



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 09:04 AM UTC

PDB ID : 8BWY / pdb_00008bwy
EMDB ID : EMD-16304
Title : In situ outer dynein arm from *Chlamydomonas reinhardtii* in a pre-power stroke state
Authors : Zimmermann, N.E.L.; Noga, A.; Obbineni, J.M.; Ishikawa, T.
Deposited on : 2022-12-07
Resolution : 38.00 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:

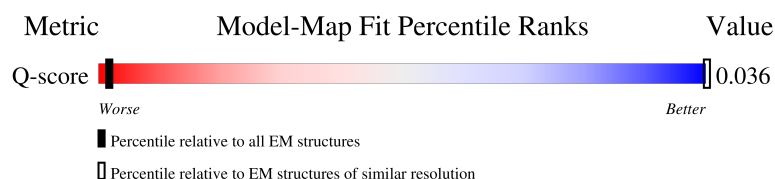
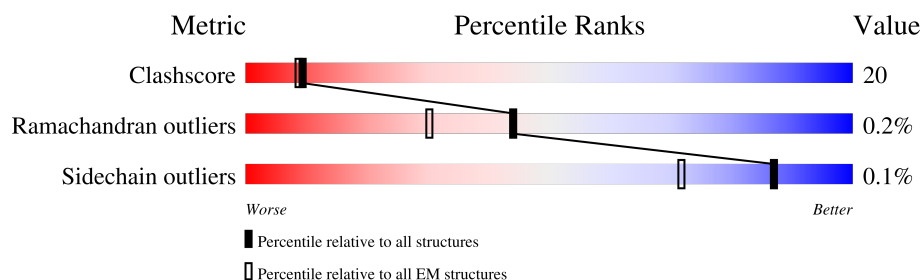
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 38.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2 (38.00 - 38.00)

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	27% 73% 9% 17%
2	B	4595	33% 73% 18% 6%
3	C	4620	28% 75% 17% 8%
4	d	667	5% 33% 36% 31%

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Mol	Chain	Length	Quality of chain
5	e	670	
6	F	133	
7	G	159	
8	H	92	
9	I	110	
10	J	93	
11	K	111	
12	L	111	
13	M	87	
14	N	132	
15	O	117	
16	P	110	
17	T	309	
18	V	130	
18	x	130	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 87003 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
1	A	3455	Total	C	N	O	S	0	0
			18127	10919	3573	3623	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4299	Total	C	N	O	S	0	0
			25545	15697	4785	5025	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	4264	Total	C	N	O	S	0	0
			25046	15335	4744	4923	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	459	Total	C	N	O	S	0	0
			3626	2316	609	680	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	545	Total	C	N	O	S	0	0
			3948	2473	697	759	19		

- 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	S	0	0
			781	493	137	149	2		

- 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	S	0	0
			744	468	128	147	1		

- Molecule 8 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	85	Total	C	N	O	S	0	0
			702	453	115	130	4		

- Molecule 9 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	89	Total	C	N	O	S	0	0
			694	443	111	136	4		

- Molecule 10 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	84	Total	C	N	O	S	0	0
			702	459	114	125	4		

- Molecule 11 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	95	Total	C	N	O	S	0	0
			803	525	134	139	5		

- Molecule 12 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	97	Total	C	N	O	S	0	0
			773	506	131	133	3		

- Molecule 13 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	86	Total	C	N	O	S	0	0
			726	472	122	128	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	109	Total	C	N	O	S	0	0
			897	581	154	159	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	111	Total	C	N	O	S	0	0
			878	558	143	174	3		

- Molecule 16 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	103	Total	C	N	O	S	0	0
			847	549	134	161	3		

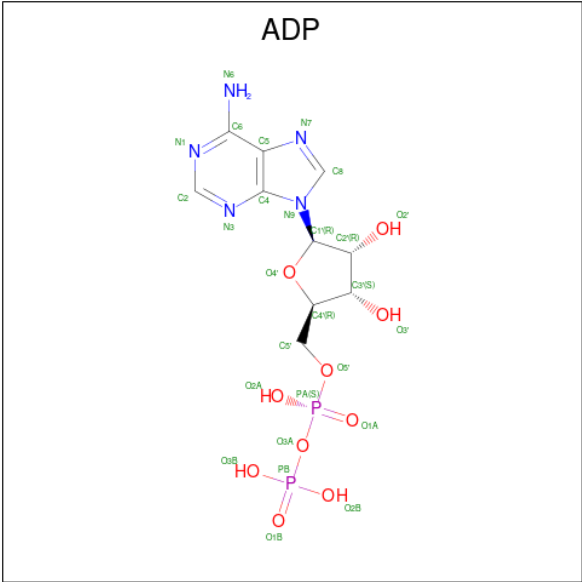
- Molecule 17 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	131	Total	C	N	O	S	0	0
			1057	655	181	215	6		

- Molecule 18 is a protein called Docking complex 1/2 protein.

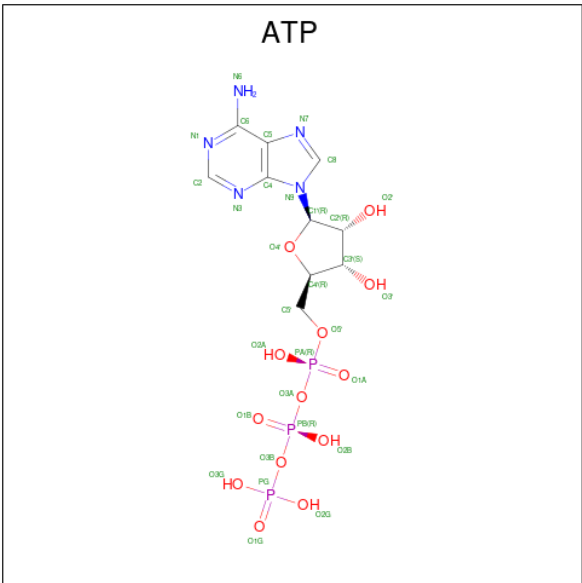
Mol	Chain	Residues	Atoms				AltConf	Trace
18	V	98	Total	C	N	O	0	0
			490	294	98	98		
18	x	101	Total	C	N	O	0	0
			505	303	101	101		

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

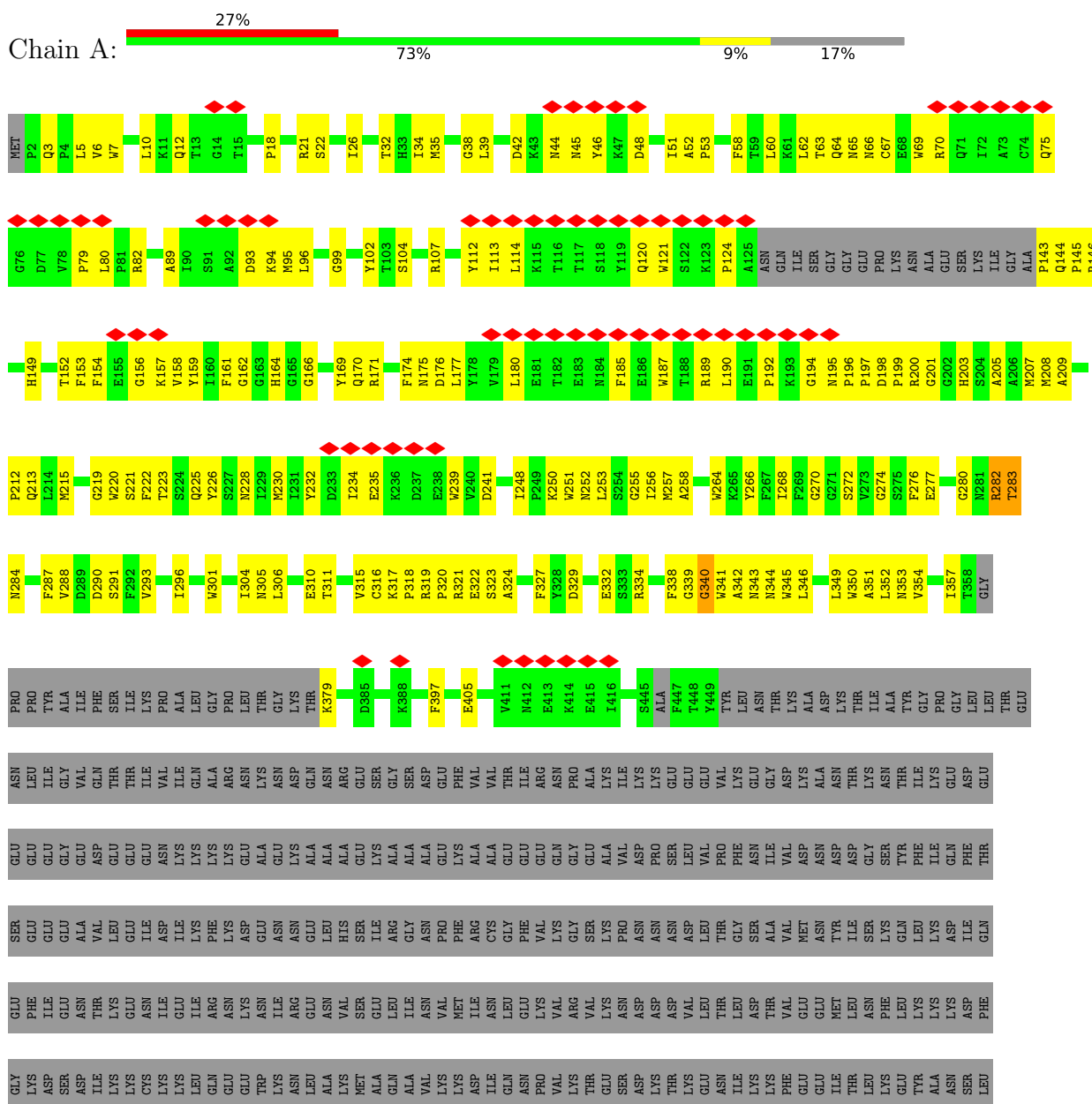


Mol	Chain	Residues	Atoms					AltConf
20	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots

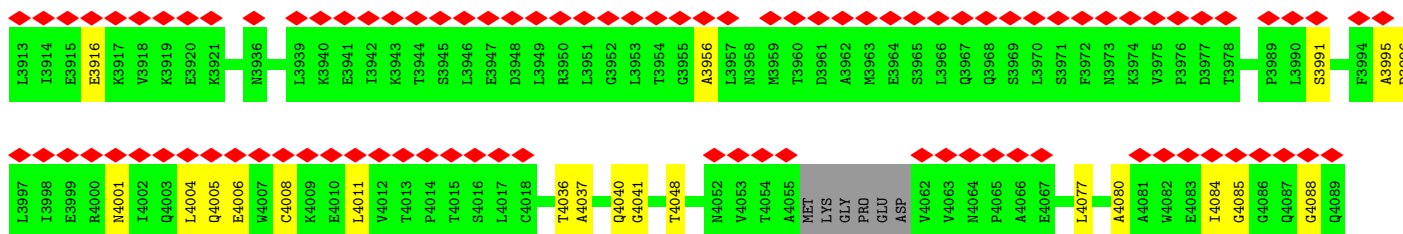
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

