



wwPDB EM Validation Summary Report ⓘ

Jul 14, 2024 – 09:24 am BST

PDB ID : 8BWY
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:

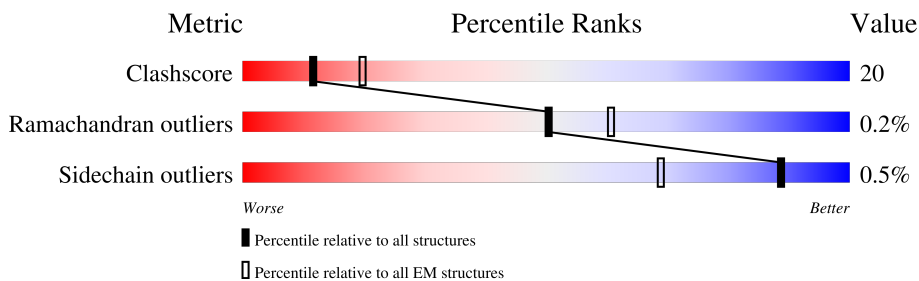
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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.



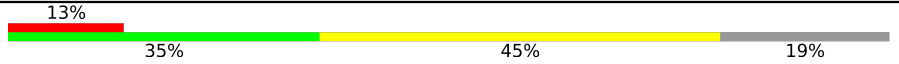
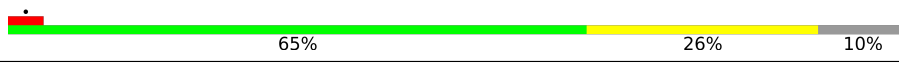
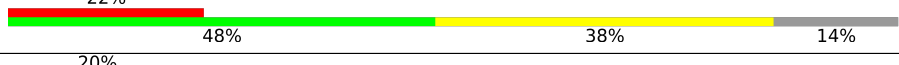
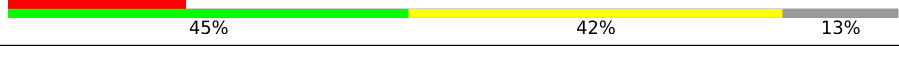


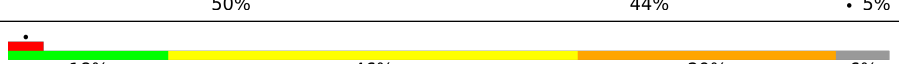
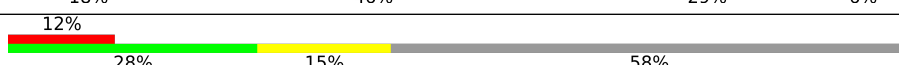
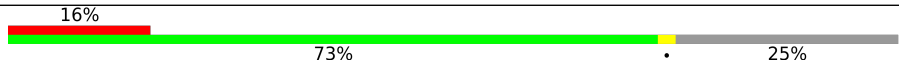
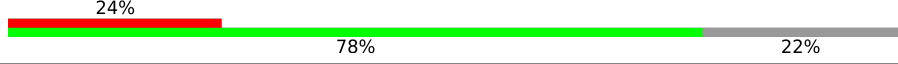

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
5	e	670	
6	F	133	
7	G	159	
8	H	92	

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Mol	Chain	Length	Quality of chain
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 [i](#)

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
			Total	C	N	O	S		
1	A	3455	18127	10919	3573	3623	12	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	459	3626	2316	609	680	21	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	S		
5	e	545	3948	2473	697	759	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	98	781	493	137	149	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	95	744	468	128	147	1	0	0

- Molecule 8 is a protein called Dynein light chain.

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

- Molecule 9 is a protein called Dynein light chain.

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

- Molecule 10 is a protein called Dynein light chain.

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

- Molecule 11 is a protein called Dynein light chain.

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

- Molecule 12 is a protein called Dynein light chain.

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

- Molecule 13 is a protein called Dynein light chain.

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

- 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.

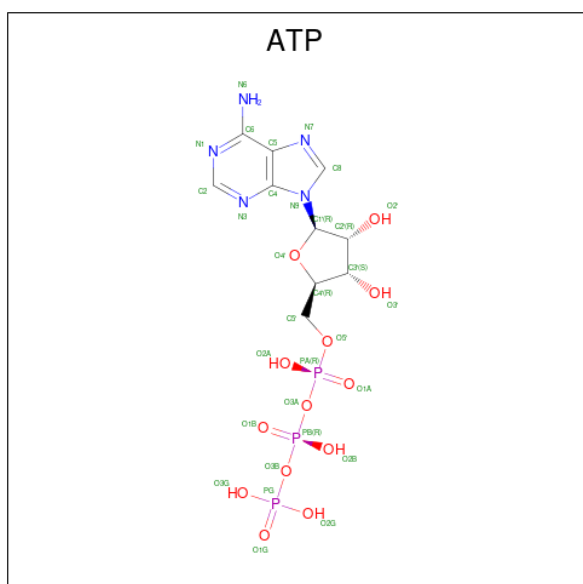
Mol	Chain	Residues	Atoms				AltConf	Trace
18	V	98	Total	C	N	O	0	0
			490	294	98	98		
18	x	101	Total	C	N	O	0	0
			505	303	101	101		

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

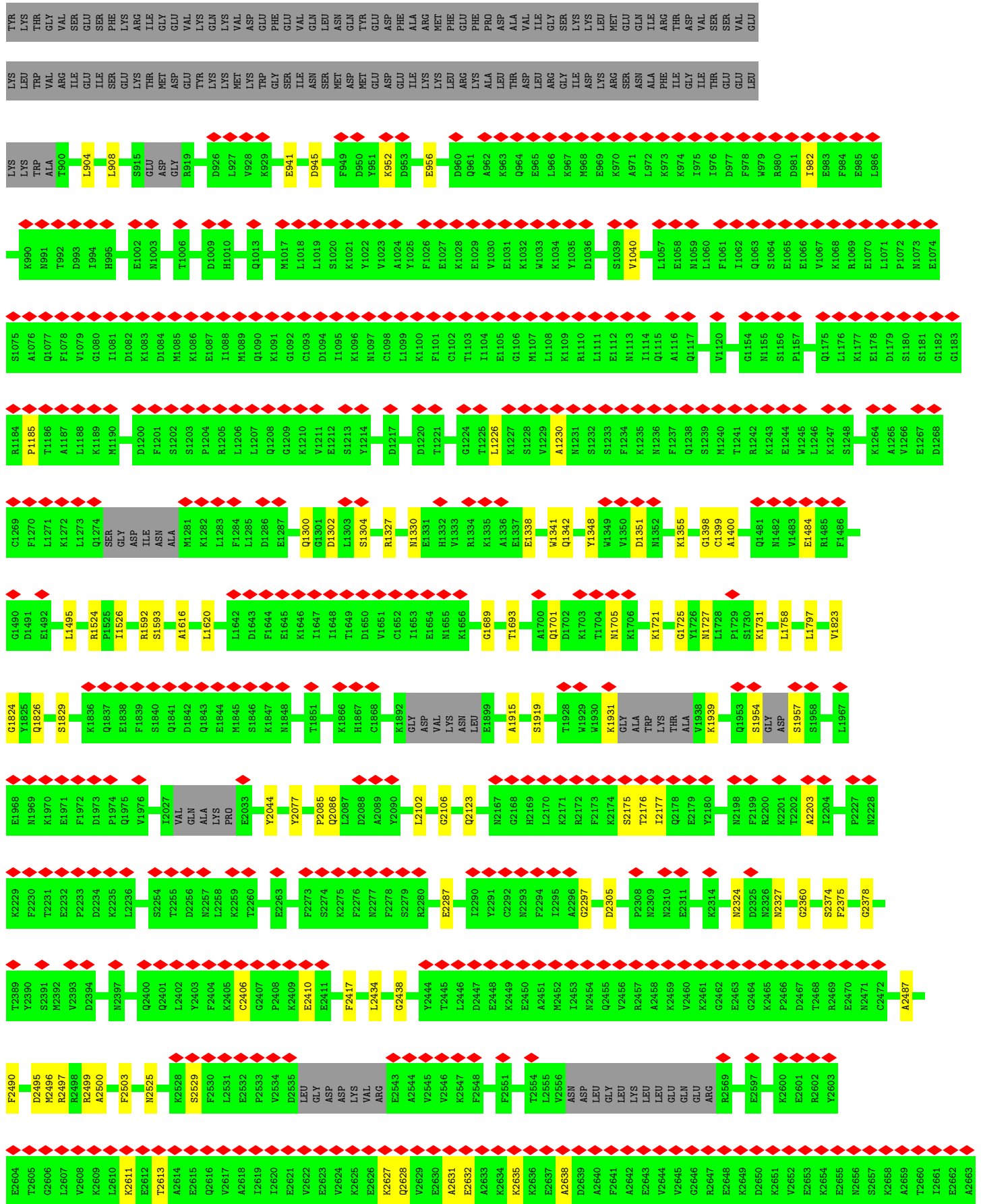


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
19	C	1	27	10	5	10	2	0
19	C	1	27	10	5	10	2	0
19	C	1	27	10	5	10	2	0

