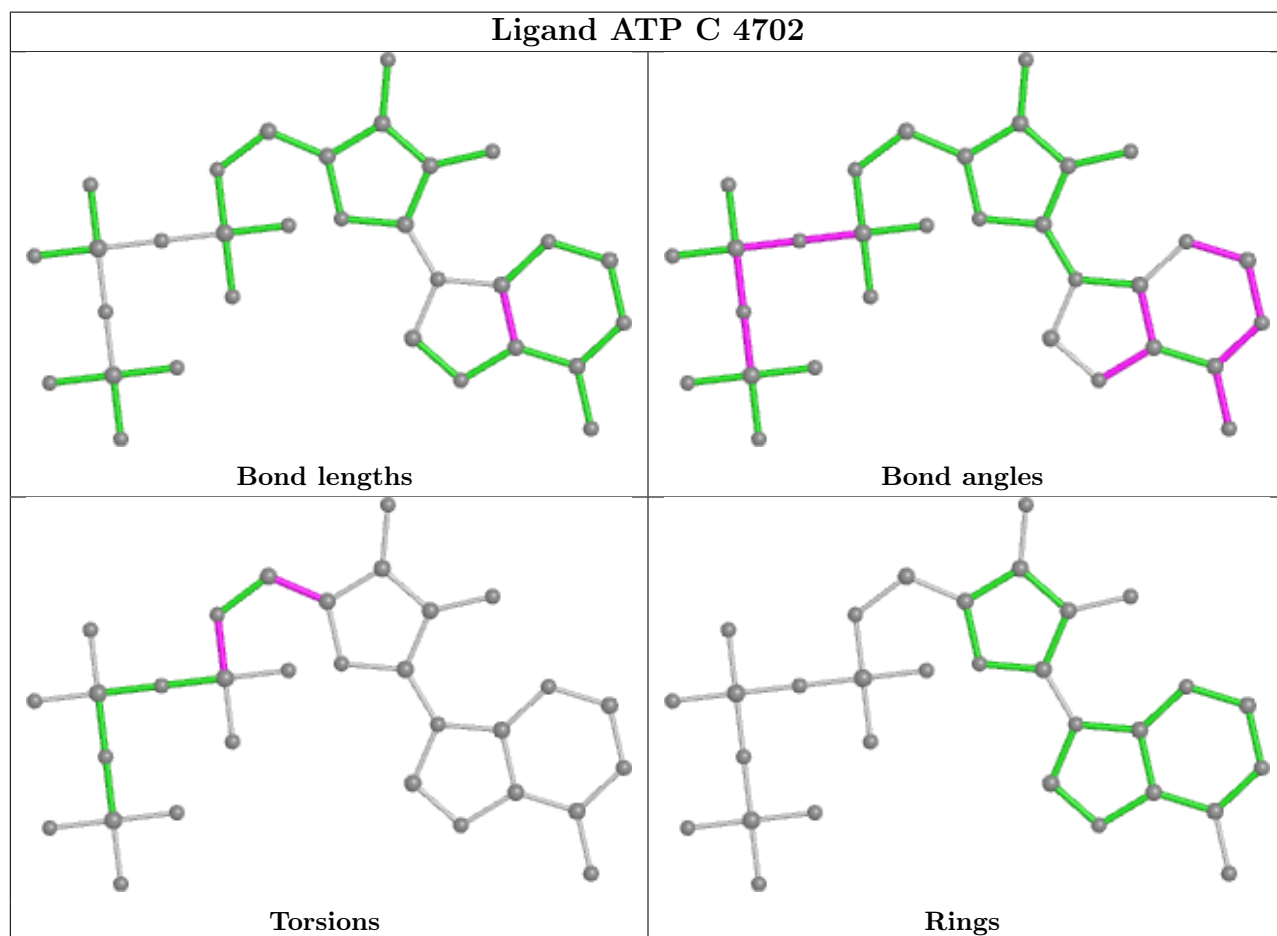
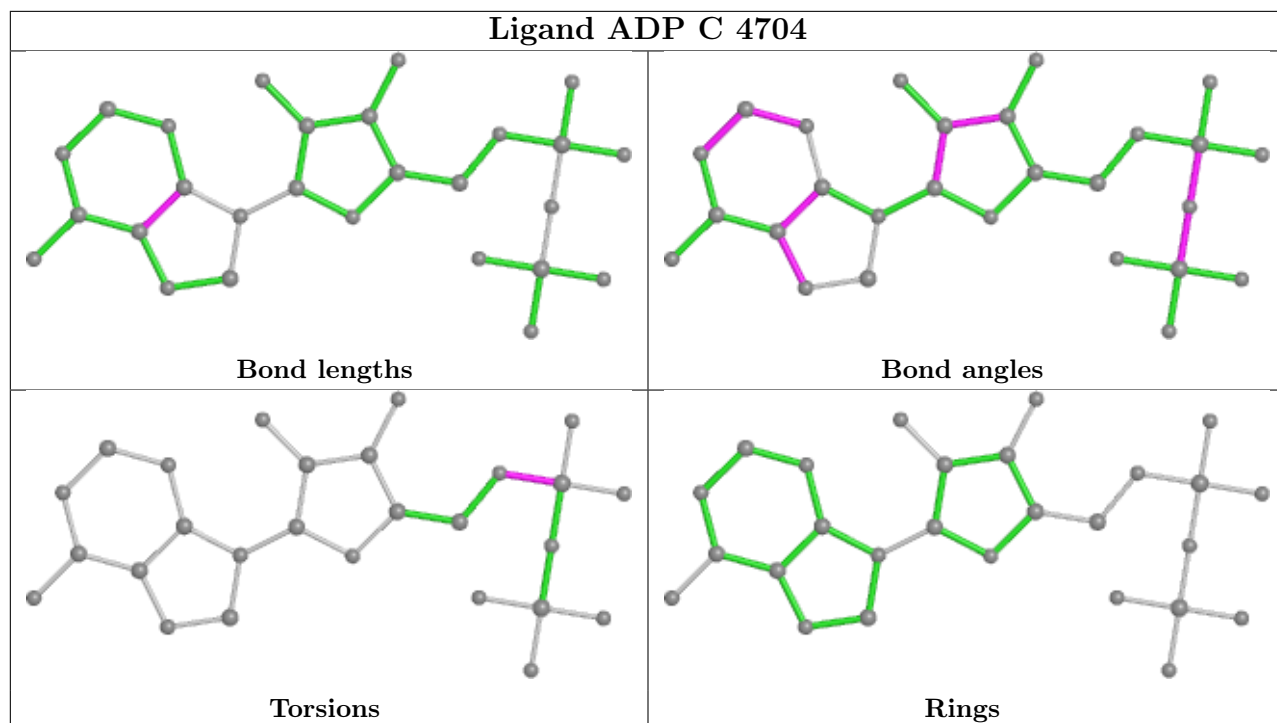
5 of 18 torsion outliers are listed below:

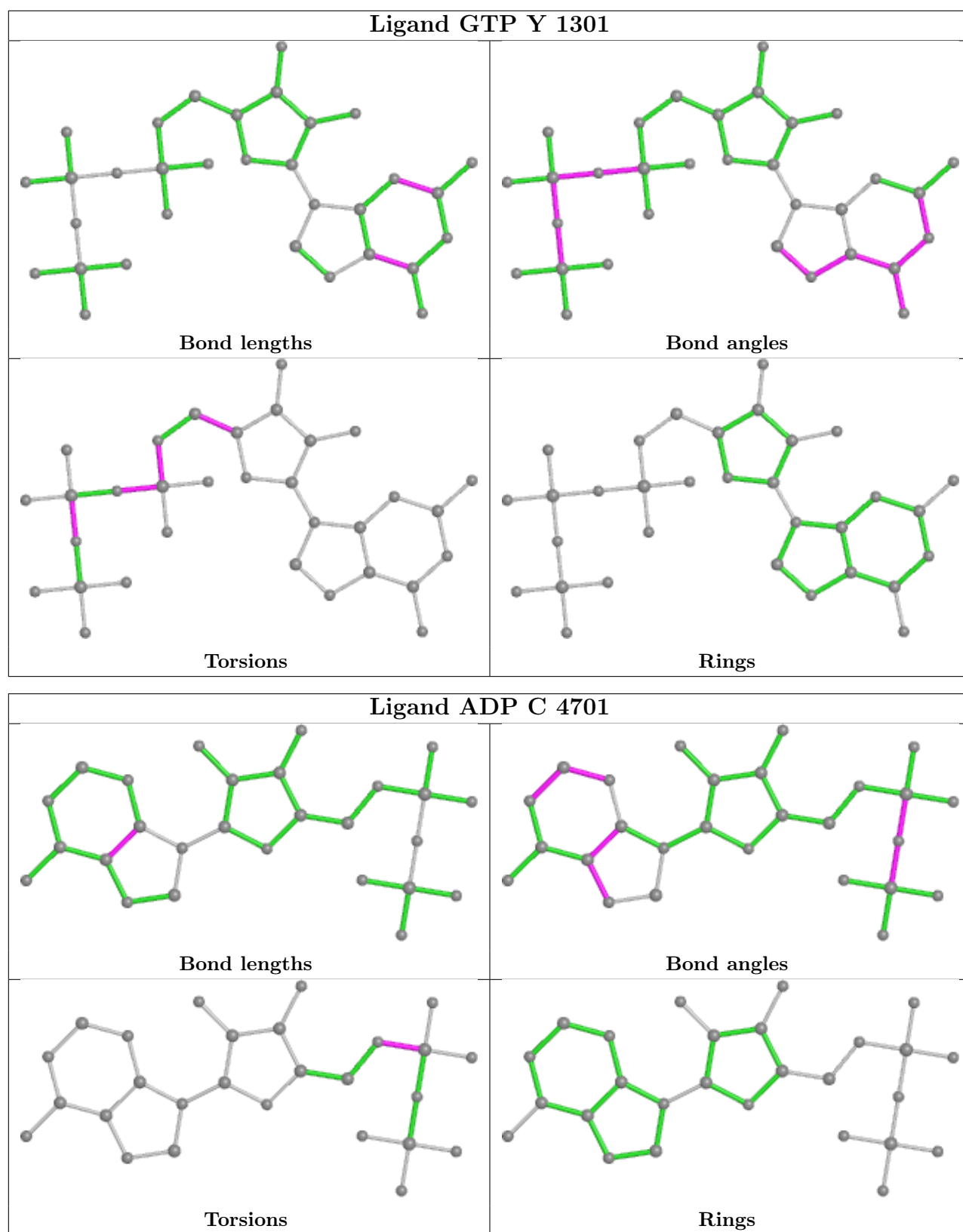
Mol	Chain	Res	Type	Atoms
18	C	4703	ADP	C5'-O5'-PA-O1A
18	C	4703	ADP	C5'-O5'-PA-O2A
18	C	4704	ADP	C5'-O5'-PA-O2A
19	C	4702	ATP	C5'-O5'-PA-O1A
19	C	4702	ATP	C5'-O5'-PA-O3A

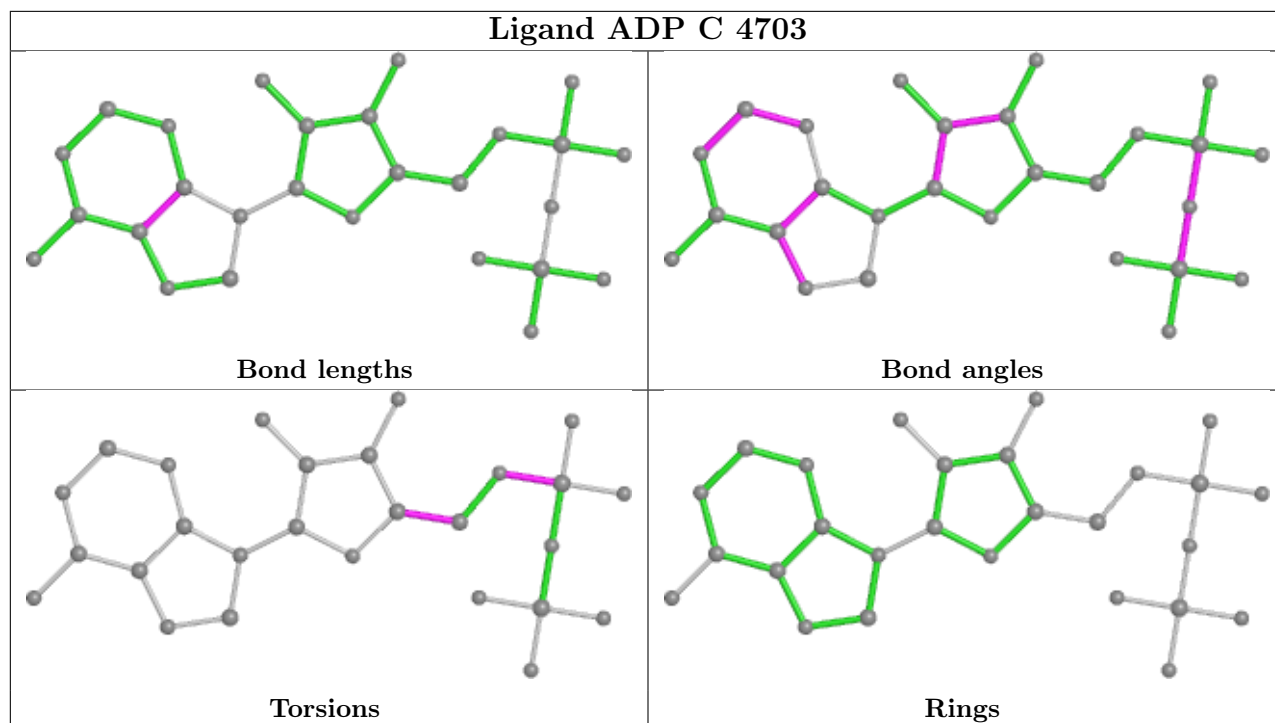
There are no ring outliers.