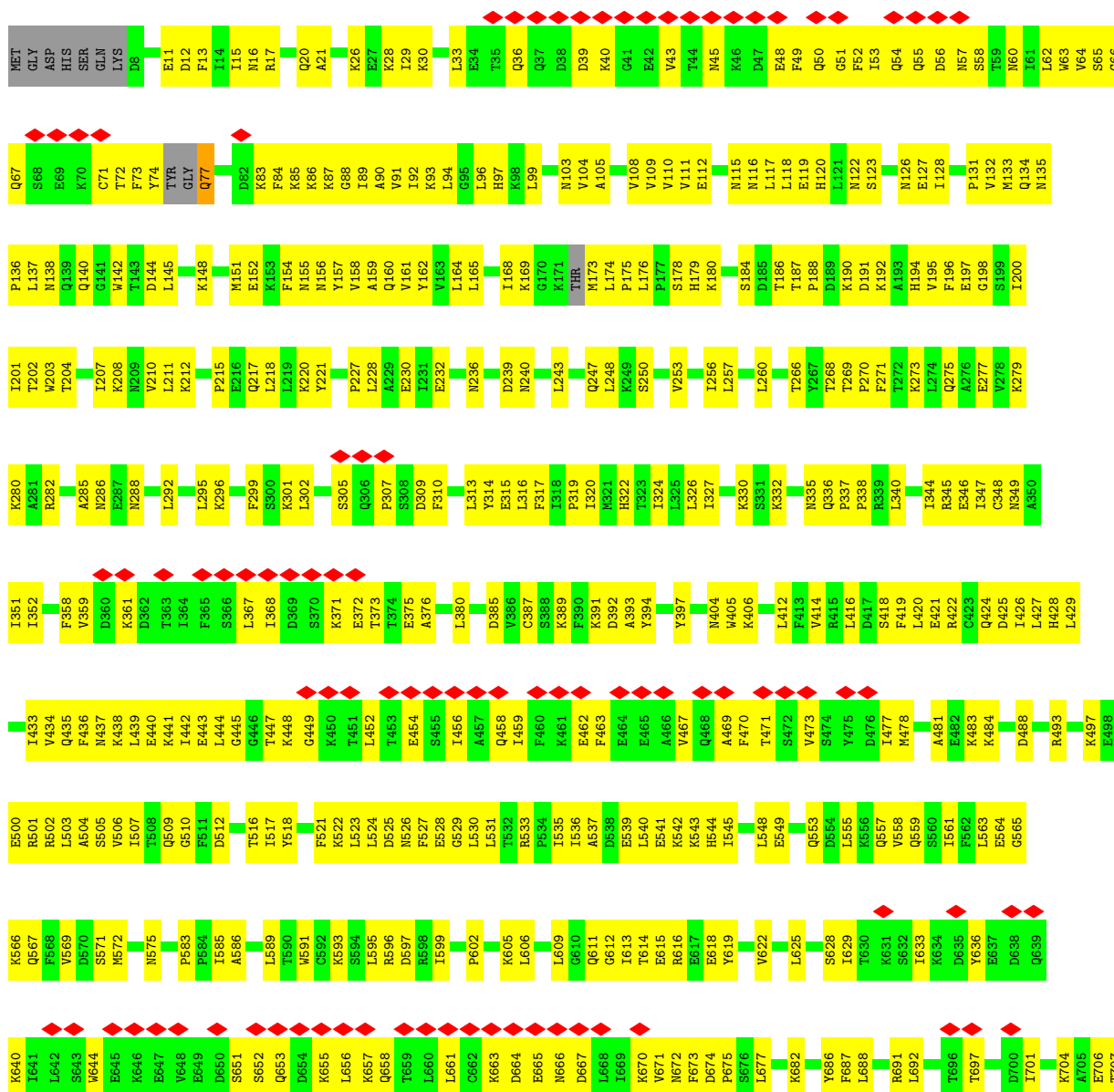




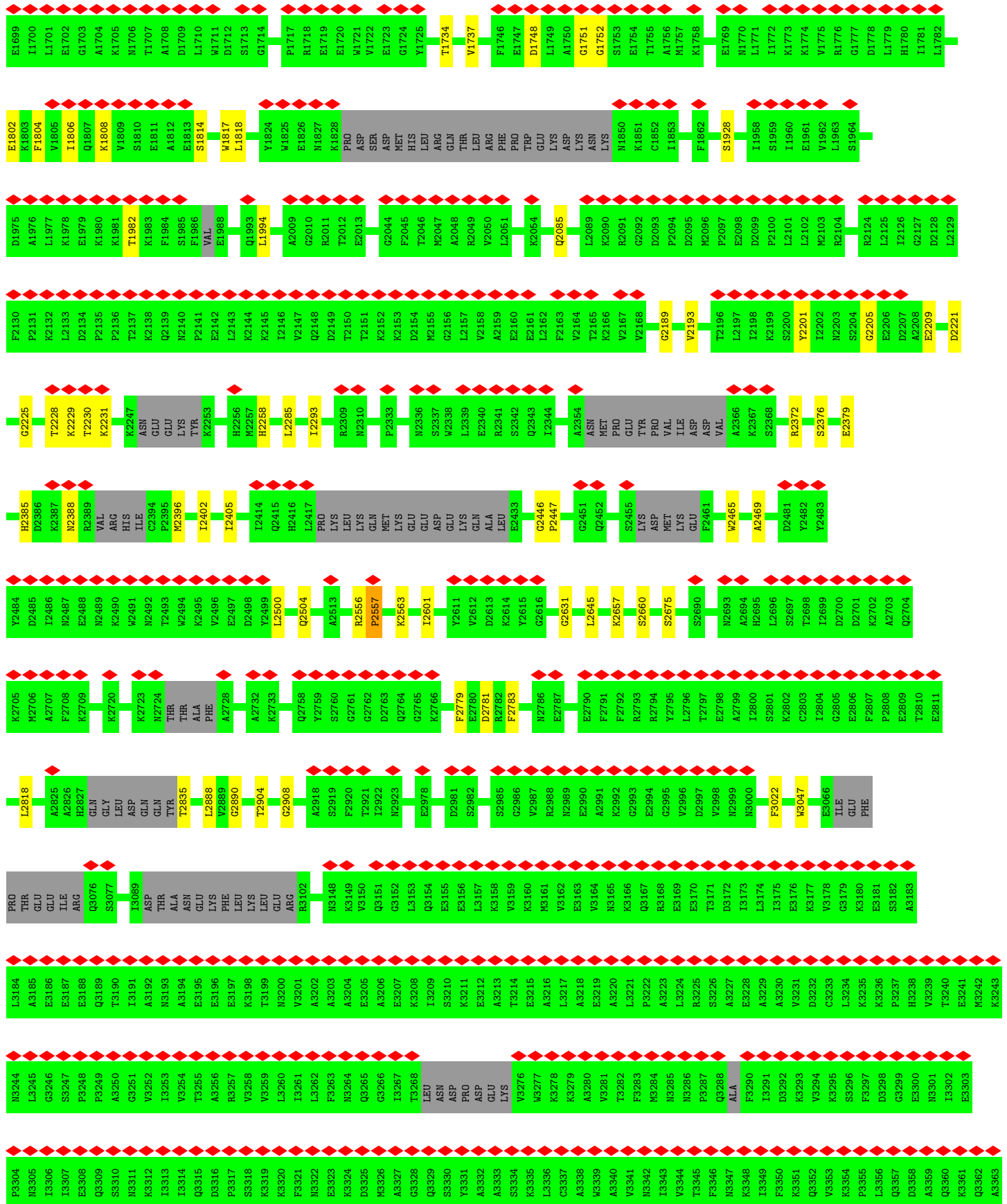
A3821	PRO	GLN	PHE	LYS	SER	PRO	D3828	P3829	S3830	K3831	F3832	F3833	L3711	Y3834	E3835	A3836	Y3837	R3838	K3839	Y3840	I3841	E3842	E3843	K3844	P3850	M3855	S3882	S3883	G3884	G3885	G3886	A3887	S3888	K3889	K3890	D3891	D3892	G3893	Y3894	M3895	Y3896	Y3897	E3785	S3811	E3812	L3813	L3814	Q3815	P3665	N3816	F3818	N3819	L3820	N3910	M3911	L3912					
LEU	LEU	PRO	LEU	MET	GLN	T3675	A3688	P3829	Q3708	E3709	F3710	F3711	D3712	K3713	C3714	K3715	K3716	K3717	P3718	T3719	E3720	F3721	K3722	S3723	S3733	G3737	G3742	W3746	L3764	L3768	S3769	K3770	Y3771	D3772	Q3773	D3777	Y3781	E3786	S3811	E3812	L3813	L3814	Q3815	P3666	N3667	VAL	F3818	N3819	L3820	N3910	M3911	L3912									
F3556	A3583	A3584	T3585	F3586	D3587	V3588	S3589	A3590	N3591	N3592	G3593	R3594	F3595	I3596	E3605	D3606	R3607	A3608	K3609	K3610	A3611	L3612	F3613	D3614	C3615	A3616	Q3617	K3618	Q3619	H3620	W3621	L3629	M3630	Q3631	F3643	L3644	SER	PHE	ALA	SER	PRO	K3652	T3653	H3654	P3665	N3656	F3657	P3665	N3667	VAL											
H3438	I3441	G3442	LYS	VAL	ASP	VAL	ASN	THR	PRO	MET	PRO	D3453	K3468	A3469	L3470	E3471	T3472	I3473	H3474	Q3475	V3487	L3488	Q3489	W3490	K3491	K3492	W3493	F3494	S3495	E3496	E3497	K3498	A3499	E3500	T3501	A3502	D3503	L3504	P3505	K3506	A3507	F3508	K3509	E3510	L3511	S3512	K3513	L3519	L3523	I3545	I3552										
PRO	VAL	GLU	GLU	GLU	ASN	ALA	GLU	ASN	GLN	GLU	GLU	GLU	GLY	GLU	LYS	GLN	GLN	ALA	LYS	ASP	ASP	SER	ASP	PRO	R3383	S3384	L3385	K3386	K3387	R3388	V3389	D3390	R3406	F3409	K3413	L3426	R3427	S3428	E3429	E3430	L3431	N3432	S3433	D3434	E3435	V3436	D3437														
HIS	GLU	LYS	GLU	GLU	GLU	GLU	GLU	GLU	HIS	GLN	GLN	ALA	GLN	GLN	GLN	ASN	ASN	GLN	ASP	ASP	GLU	GLU	GLY	PRO	R3383	S3384	L3385	K3386	K3387	R3388	V3389	D3390	R3406	F3409	K3413	L3426	R3427	S3428	E3429	E3430	L3431	N3432	S3433	D3434	E3435	V3436	D3437														
E3188	L3189	I3190	E3191	N3192	L3193	E3194	Y3195	L3196	L3197	K3197	K3198	L3199	S3200	V3201	A3204	E3205	K3206	V3207	ALA	A3208	A3209	N3210	K3211	T3212	T3213	E3214	A3215	K3216	L3217	N3218	E3219	T3220	S3221	D3091	E3222	N3223	Y3224	R3225	E3268	N3269	LYS	ILE	T3270	GLY	THR	THR	MET	VAL	PRO	T3270	GLY	ASP	GLU	GLU	THR	ILE	PRO	MET	S2966	D2968	R3023
K3027	A3028	N3029	N3030	L3031	S3038	K3039	N3040	I3041	N3042	R3043	D3044	L3045	E3046	L3047	S3048	I3049	E3050	N3051	G3052	K3078	R3079	G3080	K3081	N3082	G3089	K3090	D3091	S3092	K2943	N2947	I2948	M2949	I2950	N2951	Q2952	F2954	M2955	K2956	M2958	K2959	GLU	HIS	THR	ILE	PRO	MET	S2966	D2968	R3023												
K2833	R2834	K2835	A2836	L2837	K2838	E2839	A2840	T2841	E2842	Q2843	L2844	E2845	E2846	A2847	T2848	V2849	K2850	L2851	K2852	E2853	V2854	E2855	E2856	V2857	V2858	R2859	K2860	L2861	N2862	E2863	E2864	L2865	L2866	K2867	L2868	R2869	A2870	E2871	N2872	D2873	K2874	A2875	I2876	E2877	V2818	N2819	L2820	V2821	K2822	Y2823	Y2824	D2825	V2826	I2827	Q2828	D2829	V2830	E2831	P2832		
A2713	S2714	P2715	P2716	A2717	G2718	V2719	P2720	E2721	V2722	F2723	A2724	A2725	T2726	I2727	Y2728	L2729	L2730	A2731	G2732	Y2733	F2734	N2735	GLU	ALA	ILE	GLU	ILE	ASP	Lys	ASN	Lys	Lys	PRO	Lys	ASP	S2750	W2751	K2752	S2753	S2754	L2755	K2756	L2757	M2758	K2759	S2760	P2761	GLU	E2763	F2764	M2765	E2766	K2767	L2768	L2769	N2770	F2771	Lys			
ASP	VAL	VAL	D2776	A2777	N2778	Q2779	V2780	P2781	A2782	N2784	V2785	N2786	I2787	V2788	K2789	N2790	Q2791	V2792	L2793	N2794	P2795	S2797	T2798	T2799	P2800	E2801	Q2802	M2803	A2804	S2805	K2806	S2807	A2808	A2809	A2810	C2811	C2812	L2813	C2814	S2815	W2816	V2817	V2818	N2819	L2820	V2821	K2822	Y2823	Y2824	D2825	V2826	I2827	Q2828	D2829	V2830	E2831	P2832				