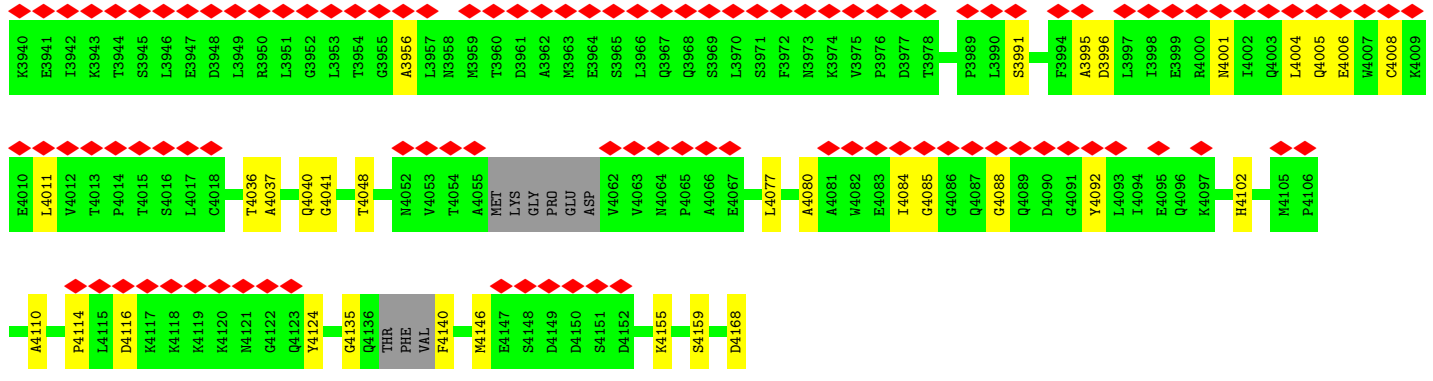
- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



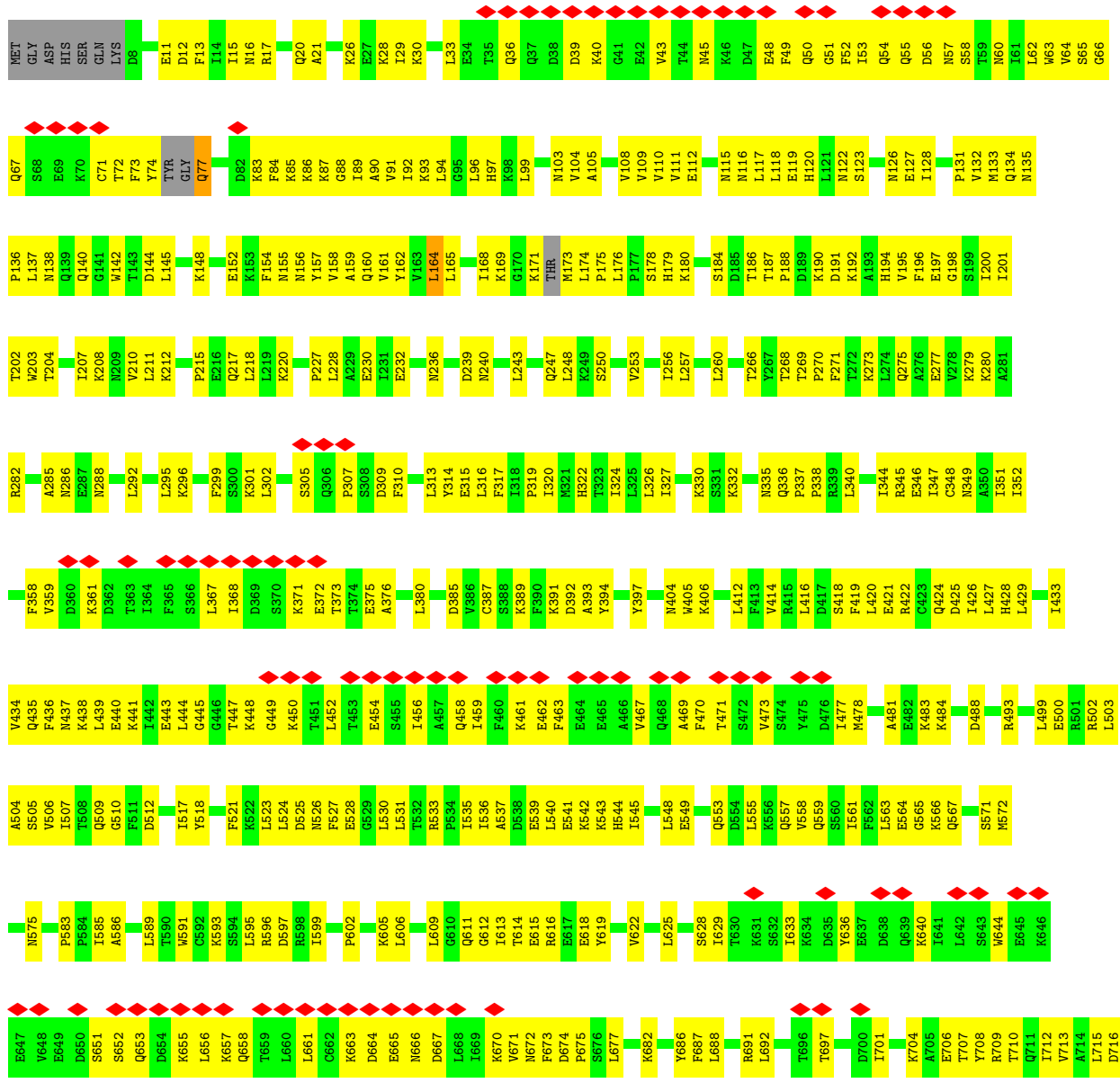
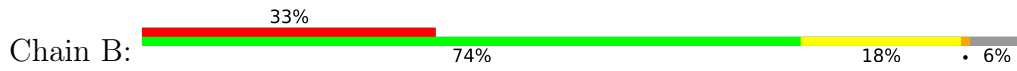
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	C	1	31	10	5	13	3	0