No monomer is involved in short contacts.

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 [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
1	A	23
2	B	12
5	e	2
4	d	1

The worst 5 of 38 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	d	201:GLN	C	235:TRP	N	31.73
1	A	389:ASP	C	390:THR	N	29.62
1	A	486:ASP	C	487:GLN	N	21.39
1	A	1299:VAL	C	1300:GLN	N	17.01
1	A	2300:SER	C	2301:ASP	N	13.90

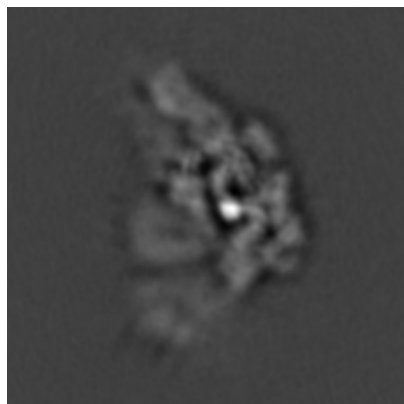
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11576. These allow visual inspection of the internal detail of the map and identification of artifacts.

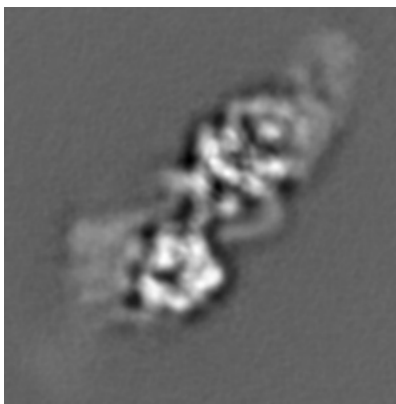
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

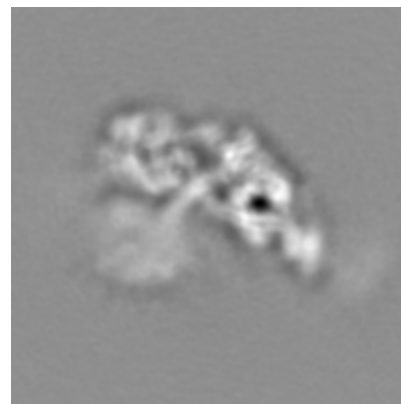
6.1.1 Primary map



X

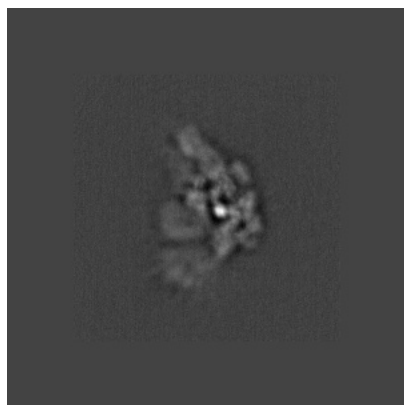


Y

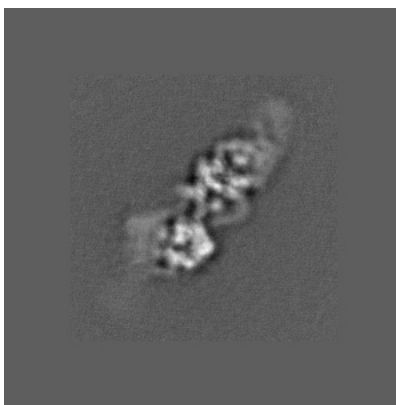


Z

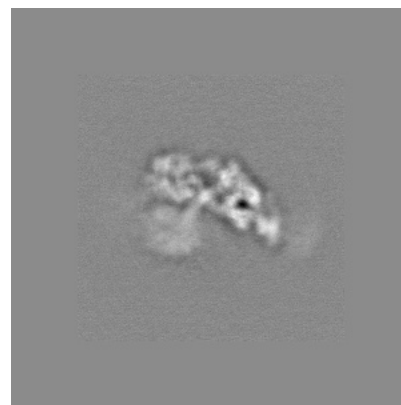
6.1.2 Raw map



X



Y

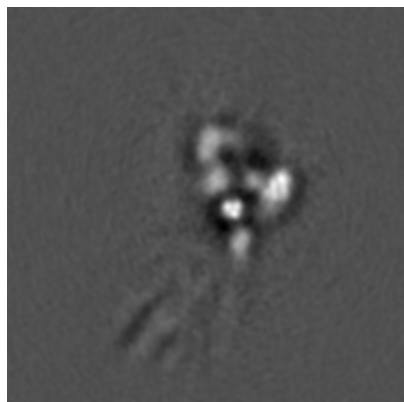


Z

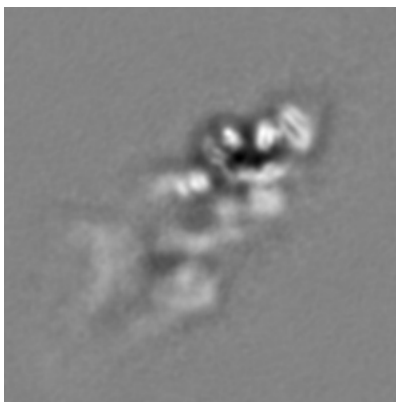
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