• Molecule 2: Outer arm dynein beta heavy chain

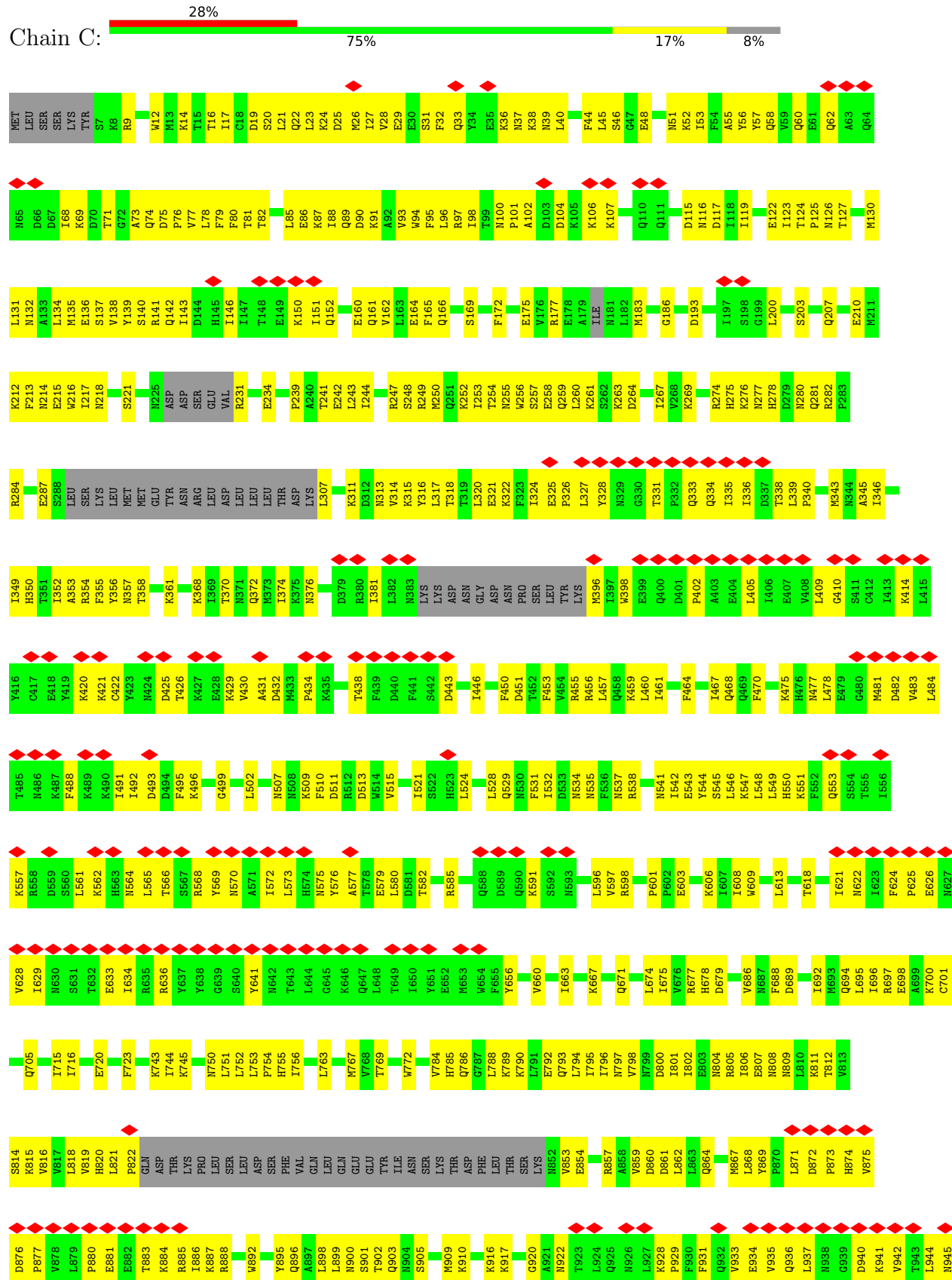


S1568	GLU	L1317	I1257	Q1188	K1125	S1065	PHE	V926	D861	L776	T710
V1569	ALA	I1318	N1258	Q1189	K1126	R1066	ASN	R927	Y862	F777	Q711
V1570	SER	H1319	M1259	I1190	M1127	I1067	ARG	T928	V863		I712
E1571	ALA	F1320	M1260		D1130	K1068	PHE	T929	N864		V713
A1572	LEU	Q1321	N1196		L1134	T1069	LEU	R930	S786		A714
C1573	HIS	Y1322	F1197		H1135	ASP	ASP	R931	L787		L715
T1574	SER	D1323			L1136	GLU	GLU	N932	Q788		D716
I1575	GLU	W1325			K1137	PRO	GLU	I934	K789		H717
I1576	PHE	K1326	R1203		L1138	D1072	ASN	N935	I790		I718
I1576	MET	T1327	V1204		L1139	I1073	LYS	D936	H791		D720
R1577	GLU	K1328			L1140	S1074	ASP	N939	L794		N721
R1578	ASP	Y1329	V1207		M1141	I1076	GLU	I940	A795		H724
D1579	ARG	H1269	K1208		S1142	L1076	GLY	P952	N796		I725
V1580	HIS	I1212			V1143	R1077	LYS		N798		K726
V1581	SER	Q1213			M1144	I1078	GLY	F955	V799		I727
L1581	GLN	L1214			K1145	N1079	GLY	L956	K800		C728
V1582	LEU	Q1215			V1146	L1080	ASP	Q957	I801		L729
G1583	LYS	A1216			L1147	Q1081	ASP	E958	I802		L730
V1584	GLN	E1217			S1148	P1082	GLU	I959	E803		P731
S1585	ILE	T1219			D1149	M1083	GLU	R960	N806		V732
Q1586	THR	G1276			V1150	Q1084	ASN	S961			E733
I1587	THR	R1277			K1151	T1085	THR	F962	S810		E734
K1465	VAL	A1278			D1152	L1086	GLU	F963	P811		P735
T1464	PHE	I1279			V1153	L1087	LYS	E964	D812		L736
K1466	ASP	E1280			E1154	D1088	GLY	F965	D813		V737
T1341	HIS	Y1281			P1155	A1089	GLN	Q967	Y814		K738
N1342	ASN	R1282			L1156	R1090	GLY	K968	D815		K739
K1343	SER	N1283			R1157	V1091	THR	C968	V829		K740
T1344	LEU	L1284			E1158	Q1092	GLY	L969	N832		I741
L1345	SER	E1285			G1159	R1093	GLY	N975	N833		Q742
G1346	PHE	K1286			I1160	T1094	GLY	C983	G833		D743
T1347	PHE	F1288			T1161	I1095	GLY	N984	N834		D745
K1348	GLY	E1289			T1162	R1096	GLY	Q985	I836		E746
I1349	ASP	Q1290			R1163	V1097	GLY	F986	Q837		E747
K1350	ASP	E1292			K1164	I1098	GLY	P987	V840		V748
N1351	ILE	E1293			K1165	T1099	GLY	A988	E842		K749
L1352	LEU	S1293			E1166	D1100	GLY	R989	V843		F750
P1353	ALA	M1294			E1167	F1101	GLY	F990	L844		G751
K1354	LEU	K1295			M1168	L1102	GLY	D991	K848		I752
E1355	ASN	K1296			V1169	V1103	GLY	T992	A849		E753
E1356	LEU	K1297			K1170	Q1104	GLY	Y993	D850		E754
I1357	TYR	Q1297			L1171	Q1105	GLY	S994	K851		I755
R1357	LYS	L1298			K1172	F1106	GLY	Y995	K852		R756
N1358	TYR	D1300			K1173	R1107	GLY	L996	Q853		W757
K1359	GLU	M1241			H1174	T1108	GLY	W997	N854		K758
K1360	GLU	Q1242			V1176	T1109	GLY	P998	W856		S759
G1361	ASN	K1243			P1177	Q1110	GLY	E999	K857		T760
Y1362	THR	L1244			T1178	K1111	GLY	D1000	N858		K761
I1363	VAL	P1245			T1179	E1112	GLY	E1001	Y859		I762
N1364	ASN	F1246			E1180	L1113	GLY	GLN	N860		D763
V1365	GLU	L1305			K1181	L1114	GLY	ILE			Q764
I1366	ILE	K1306			G1182	D1115	GLY	SER			F765
K1367	VAL	Y1248			T1183	F1116	GLY				I766
K1368	ASP	T1249			D1184	I1117	GLY				S767
K1369	VAL	E1250			P1186	E1118	GLY				K768
K1370	ALA	S1251			D1185	K1119	GLY				S769
ASN	GLN	M1252			P1187	L1120	GLY				K770
GLY	THR	G1253				D1122	GLY				
THR	VAL	Y1254				G1123	GLY				
VAL	LEU	E1255				I1124	GLY				
LEU		N1256					GLY				
T1645											
F1646											
E1647											
P1648											
P1649											
A1650											
N1651											
P1652											
A1653											
E1654											
K1657											
V1658											
F1659											
E1659											
I1660											
G1661											
K1669											
V1670											
P1671											
F1672											
S1673											
L1674											
K1675											
F1676											
I1677											
F1691											
R1692											
N1693											
R1694											
E1695											
T1696											
L1697											
Q1698											



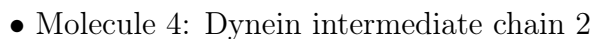


● Molecule 3: Dynein heavy chain, outer arm protein

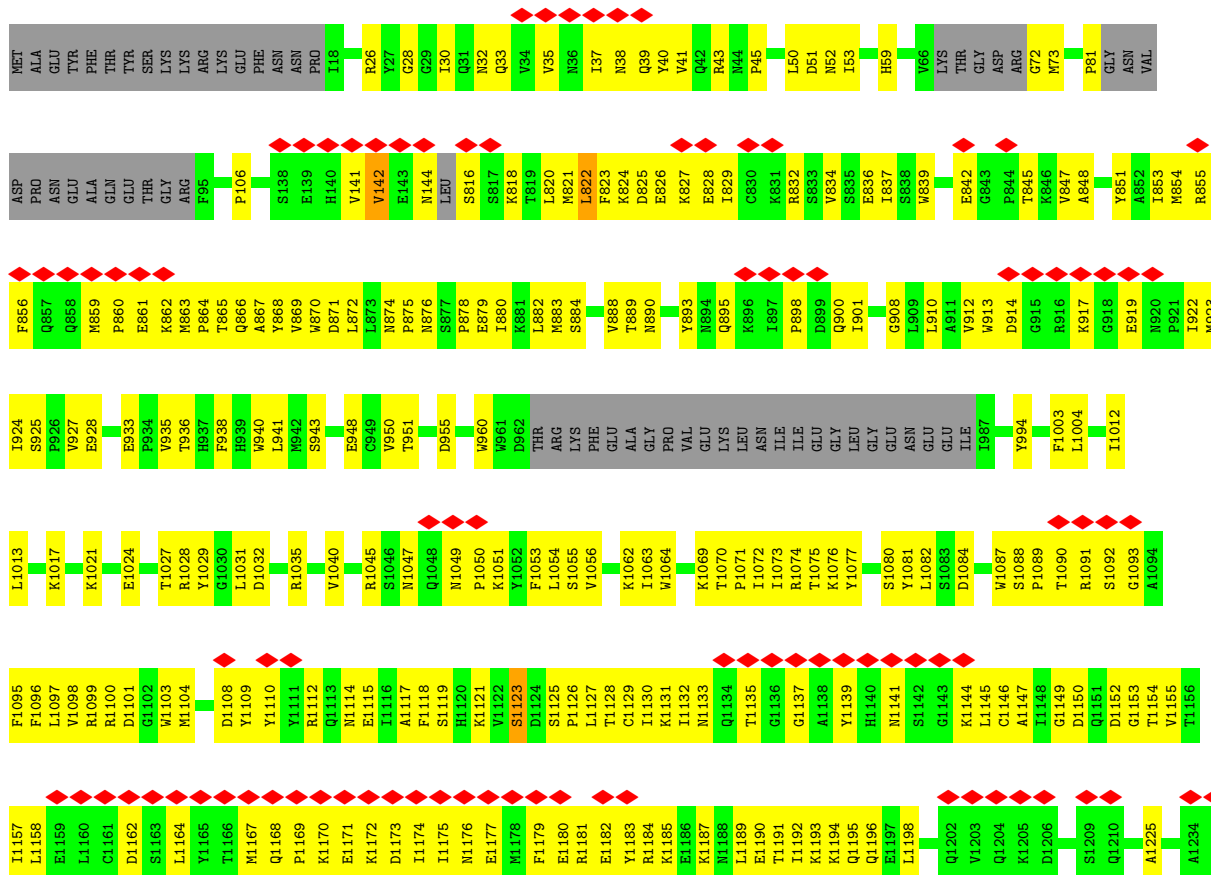




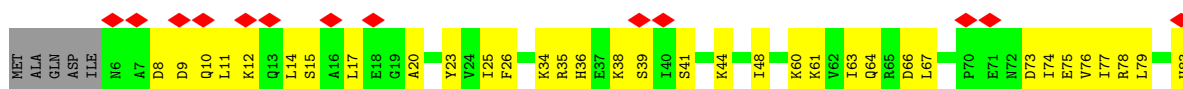
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S3927	Q3930	E3931	E3966	V3979	K3800	N3801	L3802	L3803	S3804	F3805	L3806	T3807	F3808	H3809	S3852	GLY	ASP	ALA	LEU	ASP	ILE	LYS	SER	GLU	ARG	Q3863	E3870	V3874	K3882	HIS	THR	PHE	SER	GLY	GLN	THR	LEU	P3891	E3895	L3899	I3900	S3903	E3904	N3905	Q3906	F3919	P3920	I3921	P3922	D3923	F3926	K4033	G4034	F4035	V4036	E4037	G4038	G4039
N3797	R3798	V3799	K3800	N3801	L3802	L3803	L3804	F3805	L3806	T3807	F3808	H3809	S3852	GLY	ASP	ALA	LEU	ASP	ILE	LYS	SER	GLU	ARG	Q3863	E3870	V3874	K3882	HIS	THR	PHE	SER	GLY	GLN	THR	LEU	P3891	E3895	L3899	I3900	S3903	E3904	N3905	Q3906	F3919	P3920	I3921	P3922	D3923	F3926	K4033	G4034	F4035	V4036	E4037	G4038	G4039		
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ILE	VAL	LYS	THR	GLN	PHE	ASN	VAL	VAL	ALA	GLY	THR	GLU	MET	GLU	L3617	S3618	K3619	E3620	F3621	Q3657	L3658	L3659	G3660	K3661	V3662	L3663	S3664	K3665	E3666	Q3667	K3668	A3669	E3670	E3671	D3672	S3673	L3674	N3675	Q3676	L3677	A3678	D3680	V3681	N3682	Q3683	N3684	Q3685	K3686	D3687	L3688	Q3689	S3690	L3691	D3692	K3693			
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ILE	VAL	LYS	THR	GLN	PHE	ASN	VAL	VAL	ALA	GLY	THR	GLU	MET	GLU	L3617	S3618	K3619	E3620	F3621	Q3657	L3658	L3659	G3660	K3661	V3662	L3663	S3664	K3665	E3666	Q3667	K3668	A3669	E3670	E3671	D3672	S3673	L3674	N3675	Q3676	L3677	A3678	D3680	V3681	N3682	Q3683	N3684	Q3685	K3686	D3687	L3688	Q3689	S3690	L3691	D3692	K3693			
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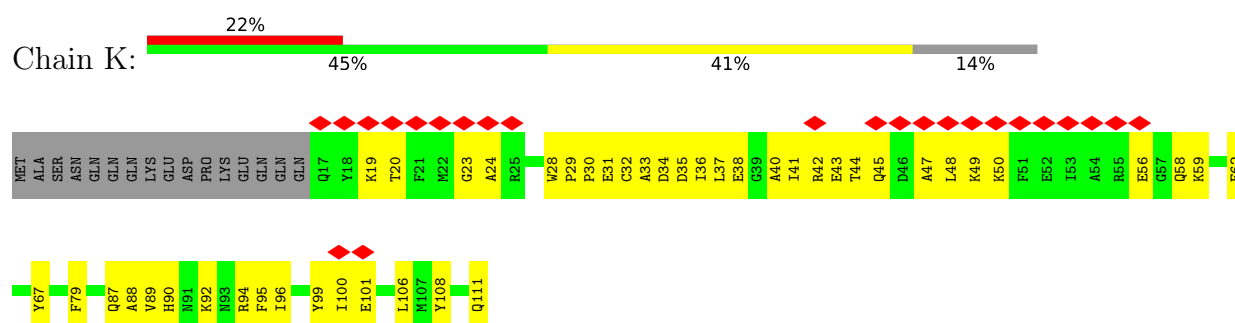