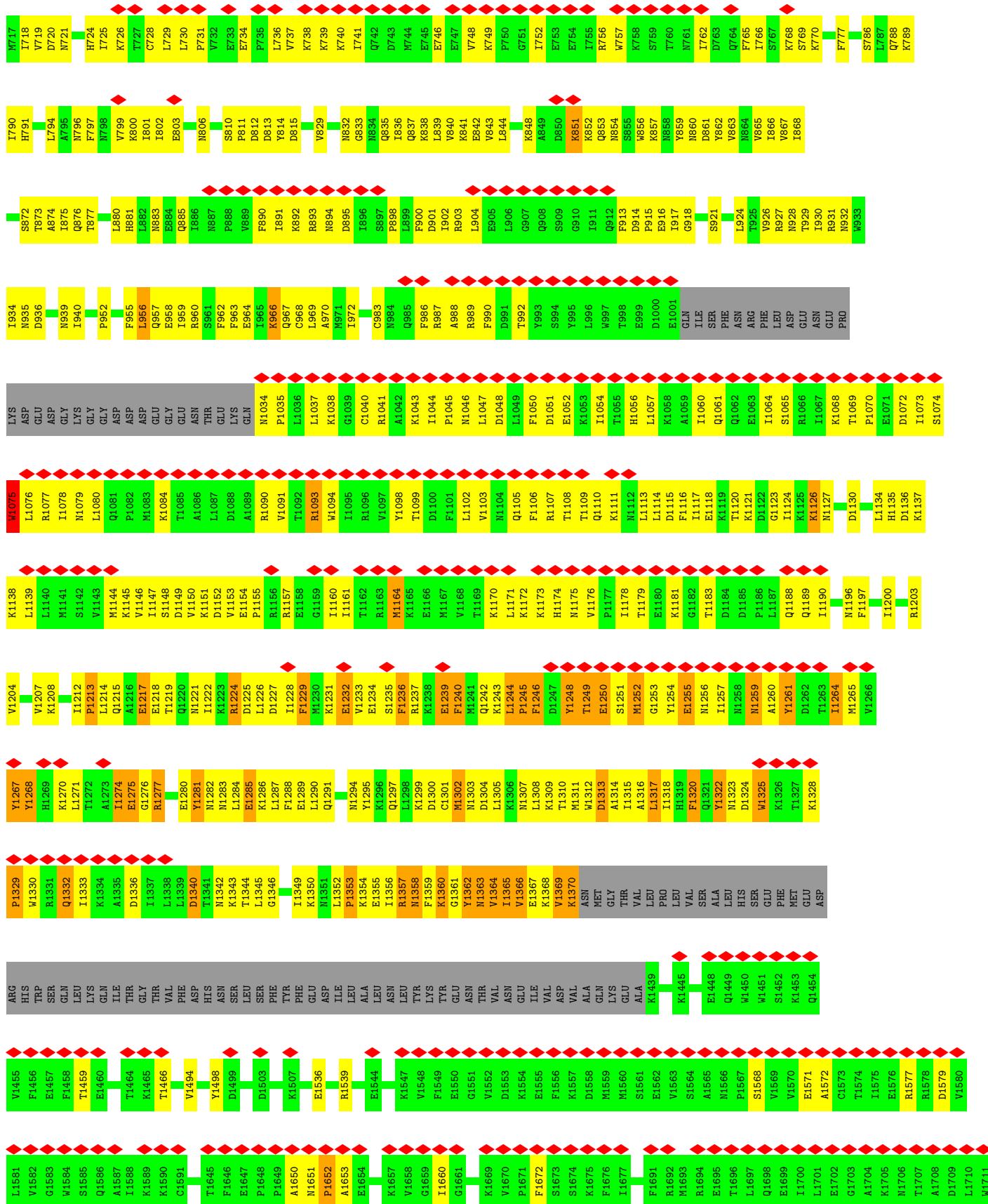


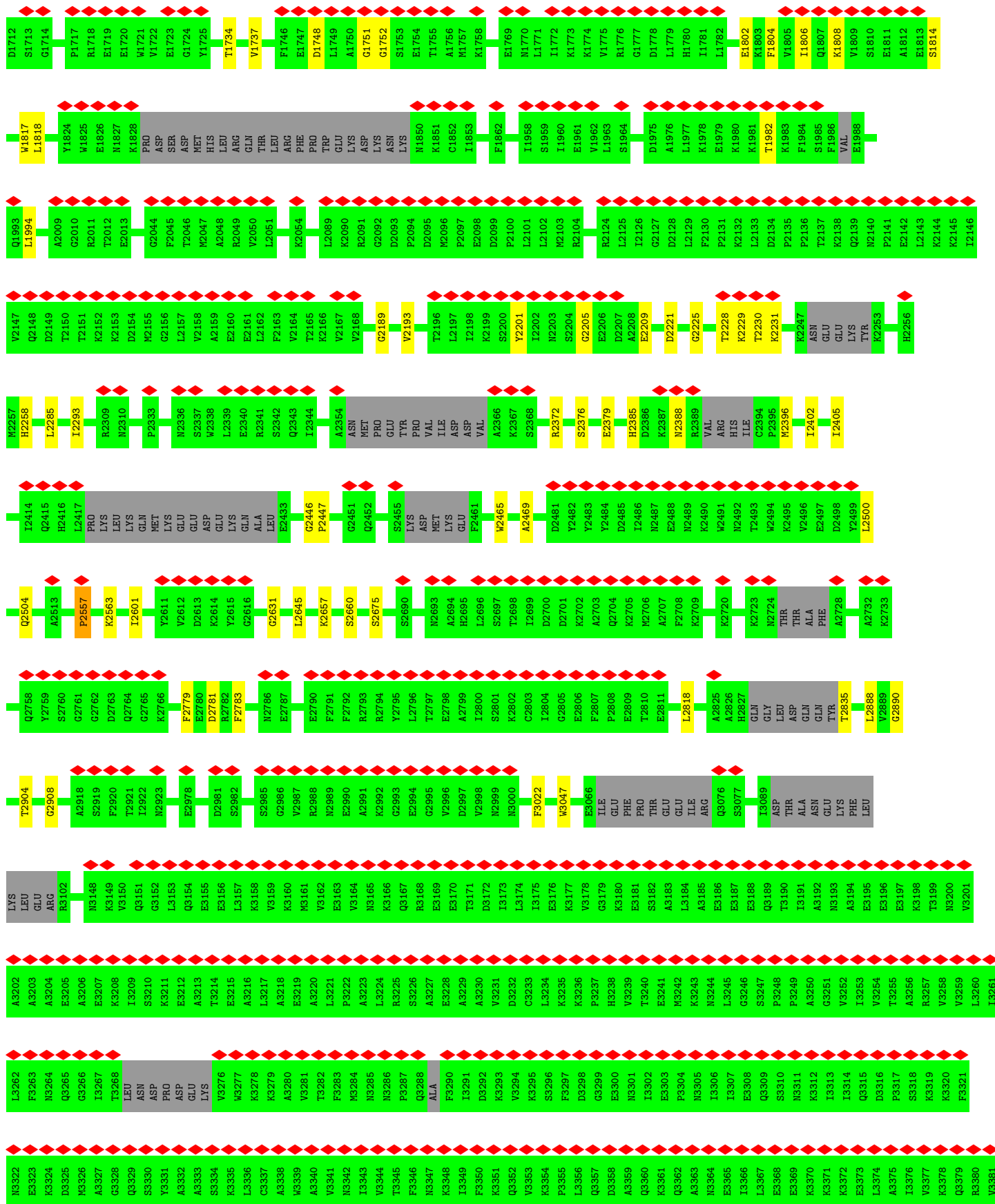
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A2724	A2725	T2726	I2727	Y2728	L2729	A2731	G2732	Y2733	F2734	N2735	GLU	ALA	ILE	GLU	ILE	ASP	LYS	ASN	ASN	PRG	LYS	VAL	S2750	W2751	Q2752	S2753	L2755	K2756	L2757	M2758	K2759	S2760	P2761	GLU	E2763	F2764	M2765	E2766	K2767	L2768	L2769	N2770	F2771	LYS	ASP	VAL	D2776	A2777	N2778	Q2779	V2780	P2781	A2782	A2783						
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L3199	S3200	V3201	A3204	E3205	V3207	A3208	A3209	A3210	K3211	I3212	T3213	A3214	A3215	K3216	I3217	N3218	E3219	T3220	S3221	E3222	Y3224	R3225	E3268	N3269	LYS	TYR	GLY	LYS	THR	MET	VAL	PRO	ALA	GLY	ASN	GLN	GLU	VAL	VAL	VAL	L3426	R3427	S3428	E3429	L3431	N3432	S3433	D3434	E3435	V3436	H3438	I3441	G3442	LYS	VAL	VAL	ASP	ASN	PRO	THR
HIS	GLN	GLN	ALA	GLN	GLN	GLN	ASN	GLN	GLU	GLN	GLN	GLU	LYS	ASP	GLU	GLU	PRO	MET	SER	ASN	PRO	R3383	S3384	L3385	K3386	K3387	R3388	V3389	D3390	R3406	F3409	K3413	L3426	R3427	S3428	E3429	L3431	N3432	S3433	D3434	E3435	V3436	H3438	I3441	G3442	LYS	VAL	VAL	ASP	ASN	PRO	THR								
GLY	GLU	GLY	GLU	GLU	GLY	GLU	LYS	GLN	GLN	ALA	LYS	ASP	SER	PRO	R3383	S3384	L3385	K3386	K3387	R3388	V3389	D3390	R3406	F3409	K3413	L3426	R3427	S3428	E3429	L3431	N3432	S3433	D3434	E3435	V3436	H3438	I3441	G3442	LYS	VAL	VAL	ASP	ASN	PRO	THR															
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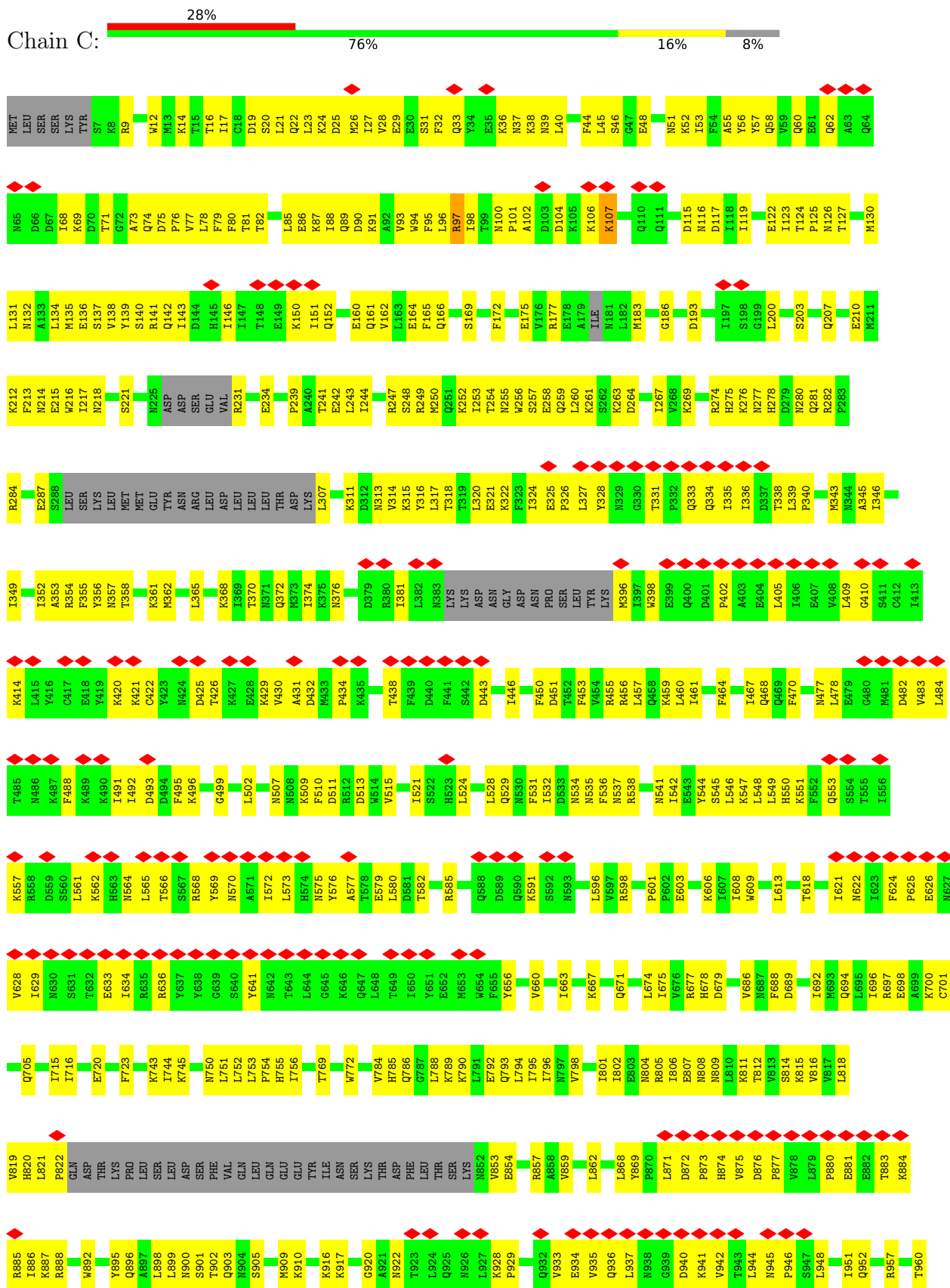