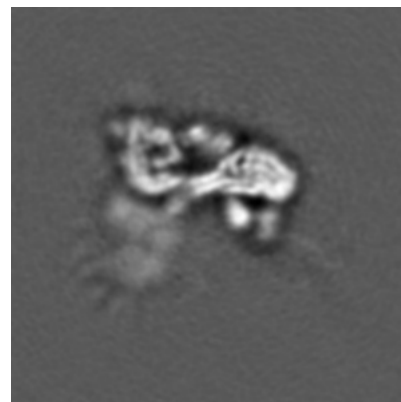
6.2.1 Primary map



X Index: 225

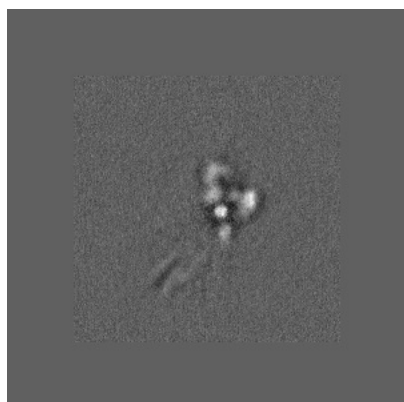


Y Index: 225

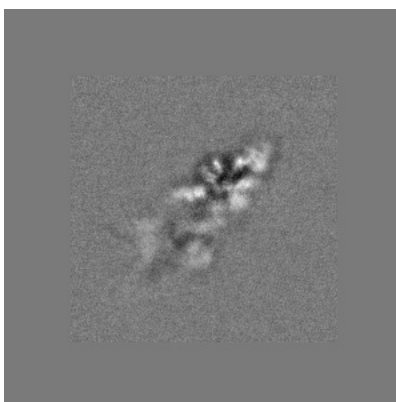


Z Index: 225

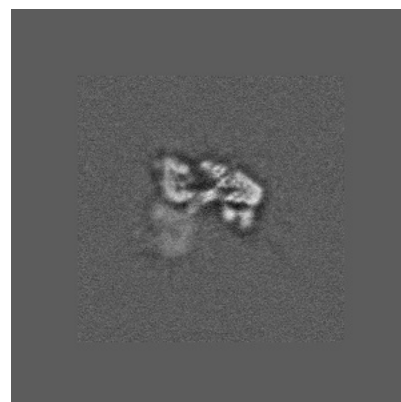
6.2.2 Raw map



X Index: 384



Y Index: 384

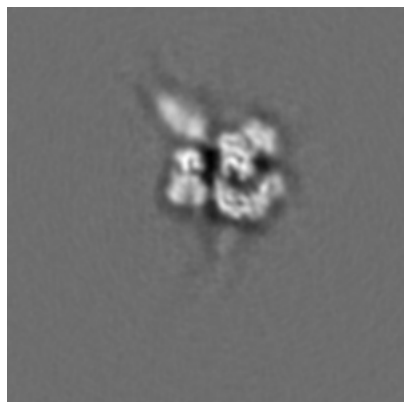


Z Index: 384

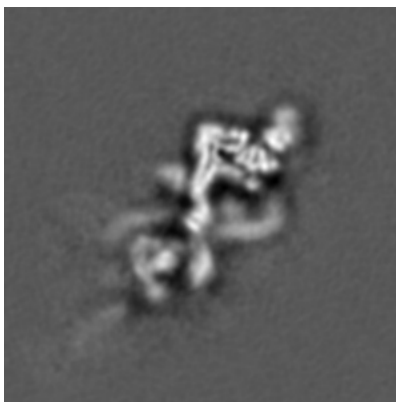
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

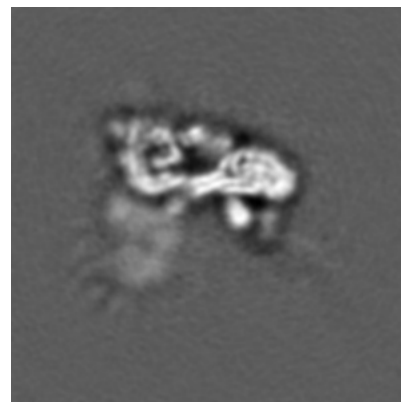
6.3.1 Primary map



X Index: 274

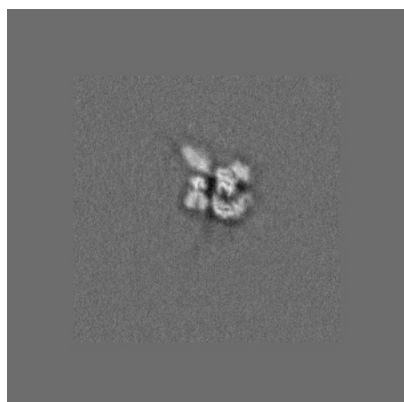


Y Index: 246

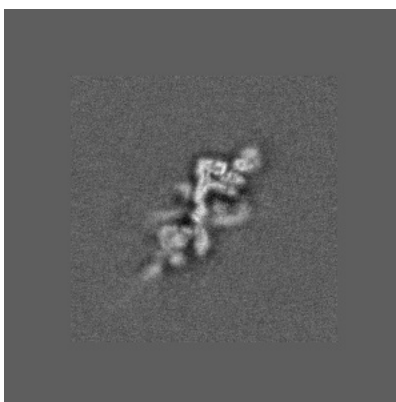


Z Index: 223

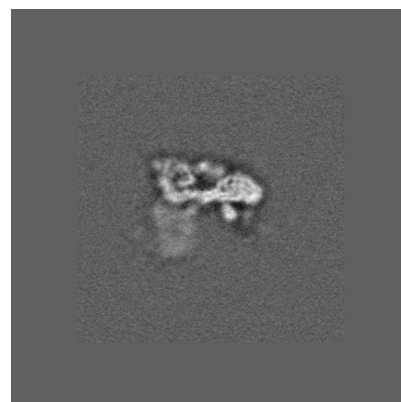
6.3.2 Raw map



X Index: 438



Y Index: 405

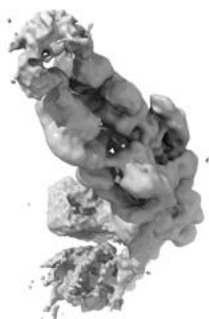


Z Index: 378

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



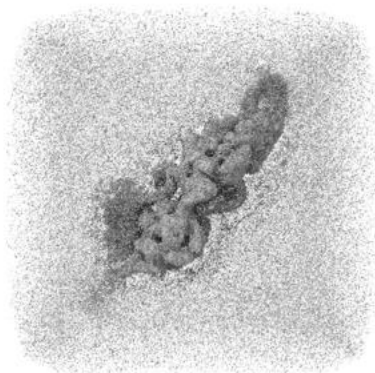
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

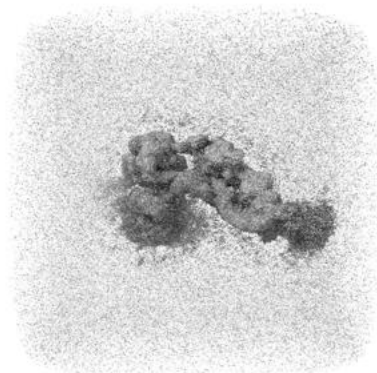
6.4.2 Raw map



X



Y



Z

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.