- Molecule 5: Flagellar outer dynein arm intermediate protein, putative

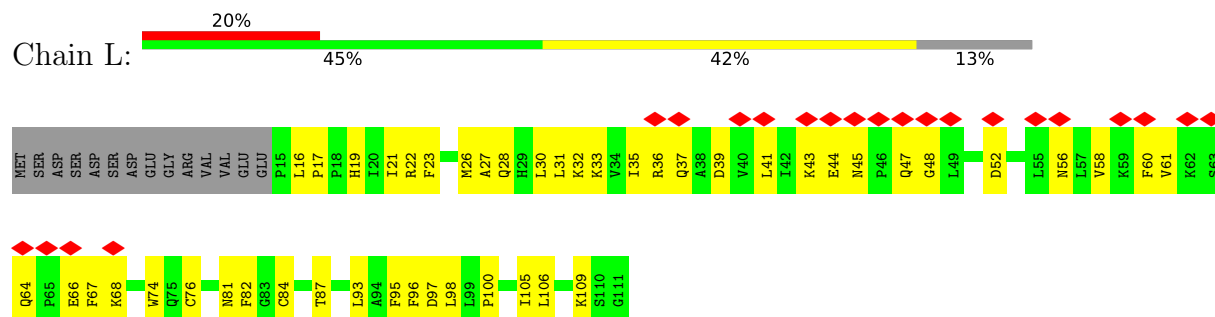


- Molecule 6: Dynein light chain roadblock-type 2 protein

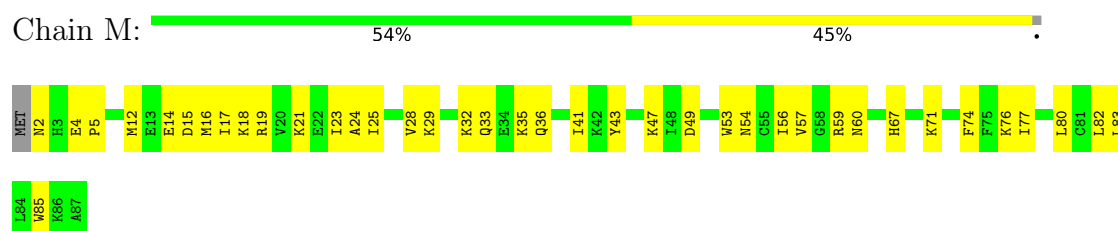




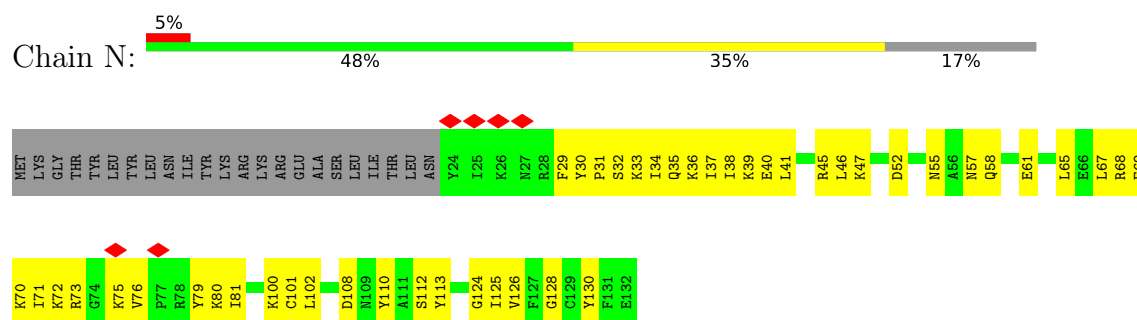
• Molecule 12: Dynein light chain



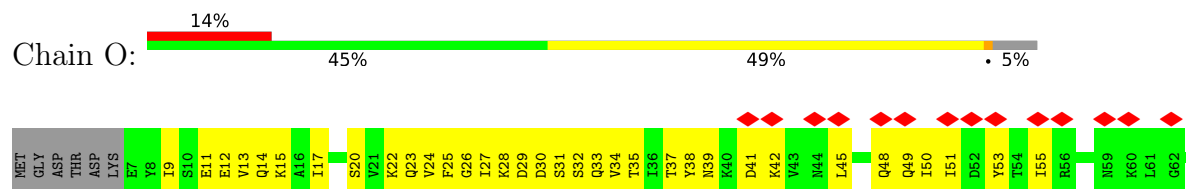
• Molecule 13: Dynein light chain

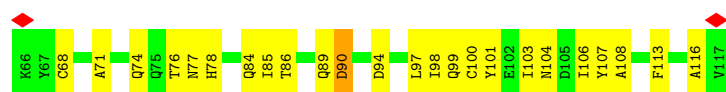


• Molecule 14: Dynein light chain 2A

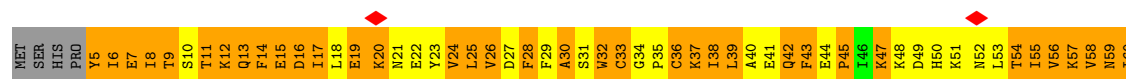


• Molecule 15: Dynein light chain tctex-type 1 protein

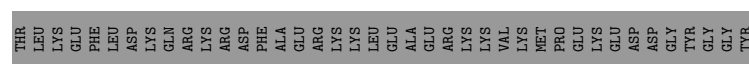
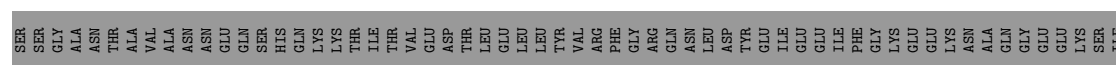
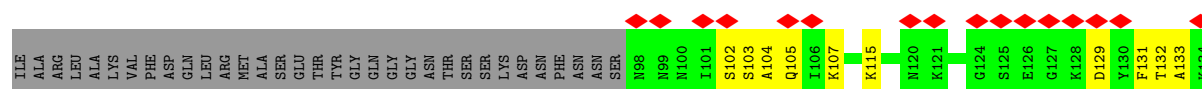
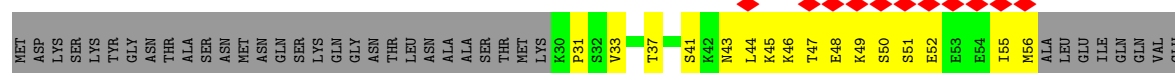




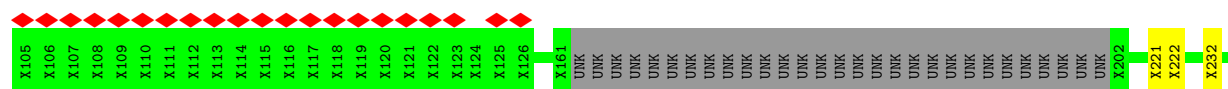
• Molecule 16: Thioredoxin



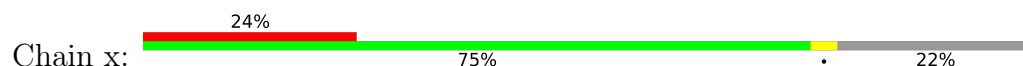
• Molecule 17: Calmodulin

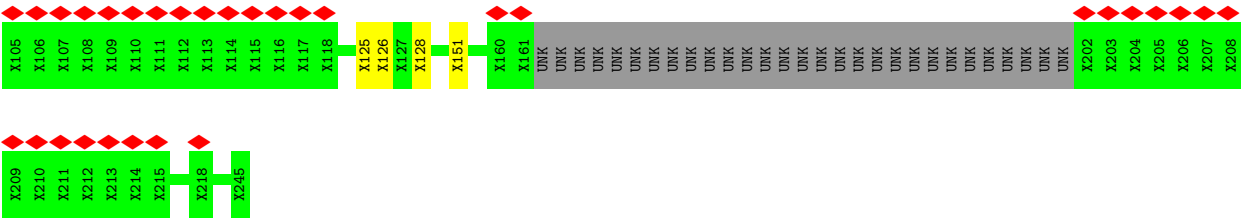


• Molecule 18: Docking complex 1/2 protein



• Molecule 18: Docking complex 1/2 protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	590	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)	4000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.383	Depositor
Minimum map value	-0.252	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	629.0, 629.0, 629.0	wwPDB
Map dimensions	74, 74, 74	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	8.5, 8.5, 8.5	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, 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	0.33	0/18167	0.78	9/25169 (0.0%)
2	B	1.01	266/25709 (1.0%)	0.87	88/35300 (0.2%)
3	C	1.07	303/25227 (1.2%)	0.85	198/34687 (0.6%)
4	d	0.24	0/3710	0.51	0/5026
5	e	0.24	0/4021	0.57	5/5463 (0.1%)
6	F	0.23	0/793	0.54	0/1070
7	G	0.20	0/751	0.45	0/1014
8	H	0.16	0/718	0.38	0/965
9	I	0.19	0/705	0.46	0/954
10	J	0.16	0/723	0.41	0/966
11	K	0.25	0/828	0.59	0/1114
12	L	0.19	0/790	0.44	0/1063
13	M	0.20	0/743	0.42	0/996
14	N	0.26	0/915	0.58	0/1229
15	O	0.19	0/891	0.47	0/1209
16	P	3.92	186/866 (21.5%)	2.58	62/1171 (5.3%)
17	T	0.19	0/1070	0.44	0/1436
All	All	0.90	755/86627 (0.9%)	0.83	362/118832 (0.3%)

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	1
2	B	0	2
3	C	0	5
All	All	0	8

The worst 5 of 755 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1075	TRP	C-O	24.46	1.54	1.24
3	C	3345	LYS	C-O	-18.77	1.00	1.24
2	B	1244	LEU	N-CA	-16.00	1.35	1.46
3	C	3307	GLU	N-CA	-15.79	1.33	1.46
3	C	3331	GLY	CA-C	15.63	1.69	1.52

The worst 5 of 362 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3355	GLN	CA-C-N	-18.06	95.72	120.46
3	C	3355	GLN	C-N-CA	-18.06	95.72	120.46
3	C	3345	LYS	N-CA-C	-14.17	80.62	110.80
5	e	106	PRO	N-CA-CB	13.43	110.44	102.92
3	C	3212	VAL	N-CA-C	-12.76	98.17	110.42

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	ARG	Peptide
2	B	1075	TRP	Mainchain
2	B	966	LYS	Peptide
3	C	3201	ALA	Mainchain
3	C	974	GLN	Peptide

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	18127	0	9379	321	0
2	B	25545	0	17415	984	0
3	C	25046	0	16445	750	0
4	d	3626	0	3455	256	0
5	e	3948	0	3485	302	0
6	F	781	0	791	46	0
7	G	744	0	771	47	0
8	H	702	0	686	55	0
9	I	694	0	684	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	702	0	671	27	0
11	K	803	0	766	79	0
12	L	773	0	806	54	0
13	M	726	0	726	36	0
14	N	897	0	911	71	0
15	O	878	0	868	57	0
16	P	847	0	836	77	0
17	T	1057	0	1033	37	0
18	V	490	0	102	5	0
18	x	505	0	105	7	0
19	C	81	0	36	0	0
20	C	31	0	12	0	0
All	All	87003	0	59983	2970	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 20.

The worst 5 of 2970 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:1212:ILE:CG2	2:B:1213:PRO:HD3	1.22	1.64
2:B:814:TYR:CA	2:B:1075:TRP:CZ2	1.79	1.58
2:B:814:TYR:HB2	2:B:1075:TRP:CE2	1.39	1.56
2:B:1148:SER:CB	2:B:1214:LEU:HB2	1.35	1.56
2:B:1148:SER:H	2:B:1214:LEU:CD1	1.01	1.55

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	3371/4168 (81%)	2907 (86%)	454 (14%)	10 (0%)	36	72
2	B	4229/4595 (92%)	3790 (90%)	429 (10%)	10 (0%)	43	78
3	C	4232/4620 (92%)	3885 (92%)	337 (8%)	10 (0%)	43	78
4	d	445/667 (67%)	400 (90%)	45 (10%)	0	100	100
5	e	529/670 (79%)	459 (87%)	69 (13%)	1 (0%)	43	78
6	F	96/133 (72%)	82 (85%)	14 (15%)	0	100	100
7	G	93/159 (58%)	81 (87%)	12 (13%)	0	100	100
8	H	83/92 (90%)	81 (98%)	2 (2%)	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%)	81 (87%)	12 (13%)	0	100	100
12	L	95/111 (86%)	90 (95%)	5 (5%)	0	100	100
13	M	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
14	N	107/132 (81%)	99 (92%)	8 (8%)	0	100	100
15	O	109/117 (93%)	103 (94%)	6 (6%)	0	100	100
16	P	101/110 (92%)	94 (93%)	7 (7%)	0	100	100
17	T	127/309 (41%)	109 (86%)	16 (13%)	2 (2%)	7	38
All	All	13963/16284 (86%)	12499 (90%)	1431 (10%)	33 (0%)	44	78

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	THR
1	A	1823	VAL
2	B	1651	ASN
2	B	1652	PRO
2	B	2557	PRO