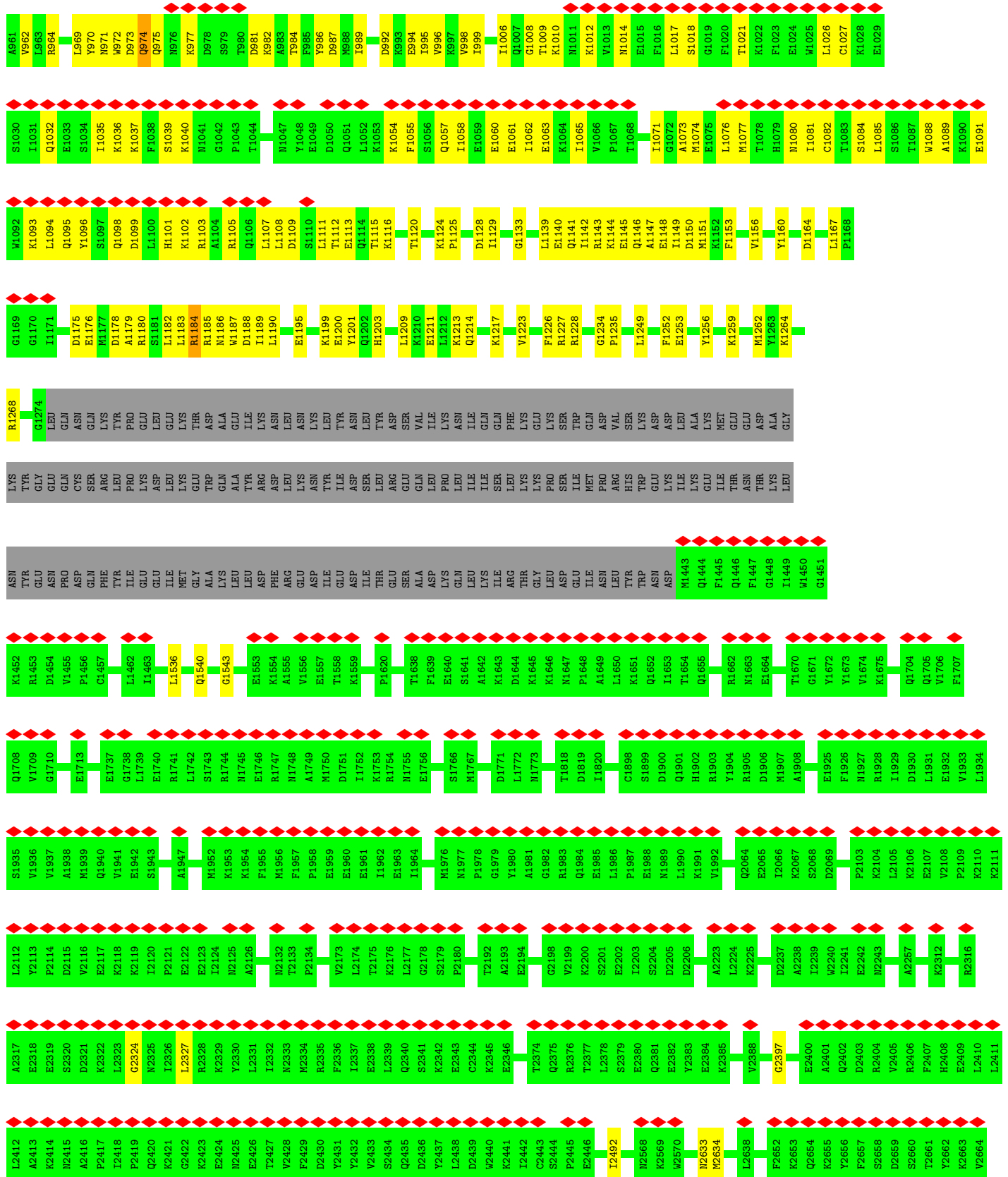
• Molecule 2: Outer arm dynein beta heavy chain