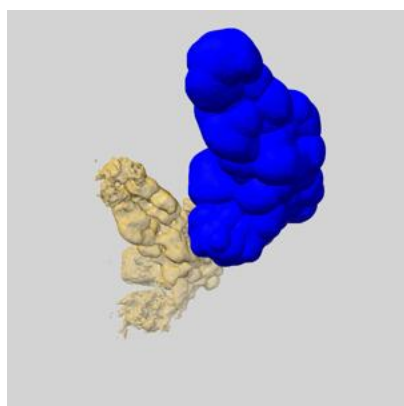
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

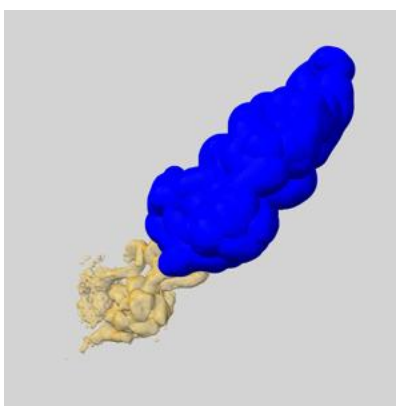
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

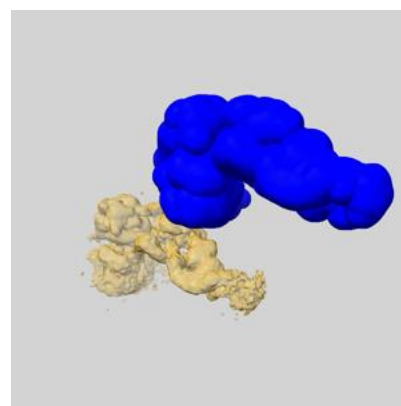
6.5.1 emd_11576_msk_1.map [i](#)