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	291/3691 (8%)	291 (100%)	0	100	100
2	B	1215/4145 (29%)	1214 (100%)	1 (0%)	88	89
3	C	1094/4196 (26%)	1094 (100%)	0	100	100
4	d	386/609 (63%)	386 (100%)	0	100	100
5	e	364/597 (61%)	363 (100%)	1 (0%)	86	86
6	F	87/109 (80%)	87 (100%)	0	100	100
7	G	86/149 (58%)	86 (100%)	0	100	100
8	H	76/83 (92%)	76 (100%)	0	100	100
9	I	76/95 (80%)	76 (100%)	0	100	100
10	J	74/82 (90%)	74 (100%)	0	100	100
11	K	81/97 (84%)	81 (100%)	0	100	100
12	L	86/99 (87%)	86 (100%)	0	100	100
13	M	77/78 (99%)	77 (100%)	0	100	100
14	N	96/119 (81%)	96 (100%)	0	100	100
15	O	98/104 (94%)	97 (99%)	1 (1%)	68	78
16	P	97/104 (93%)	97 (100%)	0	100	100
17	T	118/271 (44%)	118 (100%)	0	100	100
All	All	4402/14628 (30%)	4399 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1315	ILE
5	e	1123	SER
15	O	90	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	575	ASN
13	M	26	ASN
3	C	1098	GLN
12	L	81	ASN
15	O	48	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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$
19	ADP	C	4703	-	28,29,29	1.35	5 (17%)	43,45,45	1.84	10 (23%)
19	ADP	C	4702	-	28,29,29	1.32	4 (14%)	43,45,45	1.99	10 (23%)
19	ADP	C	4701	-	28,29,29	1.33	4 (14%)	43,45,45	1.89	10 (23%)
20	ATP	C	4704	-	32,33,33	1.24	5 (15%)	48,52,52	1.80	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ADP	C	4703	-	-	1/16/32/32	0/3/3/3
19	ADP	C	4702	-	-	3/16/32/32	0/3/3/3
19	ADP	C	4701	-	-	3/16/32/32	0/3/3/3
20	ATP	C	4704	-	-	4/22/38/38	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	4701	ADP	C5-C4	4.30	1.46	1.39
19	C	4702	ADP	C5-C4	4.21	1.46	1.39
19	C	4703	ADP	C5-C4	4.21	1.46	1.39
20	C	4704	ATP	C5-C4	4.09	1.46	1.39
20	C	4704	ATP	C5-N7	-2.60	1.34	1.39

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	4702	ADP	C5-C4-N3	-6.28	118.06	126.72
19	C	4701	ADP	C5-C4-N3	-6.04	118.41	126.72
20	C	4704	ATP	C5-C4-N3	-5.88	118.61	126.72
19	C	4703	ADP	C5-C4-N3	-5.51	119.12	126.72
19	C	4702	ADP	N3-C4-N9	5.29	136.17	127.17

There are no chirality outliers.

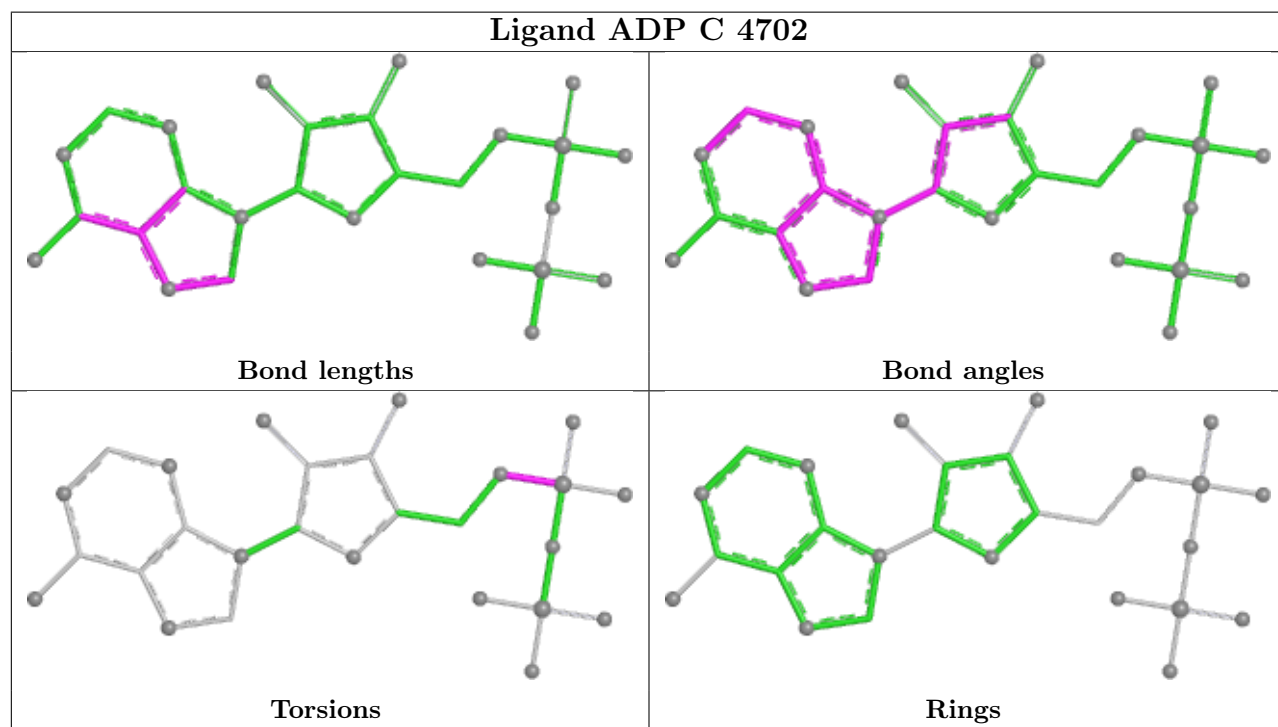
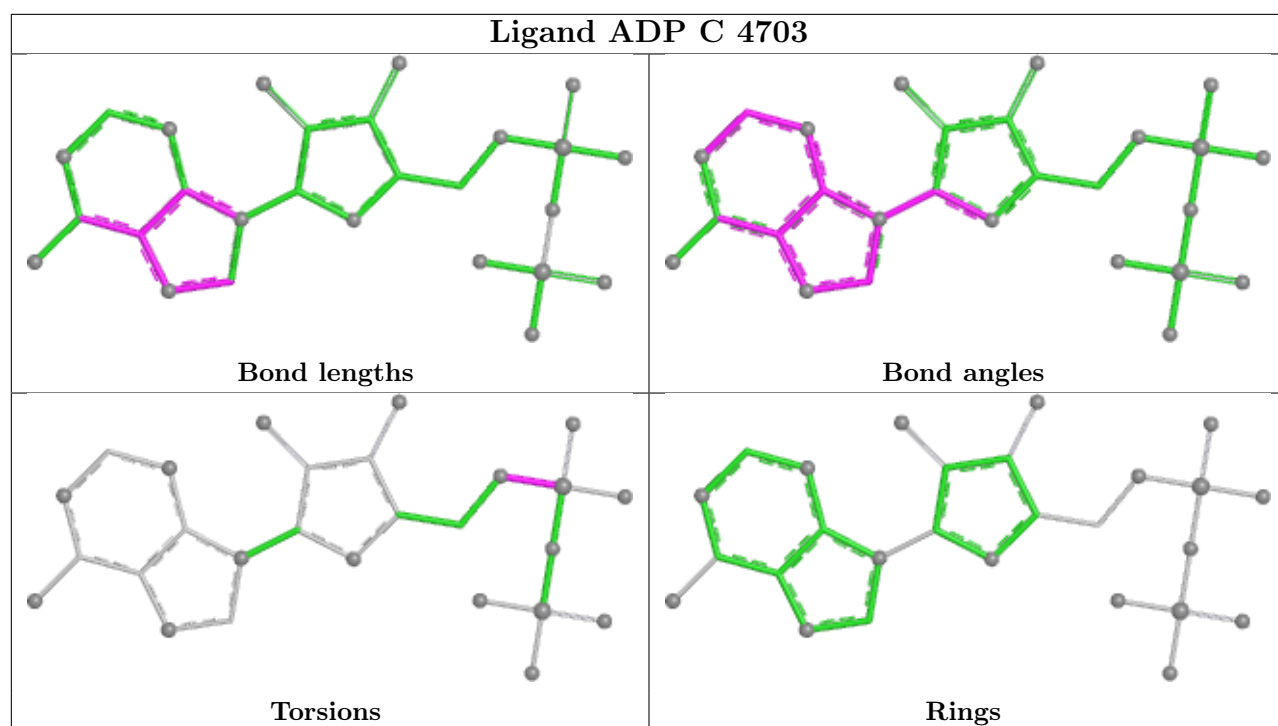
5 of 11 torsion outliers are listed below:

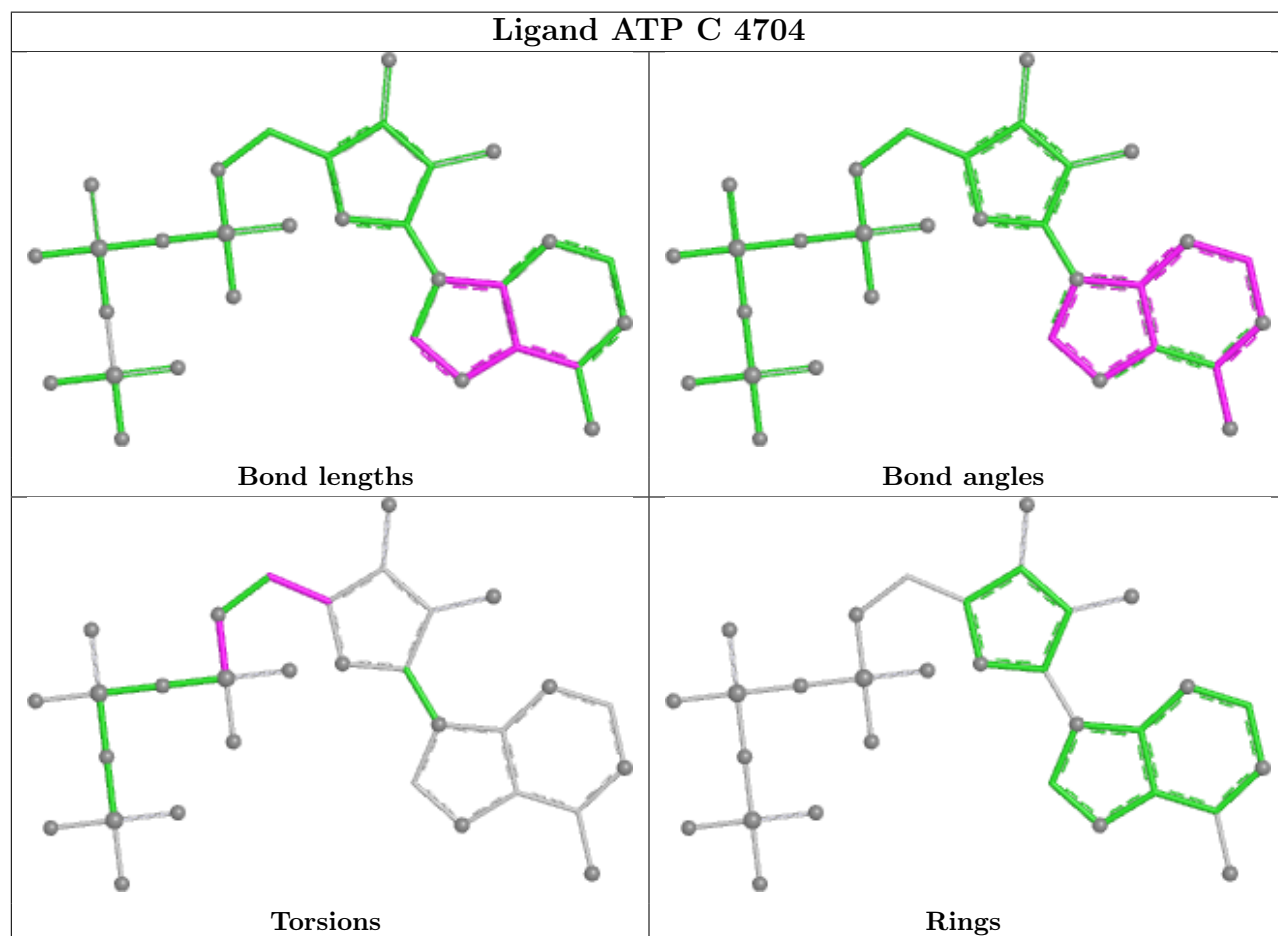
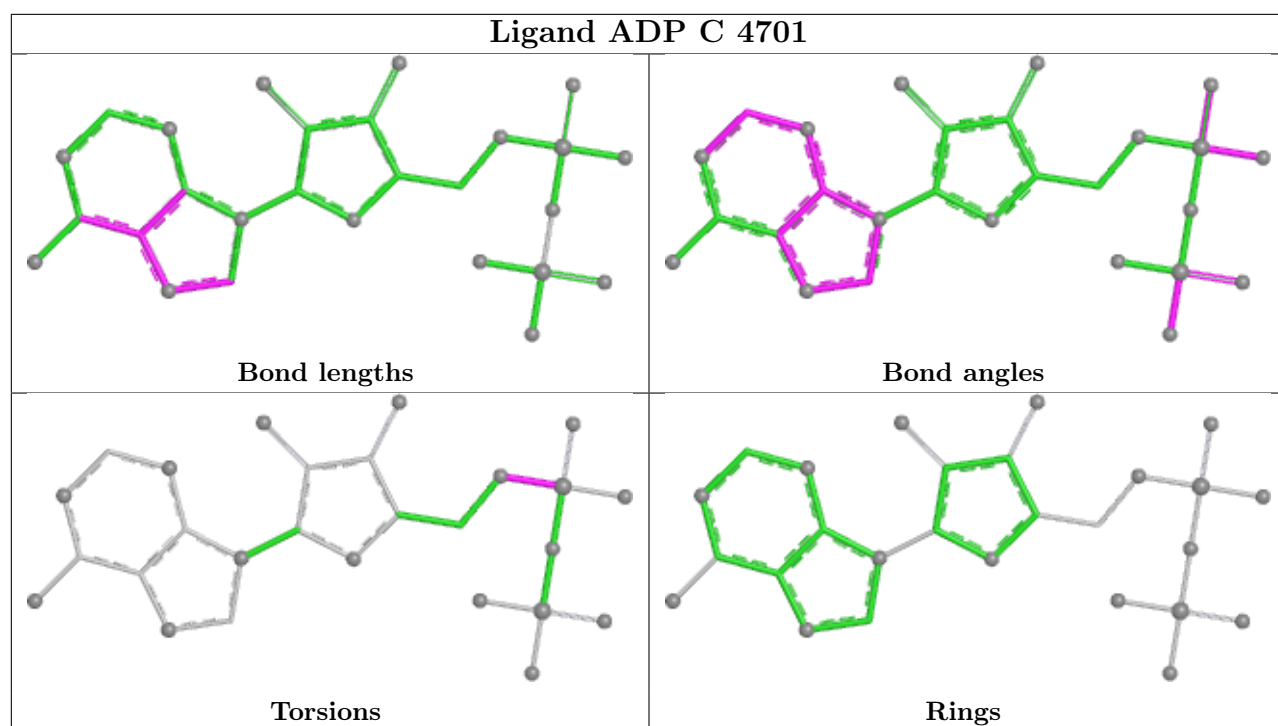
Mol	Chain	Res	Type	Atoms
19	C	4701	ADP	C5'-O5'-PA-O1A
19	C	4701	ADP	C5'-O5'-PA-O3A
19	C	4702	ADP	C5'-O5'-PA-O1A
19	C	4702	ADP	C5'-O5'-PA-O2A
19	C	4702	ADP	C5'-O5'-PA-O3A

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	22
2	B	13
3	C	9
5	e	3

The worst 5 of 47 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	389:ASP	C	390:THR	N	29.62
1	e	1233:LEU	C	1234:ALA	N	29.14
1	e	1201:ARG	C	1202:GLN	N	19.87
1	A	1299:VAL	C	1300:GLN	N	17.01
1	e	1251:GLU	C	1252:LYS	N	15.83

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16304. These allow visual inspection of the internal detail of the map and identification of artifacts.