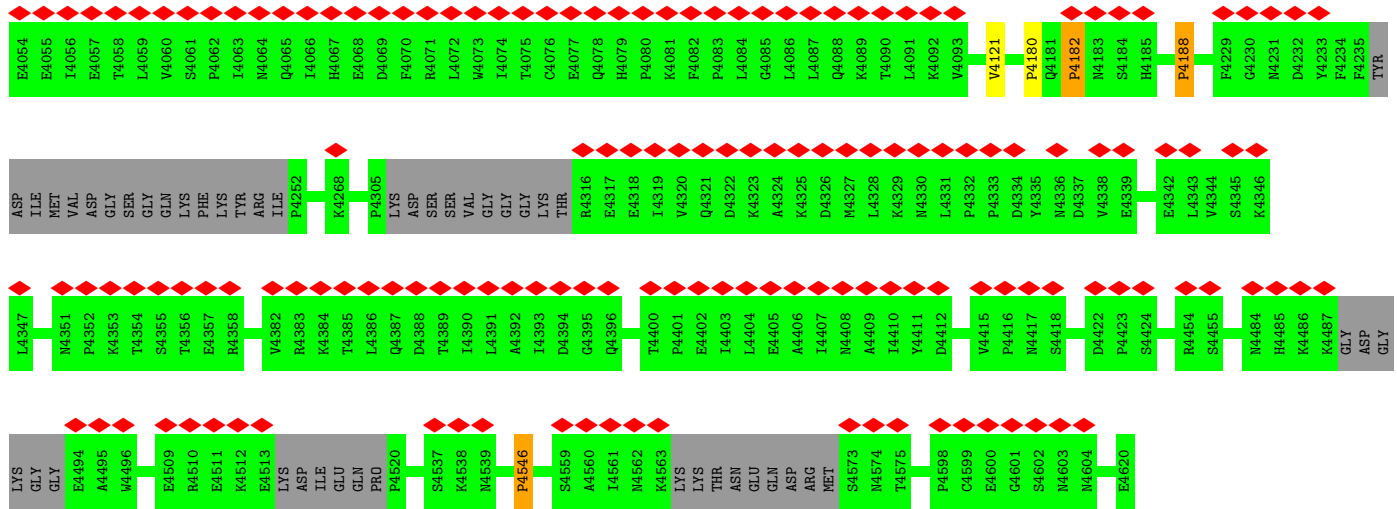




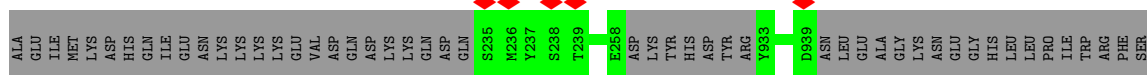
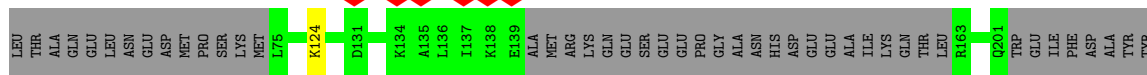
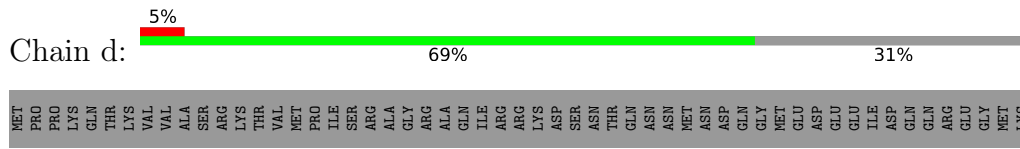




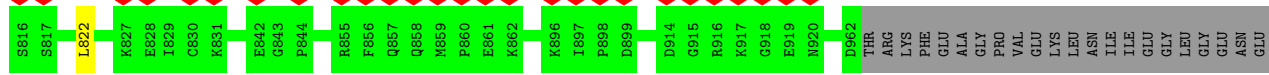
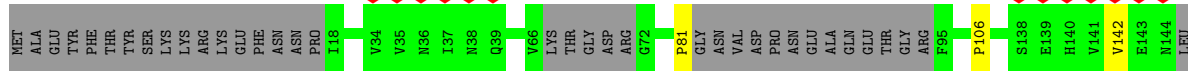
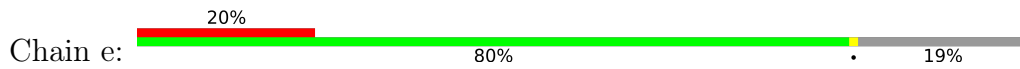
D3986	F3987	V3988	L3989	F3990	L3991	L3992	S3993	A3994	G3995	A3996	D3997	F3998	T3999	I4002	D4003	F4012	P4013	C4014	E4015	V4016	V4017	S4018	M4019	G4020	G4022	Q4023	E4024	R4025	V4026	A4027	R4028	Q4029	P3922	D3923	F3919	P3920	I3921	P3922	D3923	E3926	S3927	Q3930	E3931	E3966	W3979	Q3980	E3981	S3982	S3983	N3984	M3985	L4002	L4004	L4043	Q4044	N4045	C4046	L4047	L4048	G4049	L4050	K4051	F4052																				
S3862	GLY	ASP	ALA	LEU	ASP	ILE	LYS	SER	GLU	ARG	Q3863	E3870	W3874	K3882	HIS	THR	THR	PHE	SER	SER	GLY	GLN	THR	P3891	K3769	M3770	V3771	N3772	S3773	E3776	Q3777	F3778	L3779	K3780	L3781	F3782	I3783	E3784	S3785	P3922	D3923	F3919	P3920	I3921	P3922	D3923	E3926	S3927	Q3930	E3931	E3966	W3979	Q3980	E3981	S3982	S3983	N3984	M3985	L4002	L4004	L4043	Q4044	N4045	C4046	L4047	L4048	G4049	L4050	K4051	F4052													
D3708	D3709	T3710	E3711	L3712	M3713	D3714	V3715	V3726	L3730	L3740	N3741	E3742	K3743	R3744	E3745	Q3746	V3747	R3748	M3769	M3770	V3771	N3772	S3773	E3776	Q3777	F3778	L3779	K3780	L3781	F3782	I3783	E3784	S3785	P3922	D3923	F3919	P3920	I3921	P3922	D3923	E3926	S3927	Q3930	E3931	E3966	W3979	Q3980	E3981	S3982	S3983	N3984	M3985	L4002	L4004	L4043	Q4044	N4045	C4046	L4047	L4048	G4049	L4050	K4051	F4052																			
ILE	ILE	PRO	GLU	ARG	CYS	I3555	T3556	T3557	L3558	S3559	H3560	P3561	F3562	F3563	K3564	M3565	M3566	F3567	L3568	K3569	Y3570	C3571	M3572	E3573	S3574	G3575	L3576	T3577	L3578	I3579	V3580	E3581	N3582	E3586	V3587	D3588	D3592	L3595	E3596	ARG	GLN	ILE	ILE	VAL	VAL	LYS	GLY	LYS	THR	GLN	PHE	ASN	VAL	ALA	ALA	GLY	THR	SER	ILE	ILE	PRO	GLU	GLN	ILE	ILE	GLU	GLU	ASP	TRP	F3317	N3318	D3319	T3320	F3321	T3322	T3323	I3324	K3325	S3326	K3327	A3328	A3329	A3330
G3331	I3332	K3333	K3334	W3335	A3336	F3337	A3338	I3339	E3341	Y3342	H3343	Q3344	K3345	S3346	K3347	I3348	V3349	K3350	P3351	K3352	R3353	I3354	Q3355	V3356	A3357	I3358	A3359	E3360	G3361	R3362	K3363	A3364	I3365	L3366	L3367	D3368	K3369	V3482	P3483	E3371	K3372	A3373	R3374	E3375	W3376	L3377	A3378	Q3379	I3380	Q3381	Y3382	I3383	R3384	K3385	N3386	L3387	K3388	D3389	V3390																								
GLU	S3272	Y3273	D3274	K3275	S3276	G3277	L3278	Q3279	T3280	L3281	G3282	D3283	M3284	N3285	F3286	M3287	K3288	K3289	L3290	K3291	E3292	F3293	K3294	K3295	D3296	S3297	L3298	N3299	E3300	E3301	T3302	L3303	E3304	L3305	L3306	E3307	F3308	Y3309	L3310	N3311	Q3312	S3313	E3314	ASP	TRP	F3317	N3318	D3319	T3320	F3321	T3322	T3323	I3324	K3325	S3326	K3327	A3328	A3329	A3330																								
A3211	V3212	D3213	S3214	I3215	E3216	S3217	K3218	D3219	L3220	V3221	E3222	L3223	K3224	A3225	N3226	K3227	K3228	P3229	L3230	D3231	E3232	I3233	K3234	Y3235	I3236	M3237	D3238	A3239	V3240	L3241	V3242	F3243	F3244	K3245	A3246	R3247	L3248	ILE	PRO	ILE	GLN	ILE	GLU	GLU	ARG	VAL	PHE	ASN	LYS	LYS	GLU	GLY	LYS	ALA	VAL	LEU	PHE	LEU	LEU	LYS	A3203	A3204	R3205	R3206	R3207	A3208	Q3209	E3210															
K3151	T3152	N3153	Q3154	L3155	L3156	A3157	N3158	L3159	D3160	K3161	E3162	S3163	K3164	A3165	N3167	Q3168	K3169	G3170	E3171	K3172	V3173	A3174	A3175	A3176	N3177	K3178	Q3179	C3180	E3181	I3182	Q3183	A3184	E3185	Q3186	I3187	S3188	K3189	E3190	K3191	E3192	E3193	A3194	E3195	PHE	ASN	LYS	LYS	GLU	GLY	LYS	ALA	VAL	LEU	PHE	LEU	LEU	LYS	A3203	A3204	R3205	R3206	R3207	A3208	Q3209	E3210																		
I2665	E2666	S2667	S2670	A2671	A2674	L2675	W2676	N2677	K2678	V2679	K2680	S2681	T2682	H2683	L2684	P2685	T2686	P2687	I2714	N2715	D2716	A2717	P2718	K2719	S2720	K2721	K2722	I2723	K2724	E2725	E2726	L2727	E2738	A2742	K2749	D2750	K2751	D2752	T2753	V2754	K2755	G2756	V2757	I2758	Q2759	E2760	V2761	S2762	L2763	E2764	S2765	F2766	S2767																														