X



Y

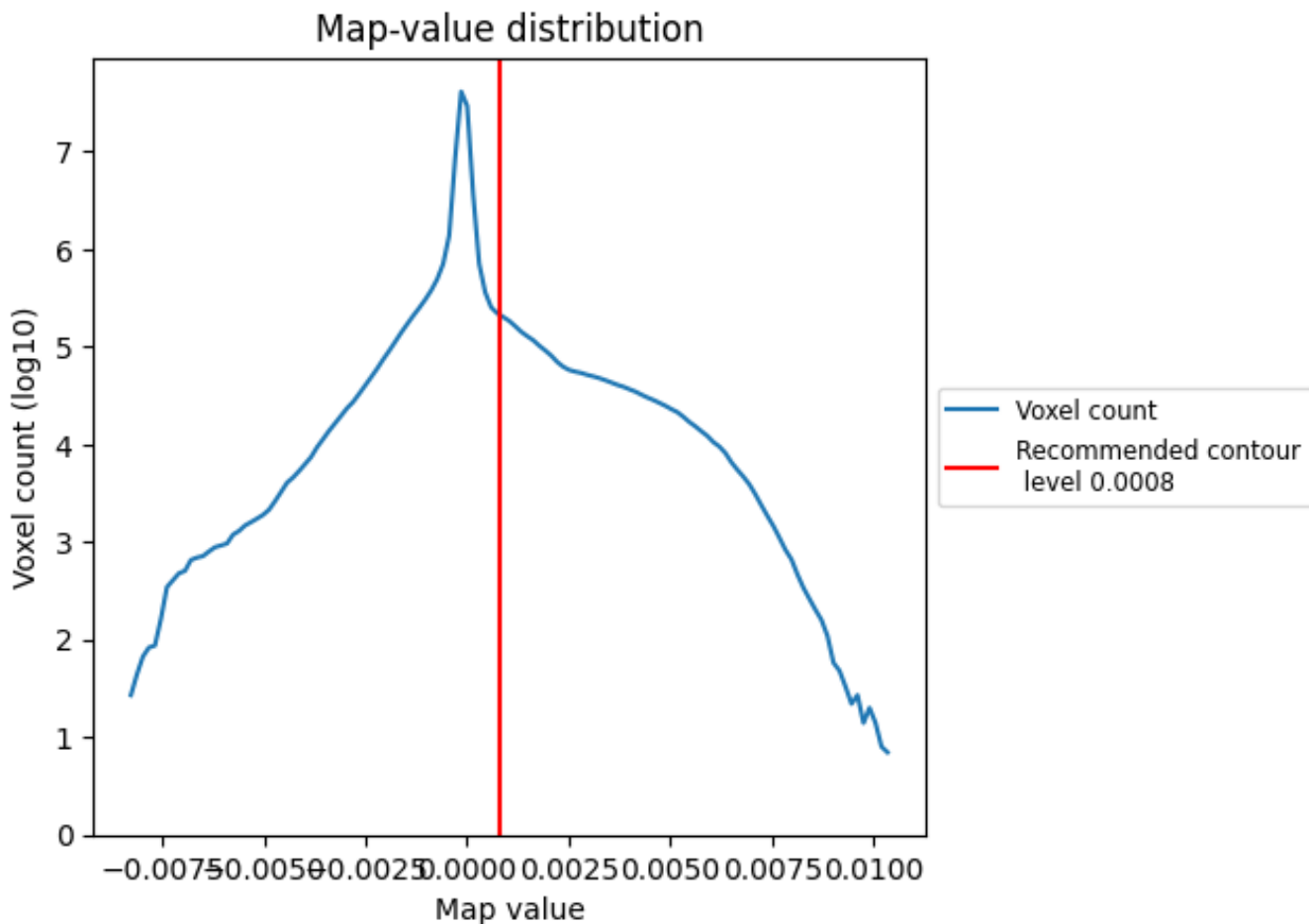


Z

7 Map analysis [i](#)

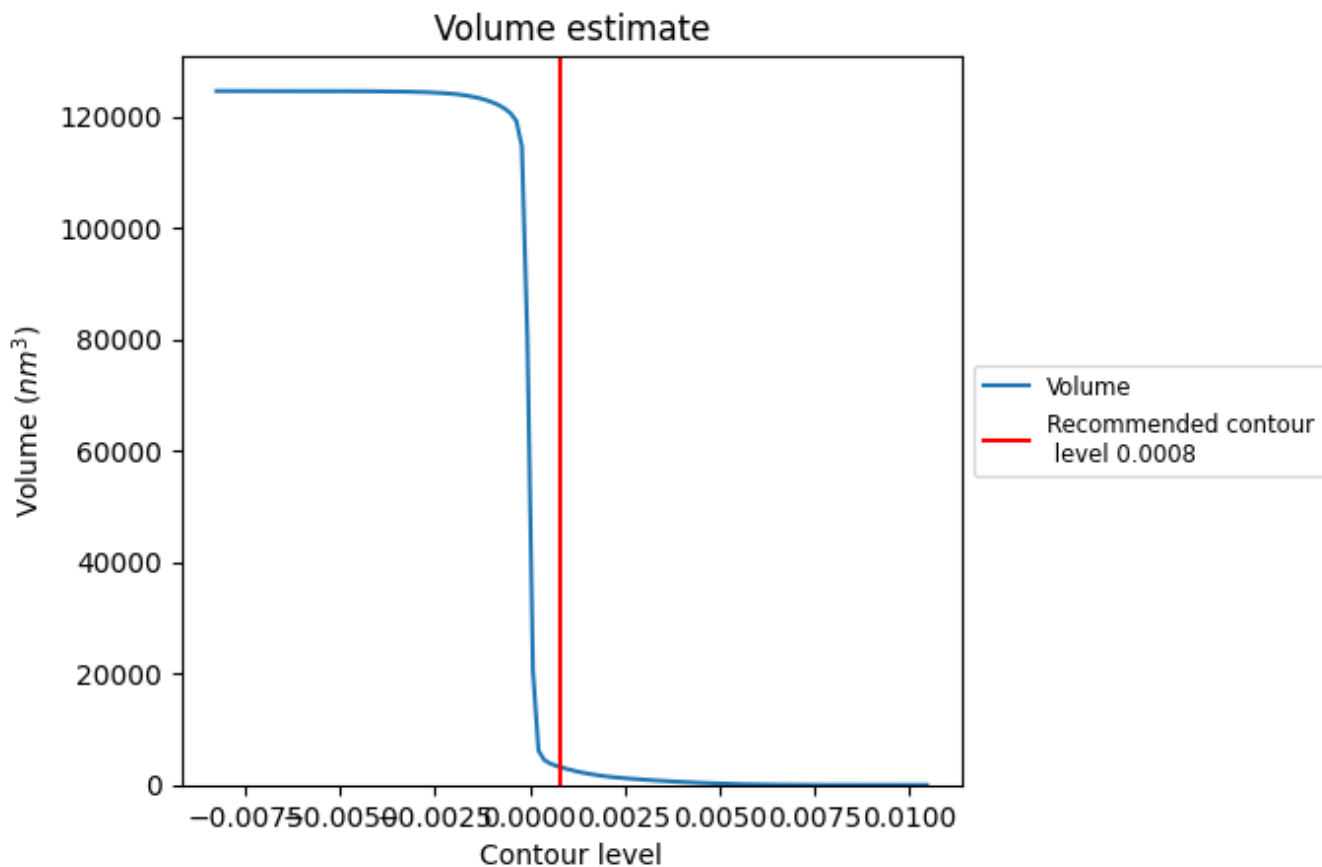
This section contains the results of statistical analysis of the map.

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.

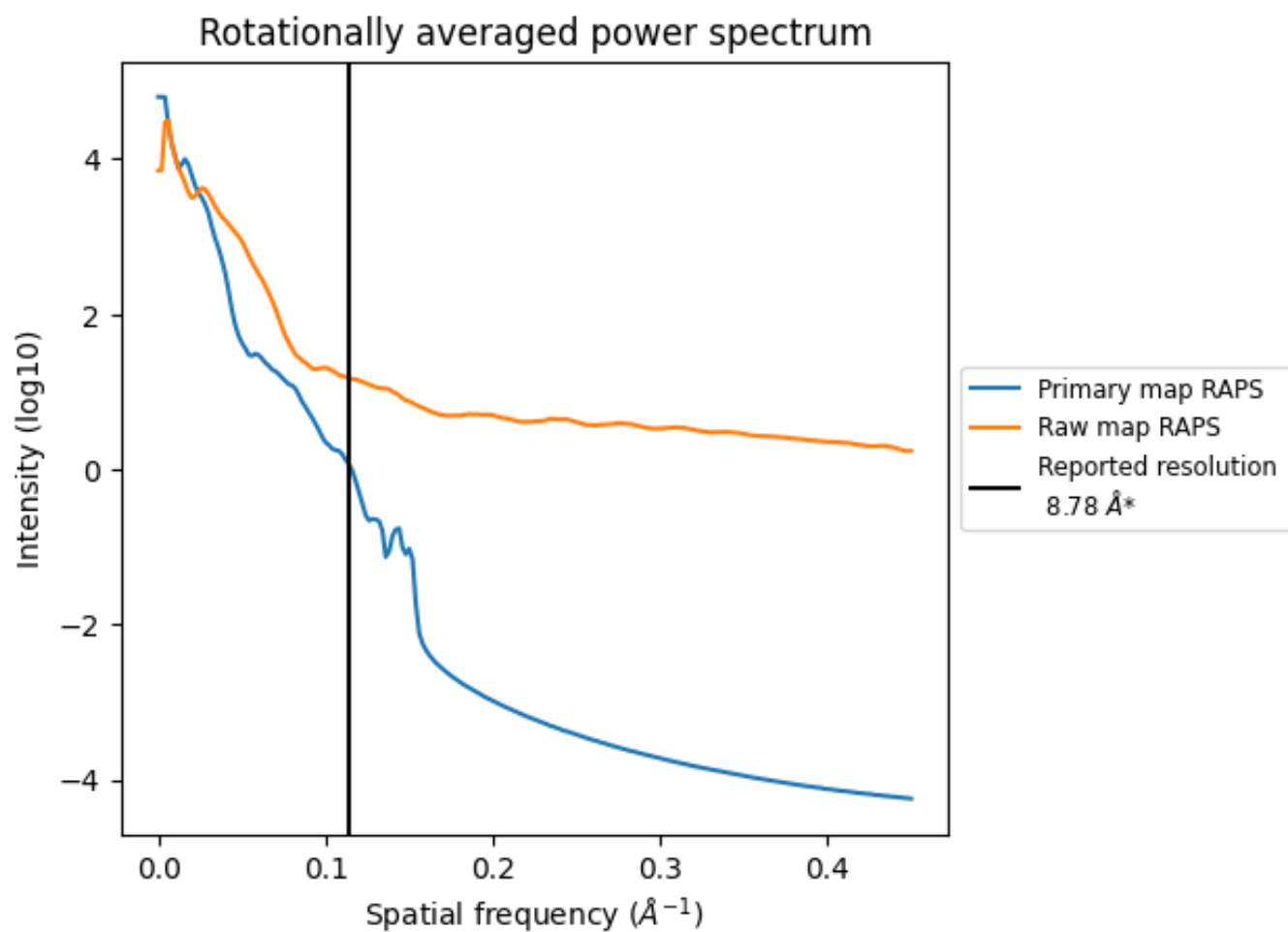
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3222 nm^3 ; this corresponds to an approximate mass of 2910 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](#)