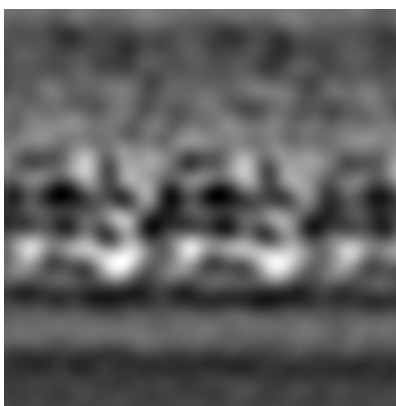
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

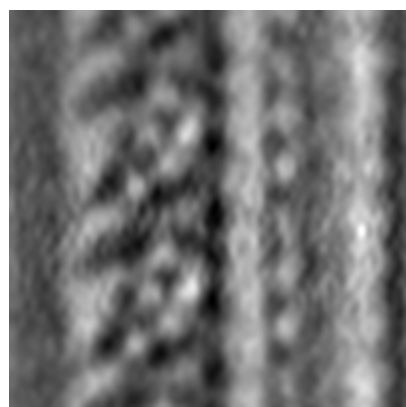


Y

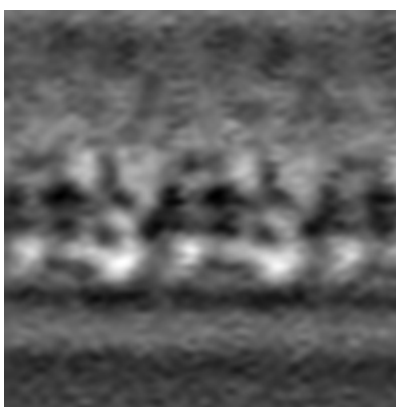


Z

6.1.2 Raw map



X



Y



Z

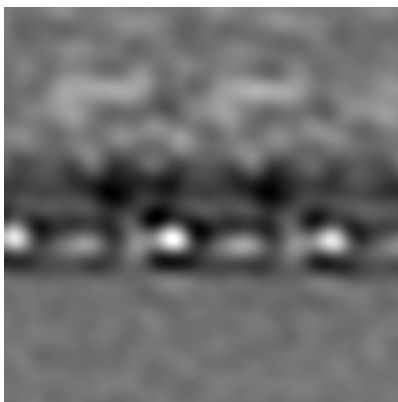
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 37

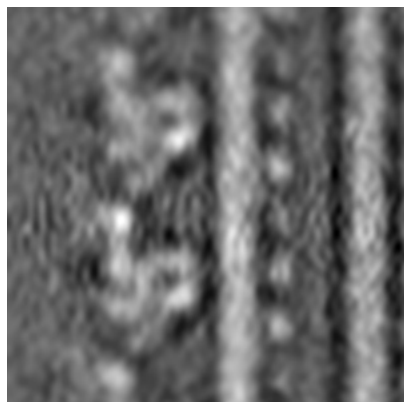


Y Index: 37

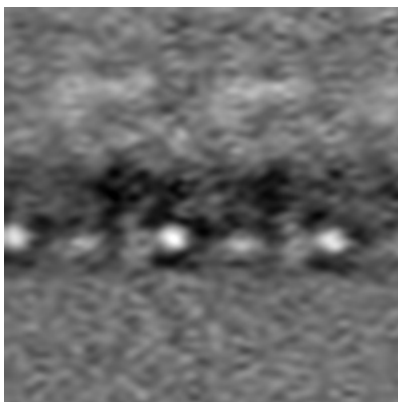


Z Index: 37

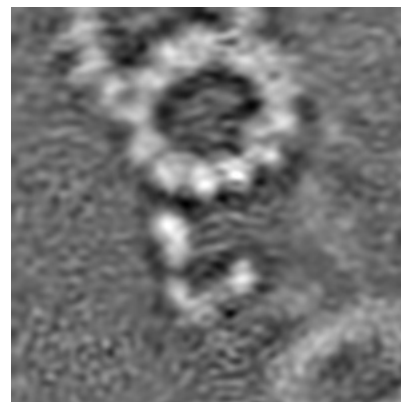
6.2.2 Raw map



X Index: 37



Y Index: 37



Z Index: 37

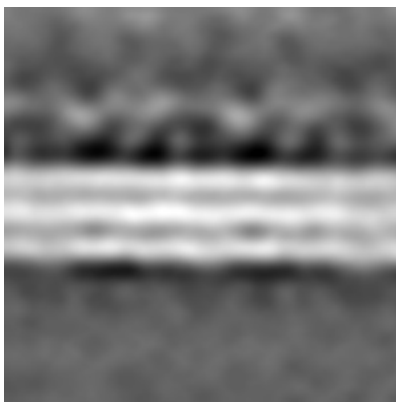
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 29

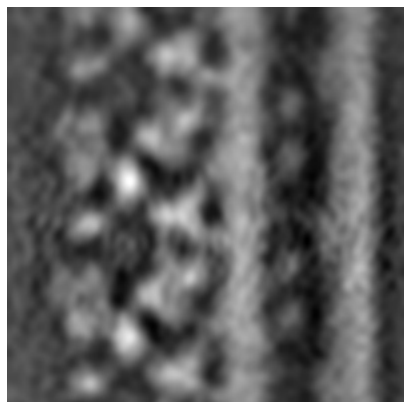


Y Index: 42

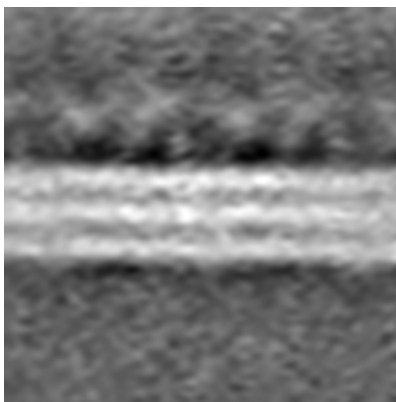


Z Index: 22

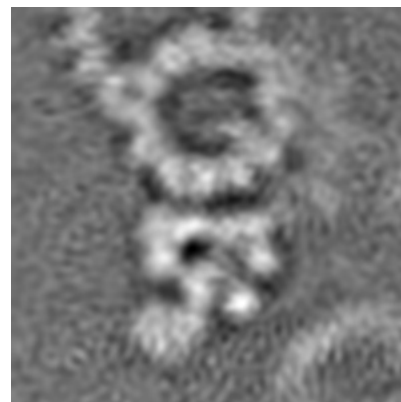
6.3.2 Raw map



X Index: 29



Y Index: 42

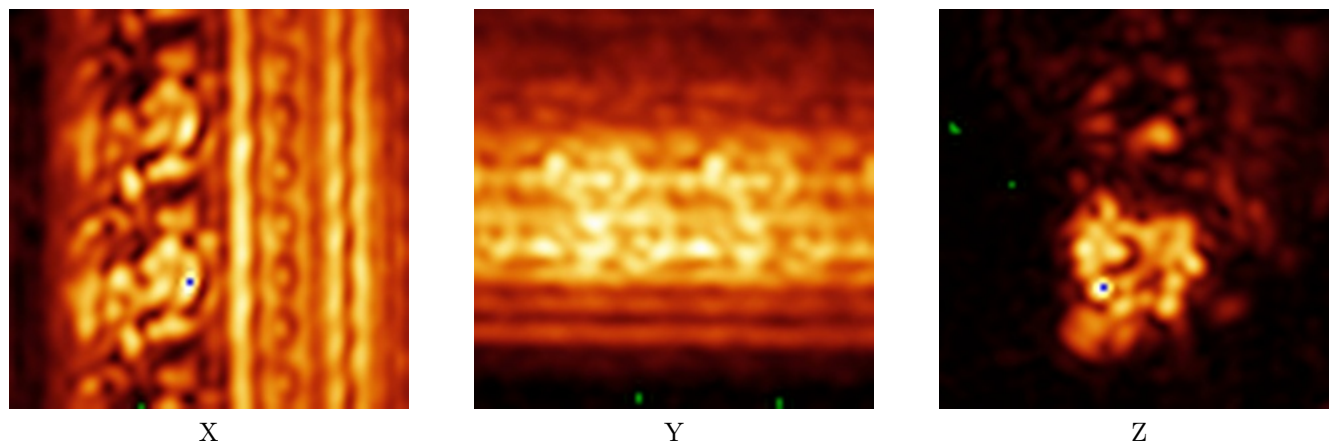


Z Index: 22

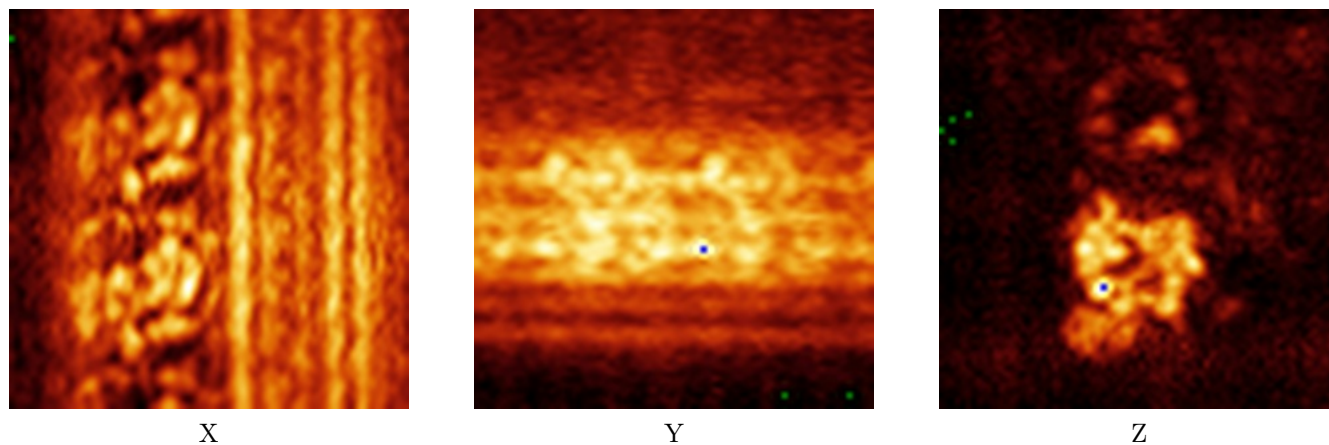
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