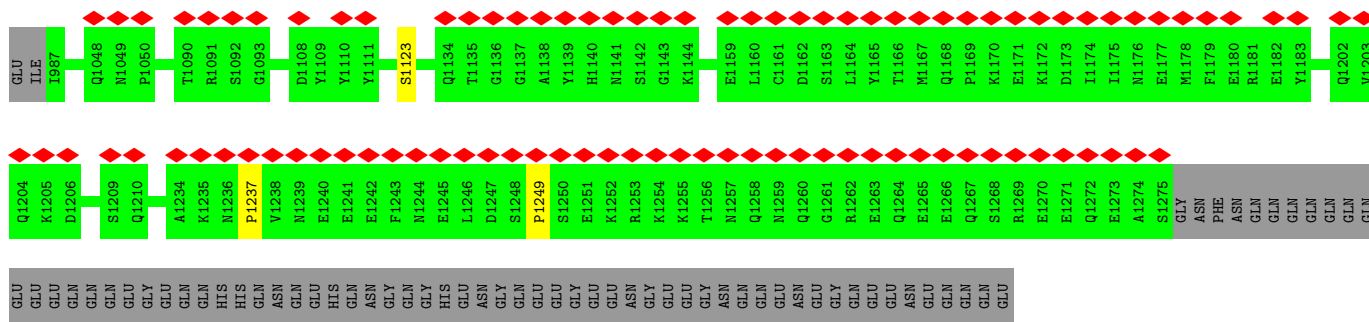


• Molecule 4: Dynein intermediate chain 2

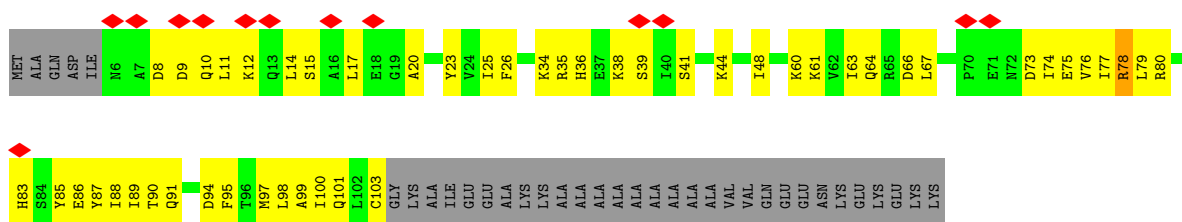


• Molecule 5: Flagellar outer dynein arm intermediate protein, putative

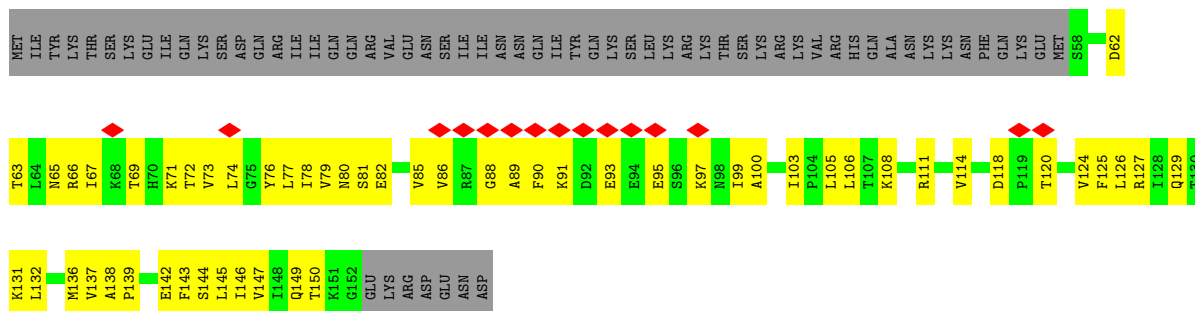
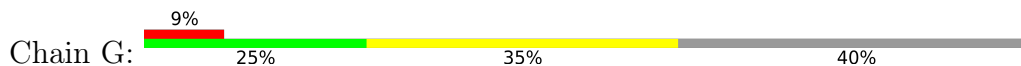




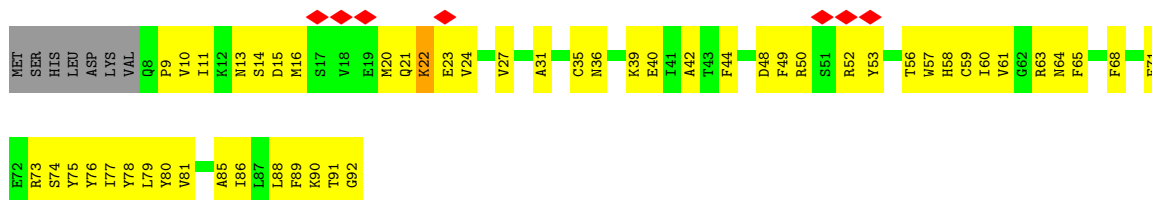
• Molecule 6: Dynein light chain roadblock-type 2 protein



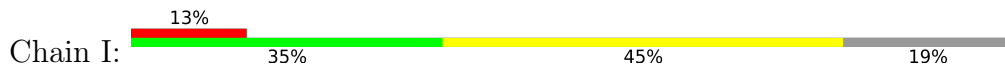
• Molecule 7: Dynein light chain roadblock-type 2 protein