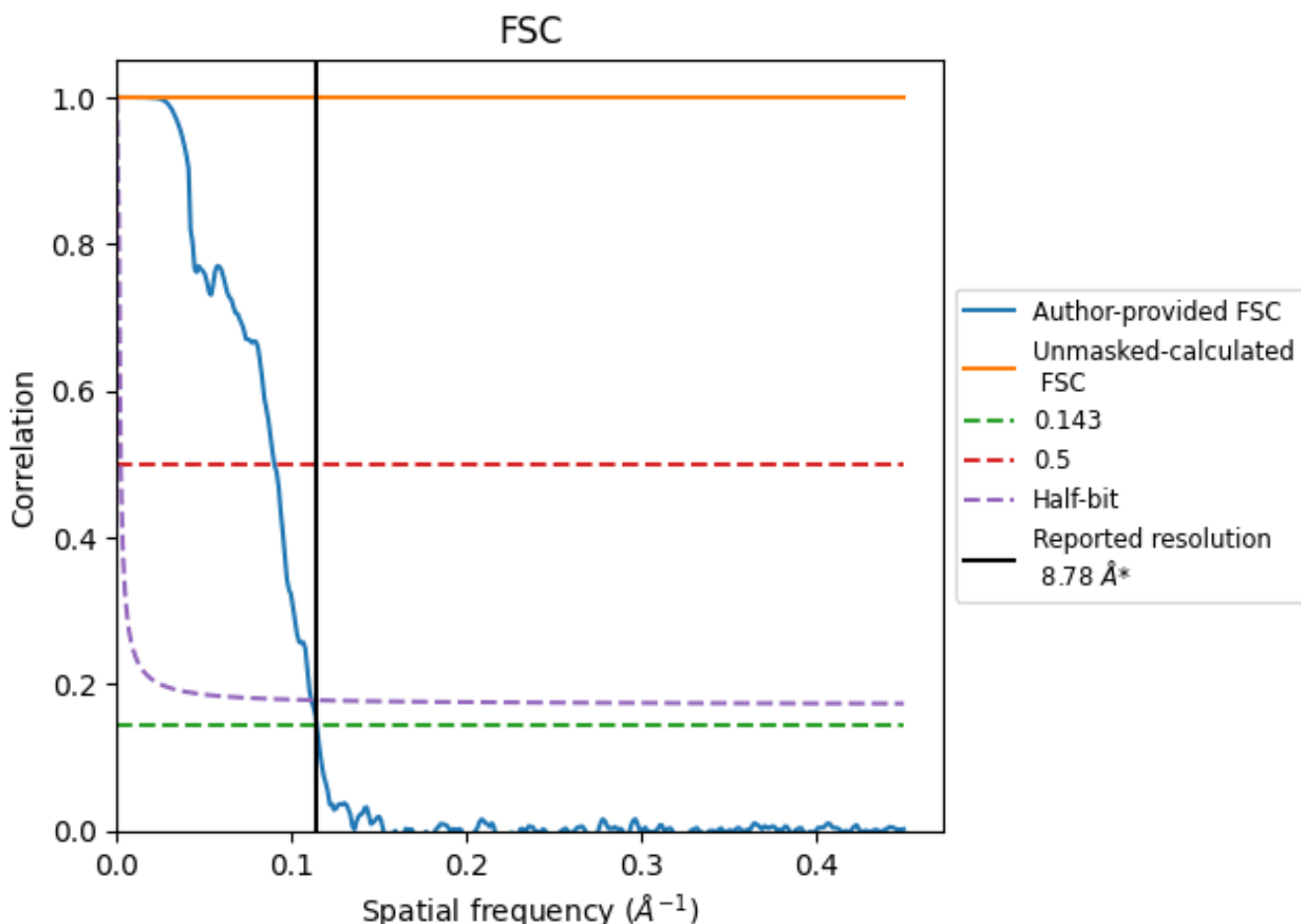


*Reported resolution corresponds to spatial frequency of 0.114 Å⁻¹

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 0.114 \AA^{-1}

8.2 Resolution estimates [i](#)

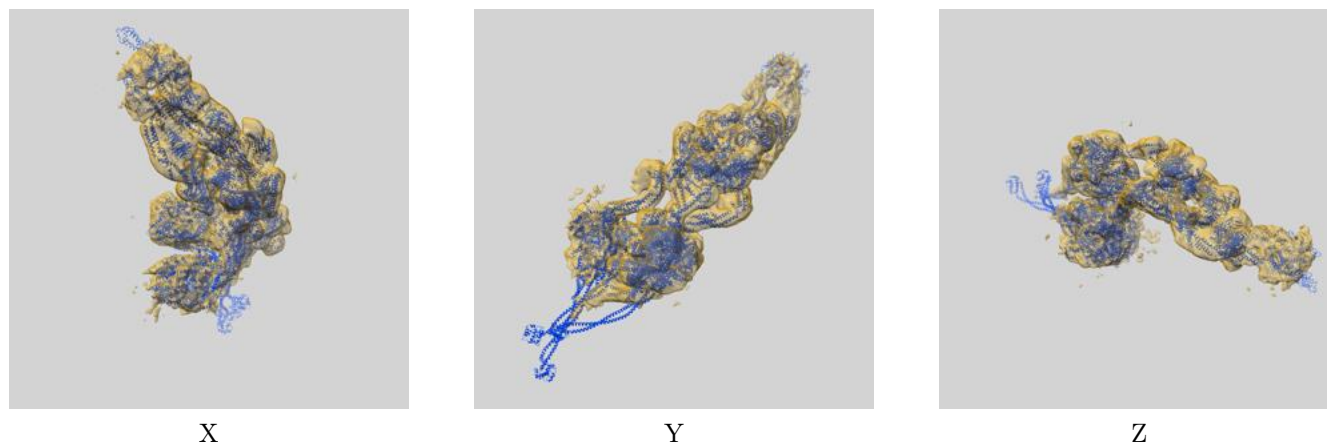
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.78	-	-
Author-provided FSC curve	8.73	11.09	8.98
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

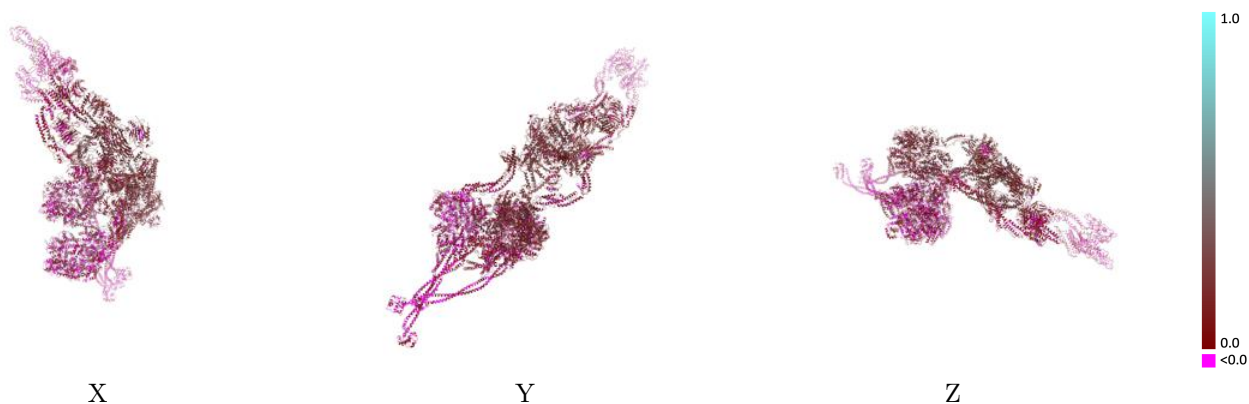
This section contains information regarding the fit between EMDB map EMD-11576 and PDB model 6ZYW. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