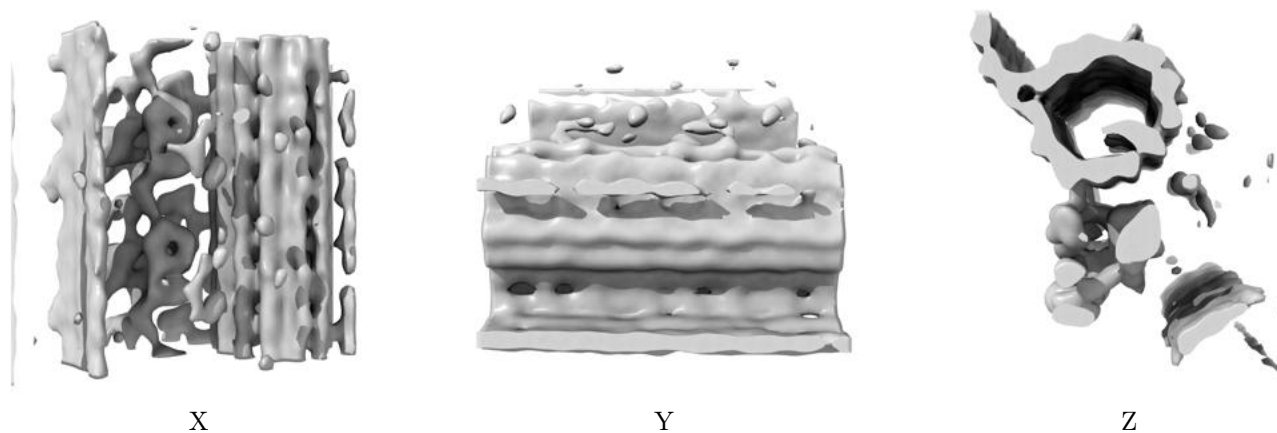
6.4.2 Raw map



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

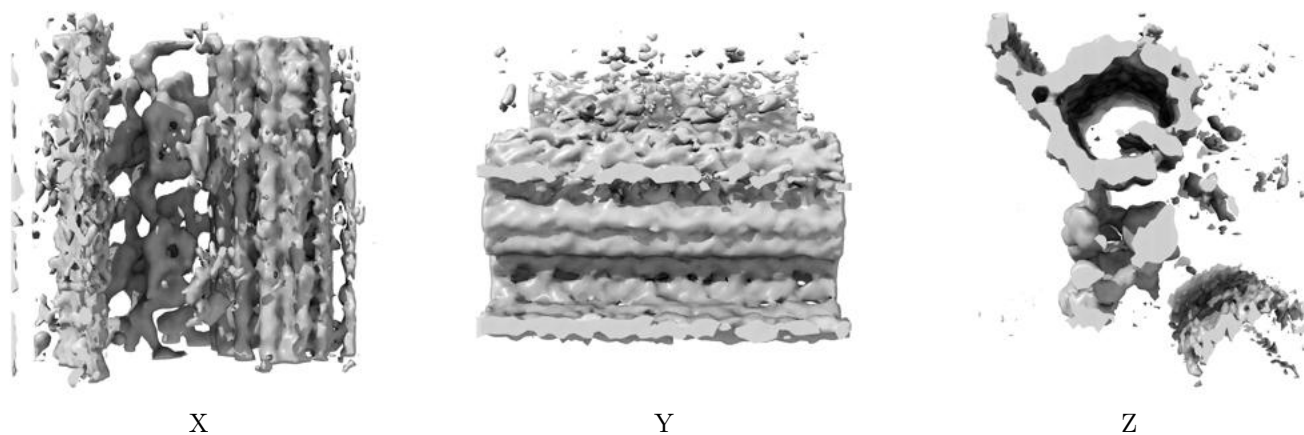
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

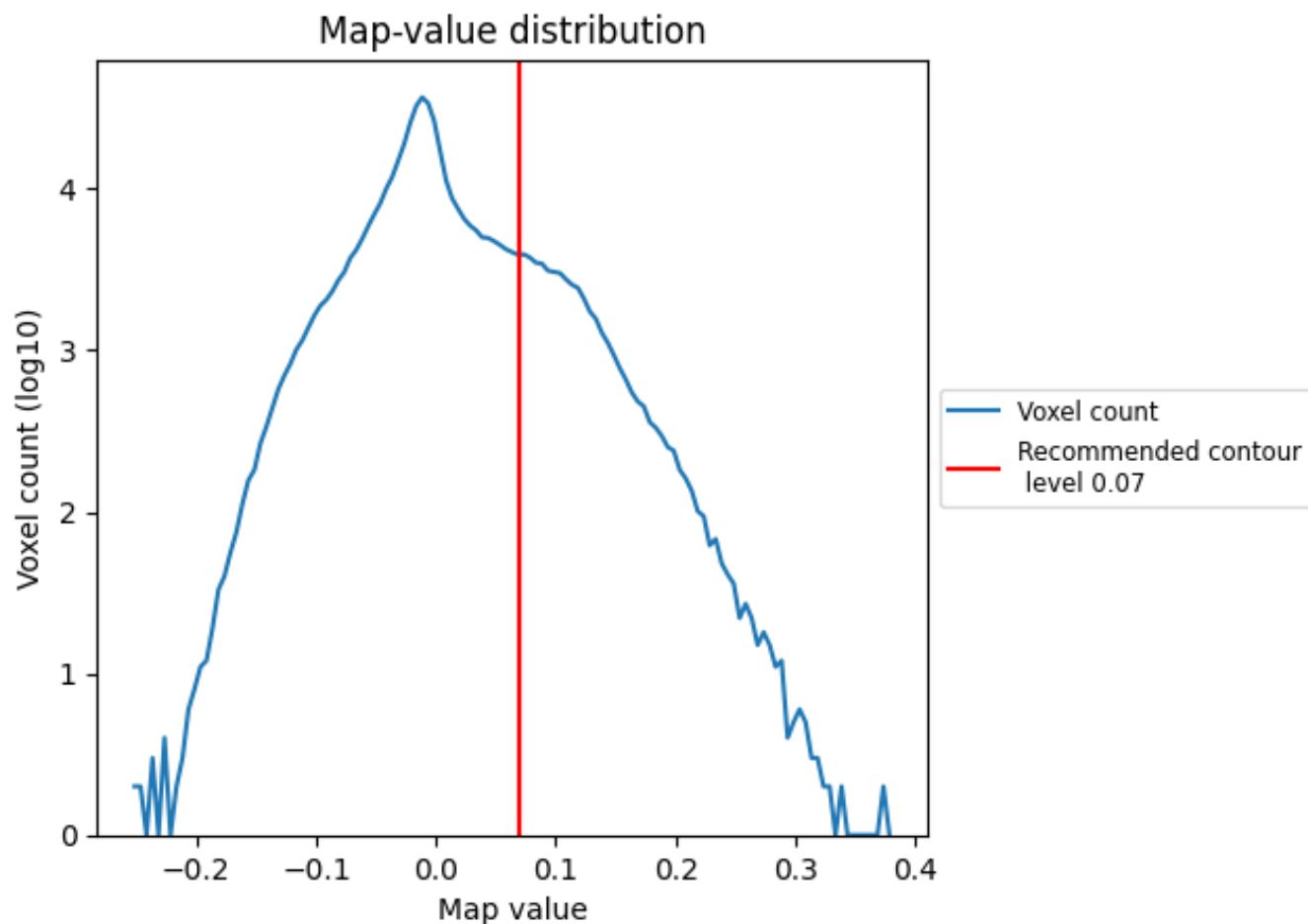
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

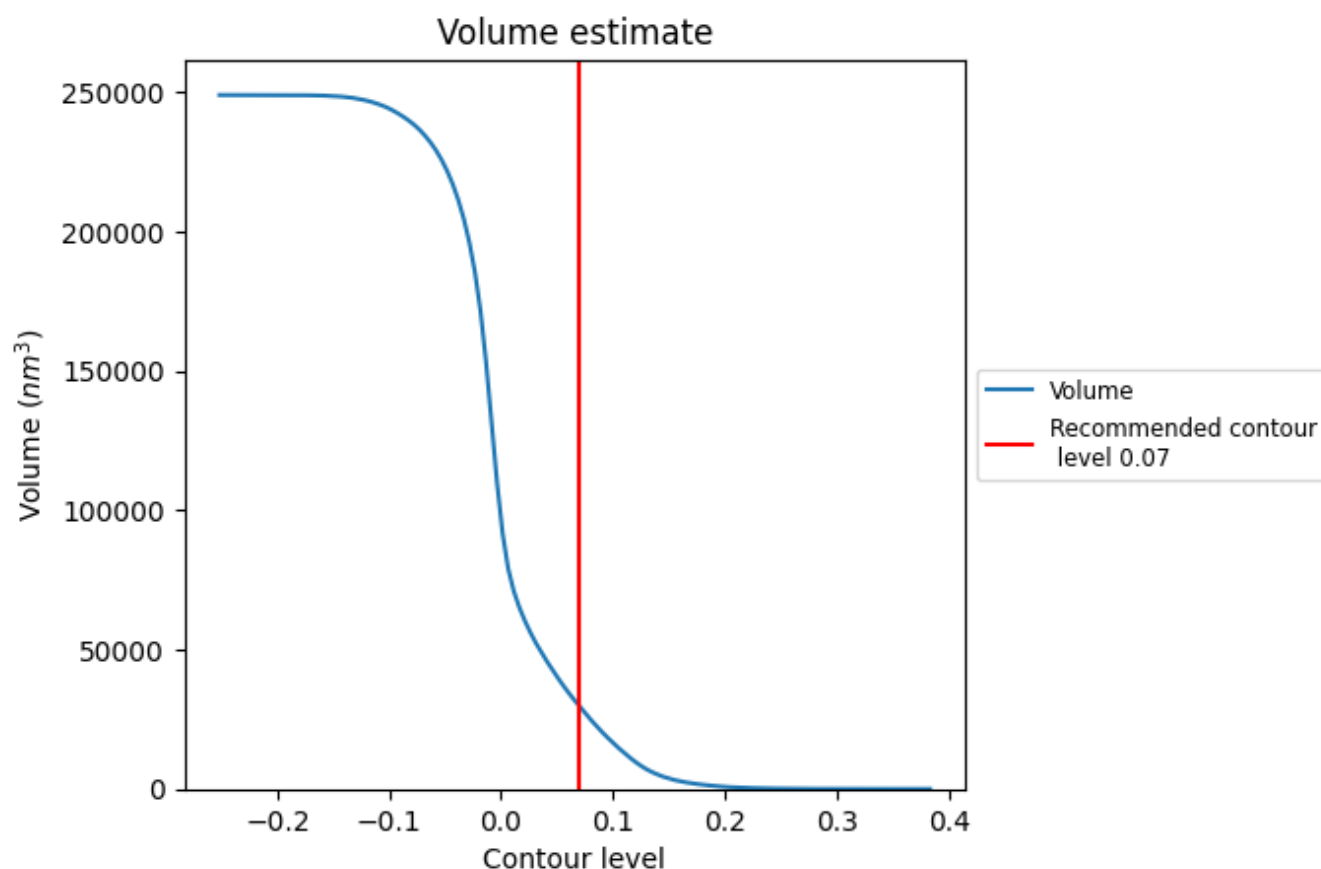
This section contains the results of statistical analysis of the map.

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.

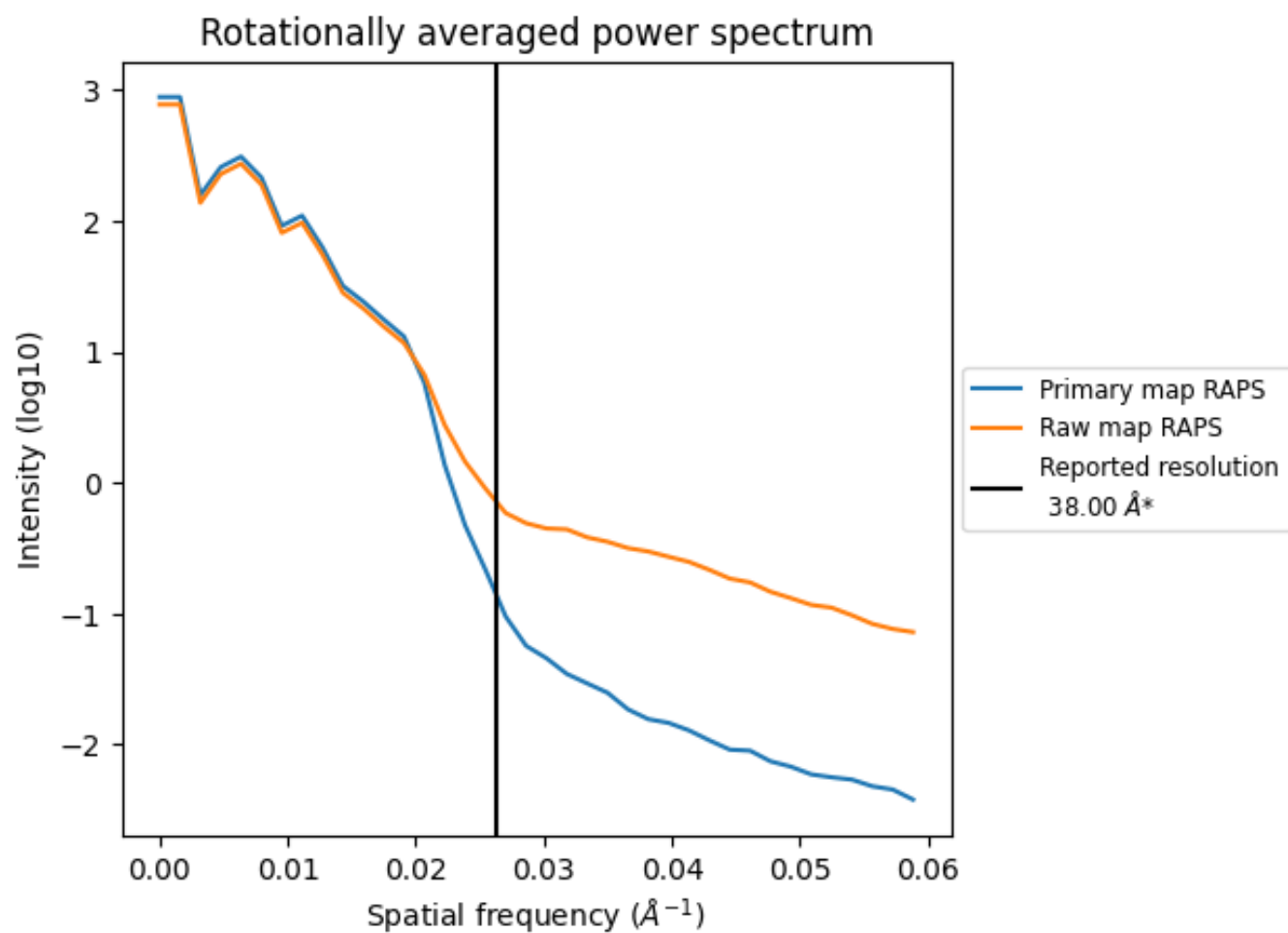
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 29745 nm^3 ; this corresponds to an approximate mass of 26870 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 ⓘ