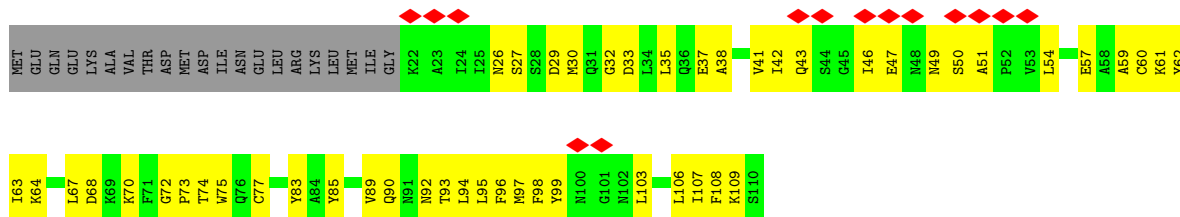


• Molecule 8: Dynein light chain

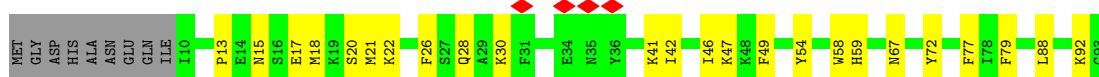


• Molecule 9: Dynein light chain

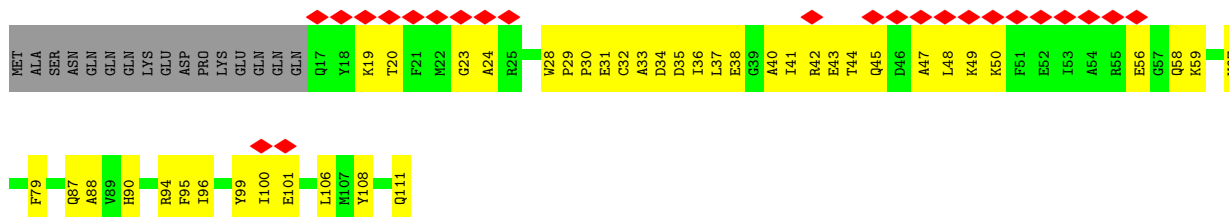




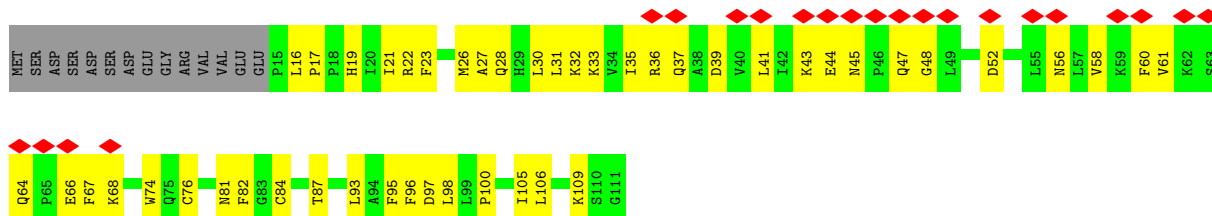
• Molecule 10: Dynein light chain



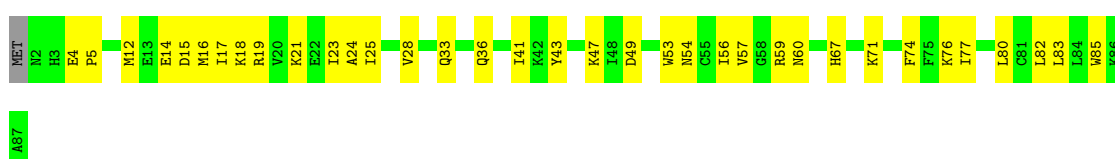
• Molecule 11: Dynein light chain



• Molecule 12: Dynein light chain



• Molecule 13: Dynein light chain

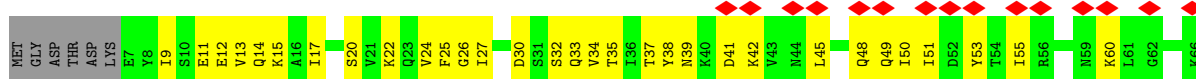


• Molecule 14: Dynein light chain 2A

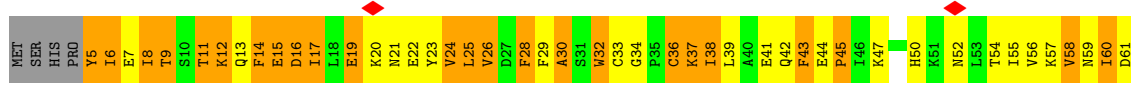
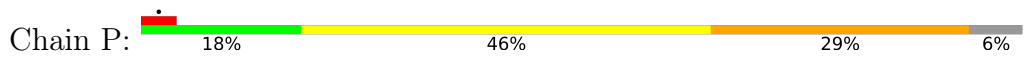




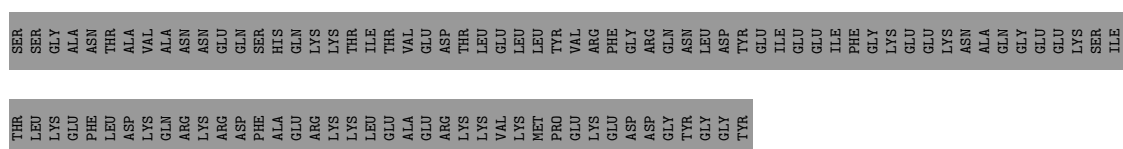
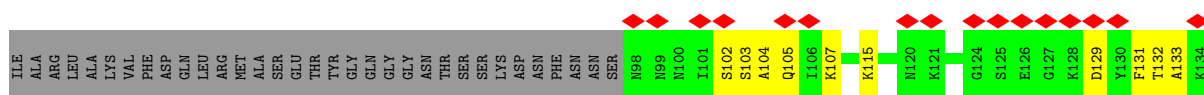
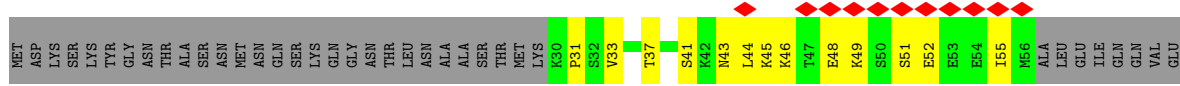
• Molecule 15: Dynein light chain tetex-type 1 protein



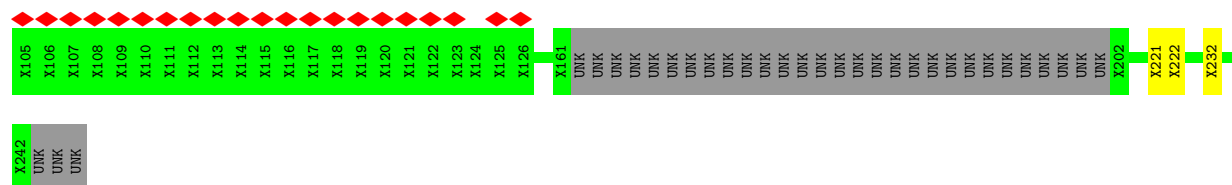
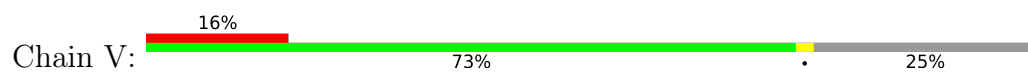
• Molecule 16: Thioredoxin



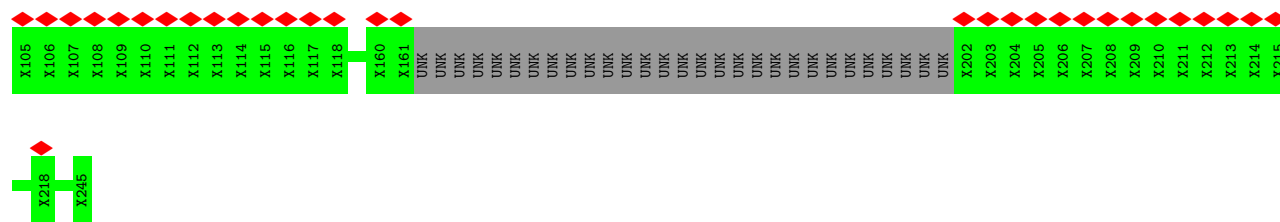
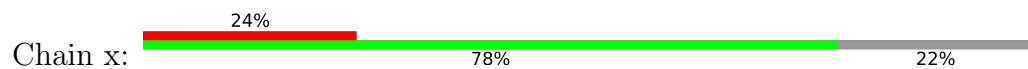
• Molecule 17: Calmodulin