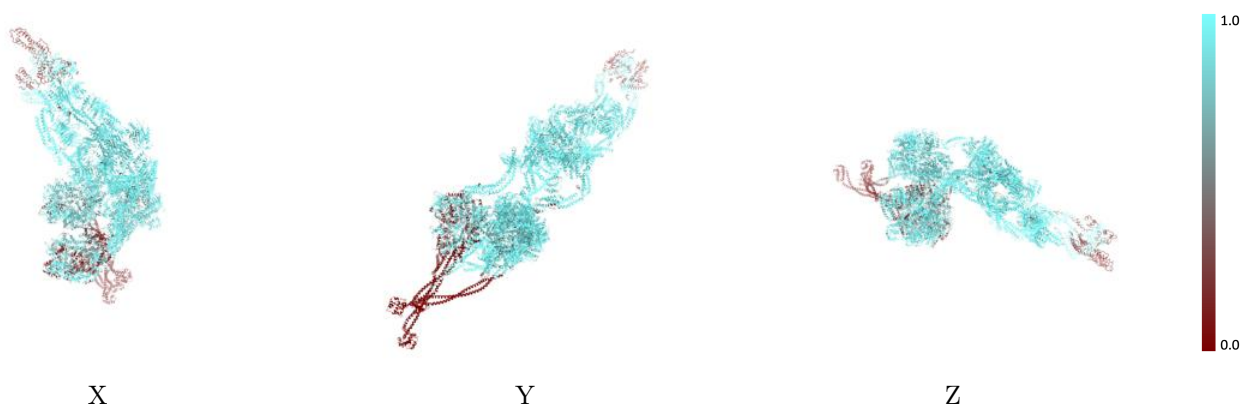
The images above show the 3D surface view of the map at the recommended contour level 0.0008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



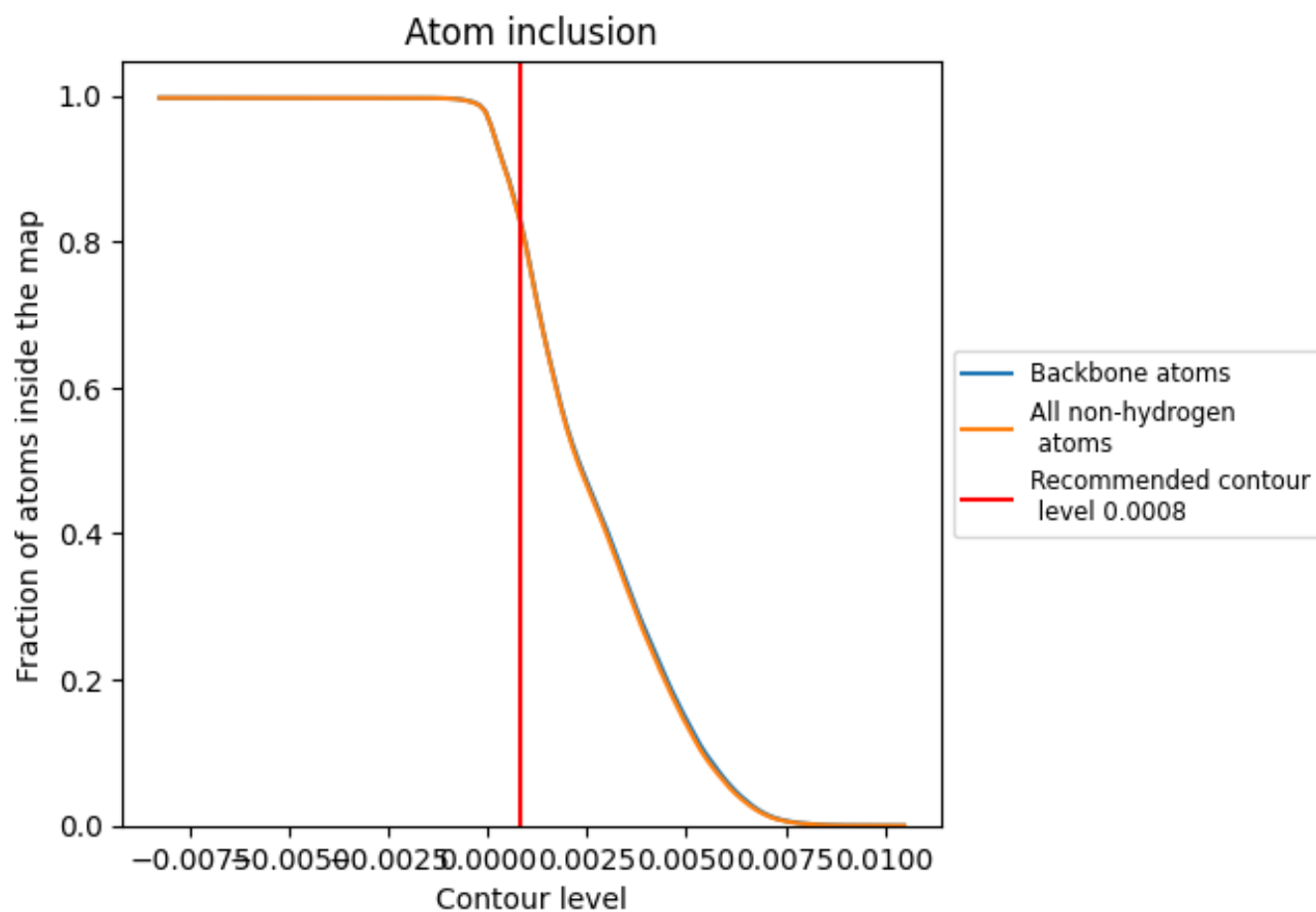
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0008).









































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 (0.0008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8305	 0.1030
A	 0.6147	 0.0490
B	 0.8391	 0.0730
C	 0.9056	 0.1350
D	 0.9994	 0.1040
E	 0.9636	 0.0940
F	 0.9979	 0.1610
G	 0.9957	 0.1840
H	 1.0000	 0.1760
I	 0.9932	 0.2000
J	 0.9952	 0.2100
K	 0.9915	 0.2000
L	 0.9937	 0.2030
M	 0.9977	 0.2150
N	 1.0000	 0.1660
O	 0.9982	 0.1580
P	 0.9552	 0.0670
Y	 0.9910	 0.2020
d	 0.9498	 0.1750
e	 0.9860	 0.1510