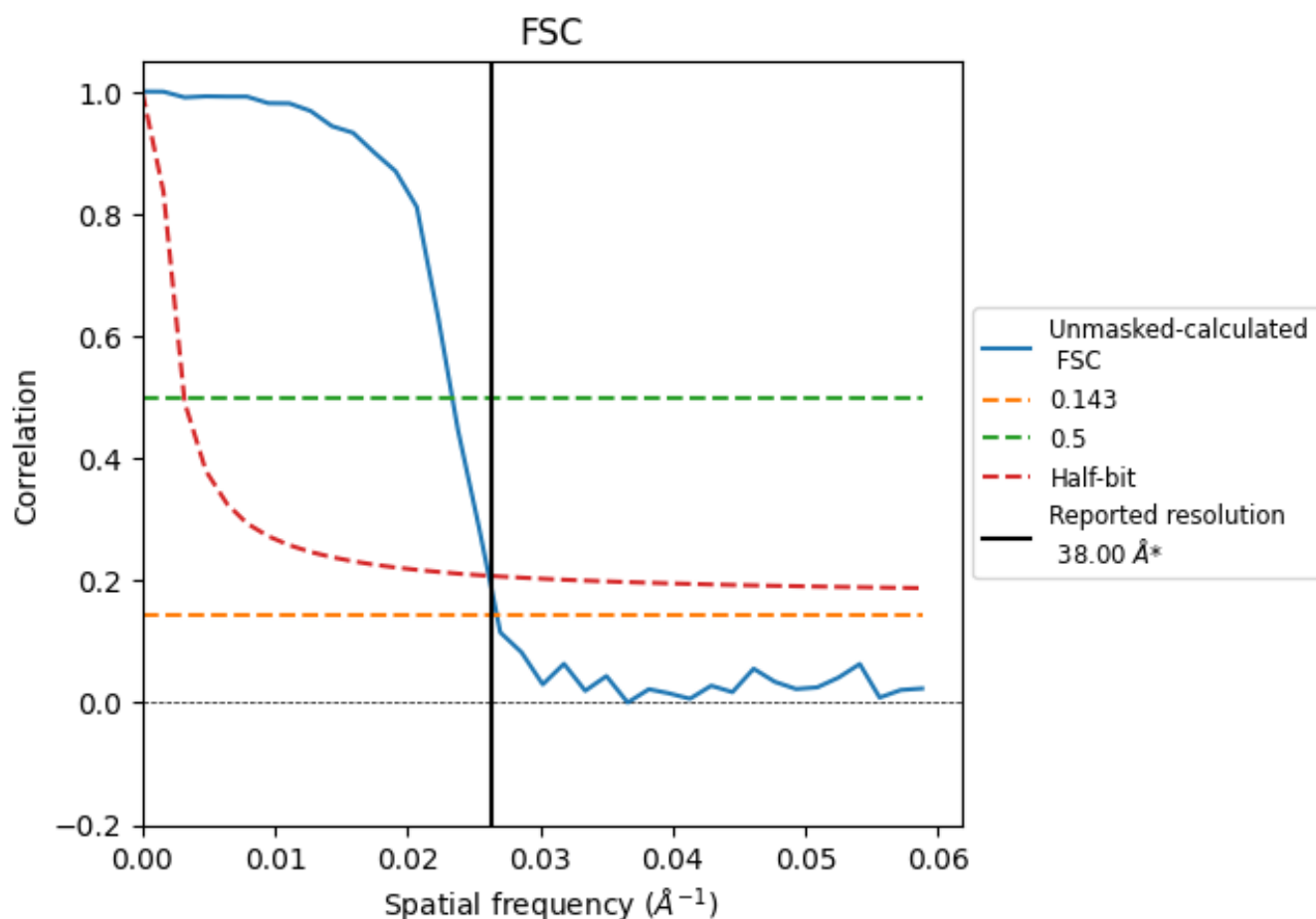


*Reported resolution corresponds to spatial frequency of 0.026 $\text{\AA}^{-1}$

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 0.026 Å⁻¹

8.2 Resolution estimates [i](#)

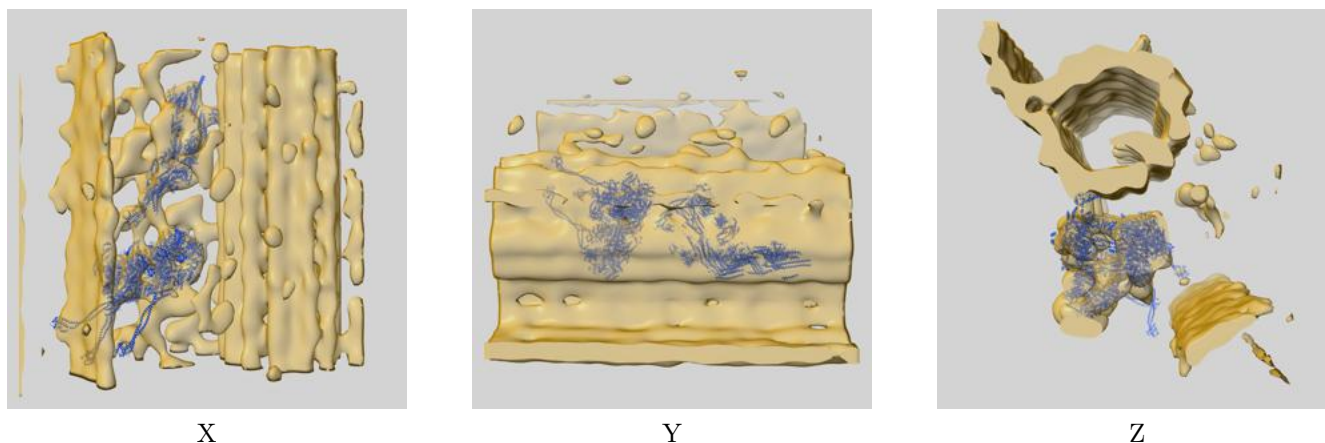
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	38.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	37.31	42.74	38.17

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

9 Map-model fit [i](#)

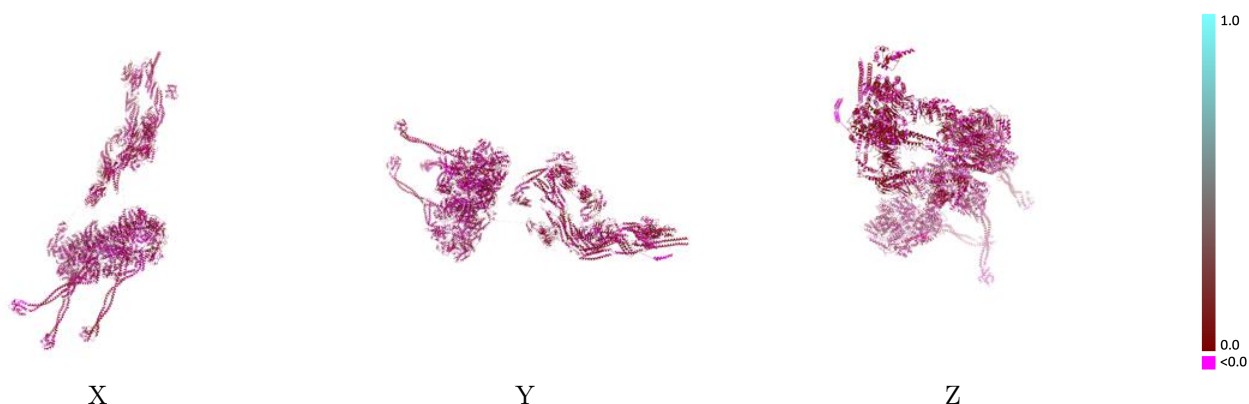
This section contains information regarding the fit between EMDB map EMD-16304 and PDB model 8BWY. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



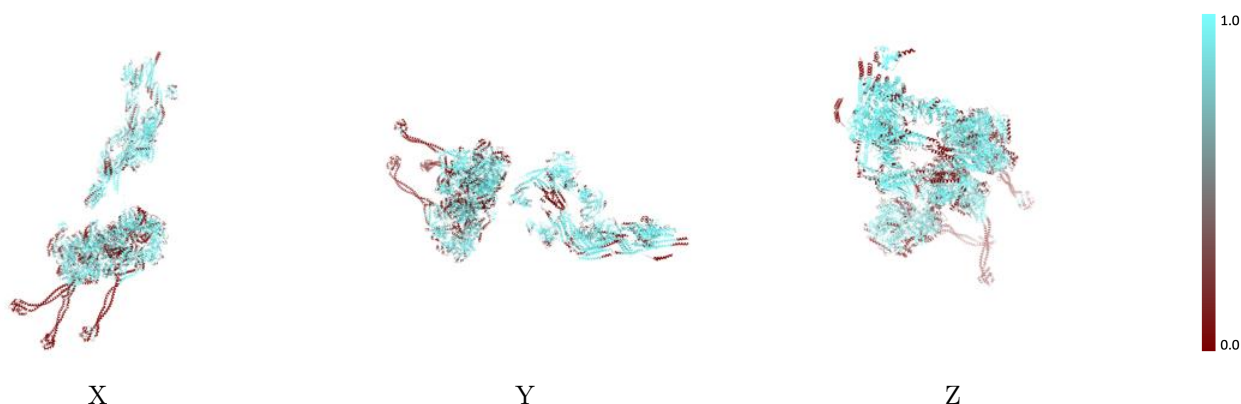
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



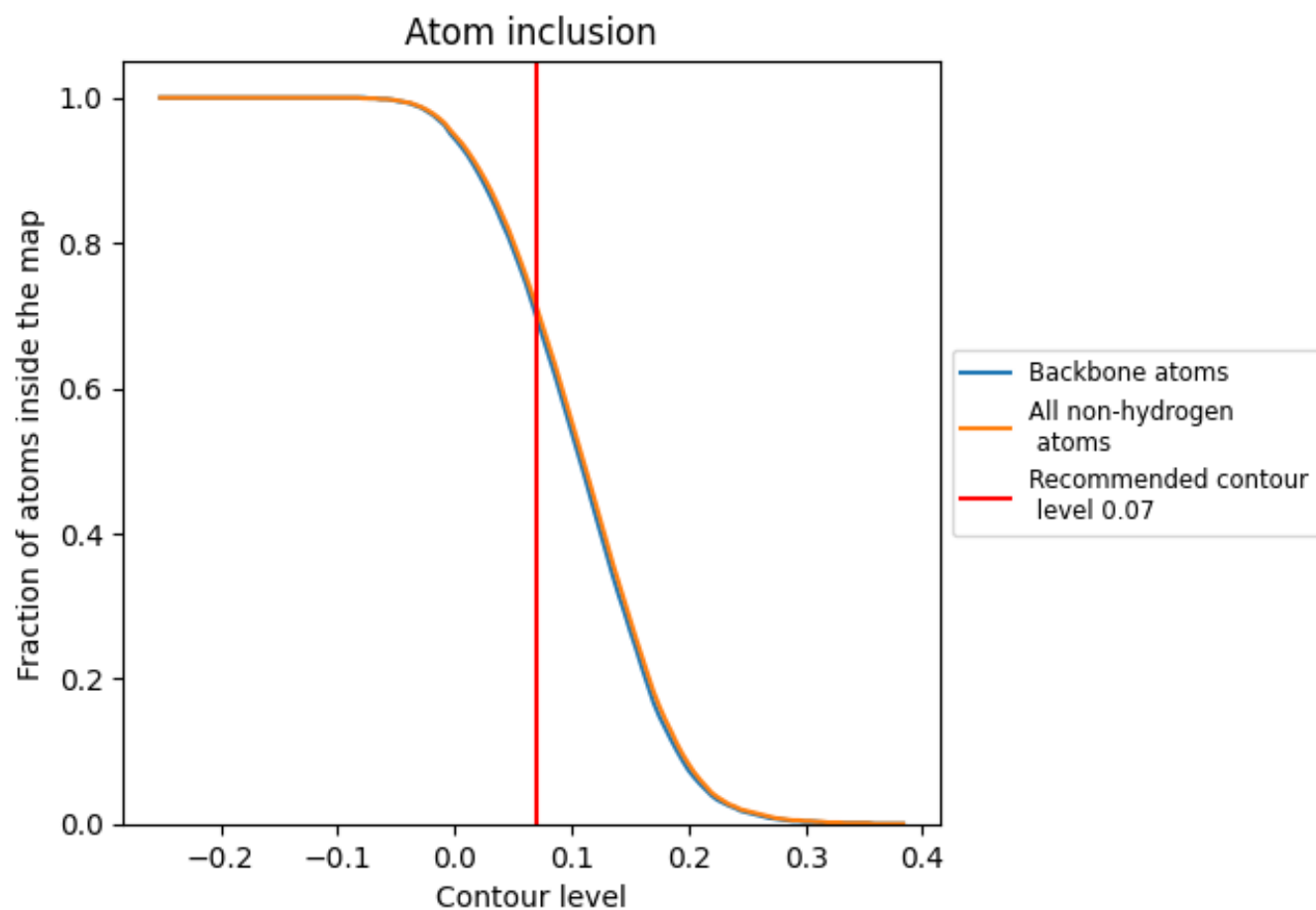
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 71% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7120	 0.0360
A	 0.6750	 0.0350
B	 0.6630	 0.0350
C	 0.7000	 0.0370
F	 0.8470	 0.0450
G	 0.8310	 0.0380
H	 0.9050	 0.0430
I	 0.8240	 0.0520
J	 0.9210	 0.0580
K	 0.7370	 0.0360
L	 0.7260	 0.0130
M	 0.9820	 0.0690
N	 0.9300	 0.0400
O	 0.8320	 0.0260
P	 0.9330	 0.0590
T	 0.6940	 0.0350
V	 0.7880	 0.0490
d	 0.9190	 0.0420
e	 0.7580	 0.0250
x	 0.6910	 0.0490