• 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 (\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 (\AA)	8.5, 8.5, 8.5	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.31	0/18167	0.63	1/25169 (0.0%)
2	B	0.79	100/25709 (0.4%)	0.77	68/35300 (0.2%)
3	C	0.70	156/25227 (0.6%)	0.68	68/34687 (0.2%)
4	d	0.32	0/3710	0.51	0/5026
5	e	0.30	0/4021	0.55	6/5463 (0.1%)
6	F	0.29	0/793	0.51	0/1070
7	G	0.27	0/751	0.52	0/1014
8	H	0.28	0/718	0.47	0/965
9	I	0.28	0/705	0.51	0/954
10	J	0.29	0/723	0.45	0/966
11	K	0.29	0/828	0.50	0/1114
12	L	0.29	0/790	0.50	0/1063
13	M	0.27	0/743	0.45	0/996
14	N	0.32	0/915	0.55	0/1229
15	O	0.28	0/891	0.47	0/1209
16	P	2.95	64/866 (7.4%)	2.22	36/1171 (3.1%)
17	T	0.27	0/1070	0.44	0/1436
All	All	0.67	320/86627 (0.4%)	0.70	179/118832 (0.2%)

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 320 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1075	TRP	C-O	16.60	1.54	1.23
3	C	3345	LYS	C-O	-12.11	1.00	1.23
3	C	3331	GLY	CA-C	10.79	1.69	1.51
16	P	41	GLU	CD-OE1	10.22	1.36	1.25
2	B	1255	GLU	CD-OE2	10.08	1.36	1.25

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3344	GLN	CA-C-N	-13.69	87.09	117.20
2	B	1224	ARG	NE-CZ-NH2	-12.33	114.14	120.30
2	B	1268	TYR	CB-CG-CD1	11.37	127.82	121.00
3	C	3345	LYS	N-CA-C	-11.25	80.62	111.00
16	P	14	PHE	CB-CG-CD2	-10.80	113.24	120.80

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	311	0
2	B	25545	0	17415	935	0
3	C	25046	0	16443	674	0
4	d	3626	0	3455	0	0
5	e	3948	0	3485	0	0
6	F	781	0	791	46	0
7	G	744	0	771	42	0
8	H	702	0	686	50	0
9	I	694	0	684	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	702	0	671	18	0
11	K	803	0	766	67	0
12	L	773	0	806	51	0
13	M	726	0	726	29	0
14	N	897	0	911	70	0
15	O	878	0	868	36	0
16	P	847	0	836	76	0
17	T	1057	0	1033	35	0
18	V	490	0	102	5	0
18	x	505	0	105	0	0
19	C	81	0	36	0	0
20	C	31	0	12	0	0
All	All	87003	0	59981	2356	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 2356 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%)	41	77
2	B	4229/4595 (92%)	3790 (90%)	429 (10%)	10 (0%)	47	81
3	C	4232/4620 (92%)	3885 (92%)	337 (8%)	10 (0%)	47	81
4	d	445/667 (67%)	400 (90%)	45 (10%)	0	100	100
5	e	529/670 (79%)	459 (87%)	69 (13%)	1 (0%)	47	81
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%)	9	44
All	All	13963/16284 (86%)	12499 (90%)	1431 (10%)	33 (0%)	50	81

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 [i](#)

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%)	288 (99%)	3 (1%)	76	86
2	B	1215/4145 (29%)	1208 (99%)	7 (1%)	86	92
3	C	1094/4196 (26%)	1091 (100%)	3 (0%)	92	95
4	d	386/609 (63%)	385 (100%)	1 (0%)	92	95
5	e	364/597 (61%)	363 (100%)	1 (0%)	92	95
6	F	87/109 (80%)	85 (98%)	2 (2%)	50	70
7	G	86/149 (58%)	85 (99%)	1 (1%)	71	83
8	H	76/83 (92%)	75 (99%)	1 (1%)	69	81
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%)	96 (98%)	2 (2%)	55	74
16	P	97/104 (93%)	96 (99%)	1 (1%)	76	86
17	T	118/271 (44%)	118 (100%)	0	100	100
All	All	4402/14628 (30%)	4380 (100%)	22 (0%)	89	93

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	1123	SER
7	G	91	LYS
6	F	80	ARG
8	H	22	LYS
2	B	461	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	971	ASN
7	G	70	HIS
3	C	975	GLN
5	e	52	ASN
9	I	26	ASN

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](#)

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	4702	-	24,29,29	0.92	1 (4%)	29,45,45	1.55	4 (13%)
20	ATP	C	4704	-	26,33,33	0.88	1 (3%)	31,52,52	1.68	5 (16%)
19	ADP	C	4701	-	24,29,29	0.91	1 (4%)	29,45,45	1.50	5 (17%)
19	ADP	C	4703	-	24,29,29	0.96	1 (4%)	29,45,45	1.51	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
19	ADP	C	4702	-	-	4/12/32/32	0/3/3/3
20	ATP	C	4704	-	-	4/18/38/38	0/3/3/3
19	ADP	C	4701	-	-	3/12/32/32	0/3/3/3
19	ADP	C	4703	-	-	1/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	4701	ADP	C5-C4	2.20	1.46	1.40
19	C	4702	ADP	C5-C4	2.14	1.46	1.40
19	C	4703	ADP	C5-C4	2.14	1.46	1.40
20	C	4704	ATP	C5-C4	2.06	1.46	1.40

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	4704	ATP	PA-O3A-PB	-5.12	115.24	132.83
19	C	4703	ADP	PA-O3A-PB	-4.58	117.12	132.83
19	C	4701	ADP	PA-O3A-PB	-4.21	118.36	132.83
20	C	4704	ATP	PB-O3B-PG	-4.15	118.57	132.83
19	C	4702	ADP	PA-O3A-PB	-4.13	118.66	132.83

There are no chirality outliers.

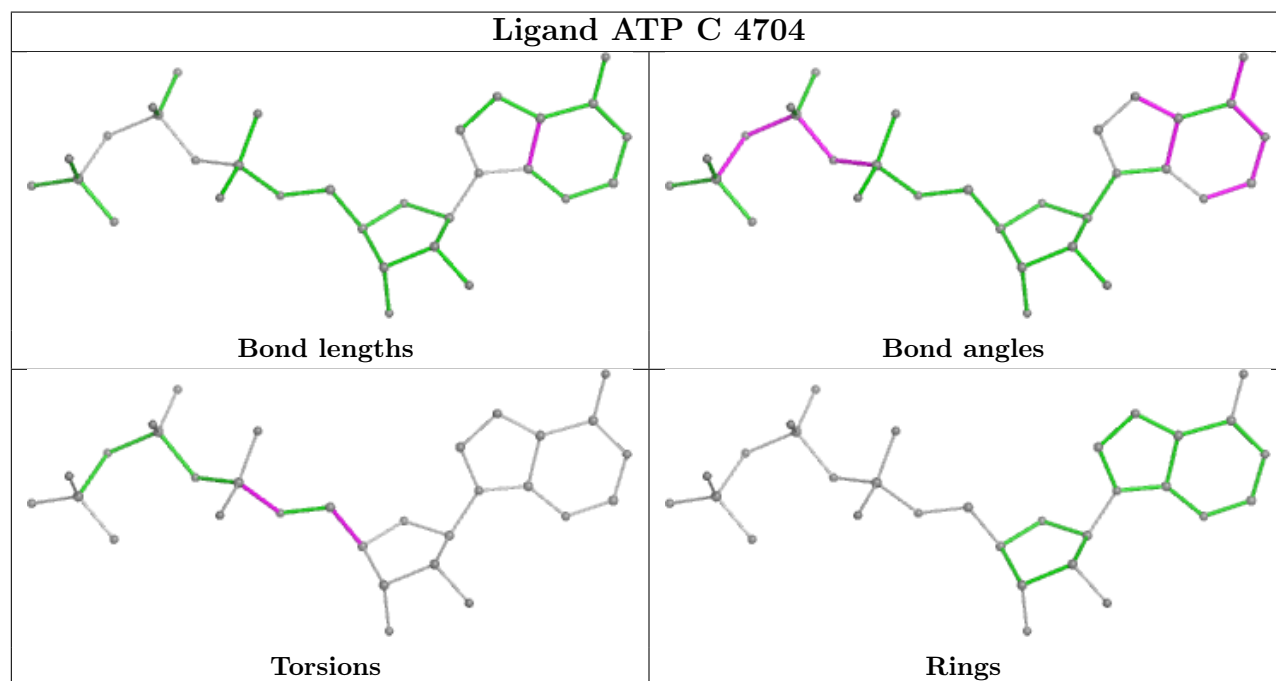
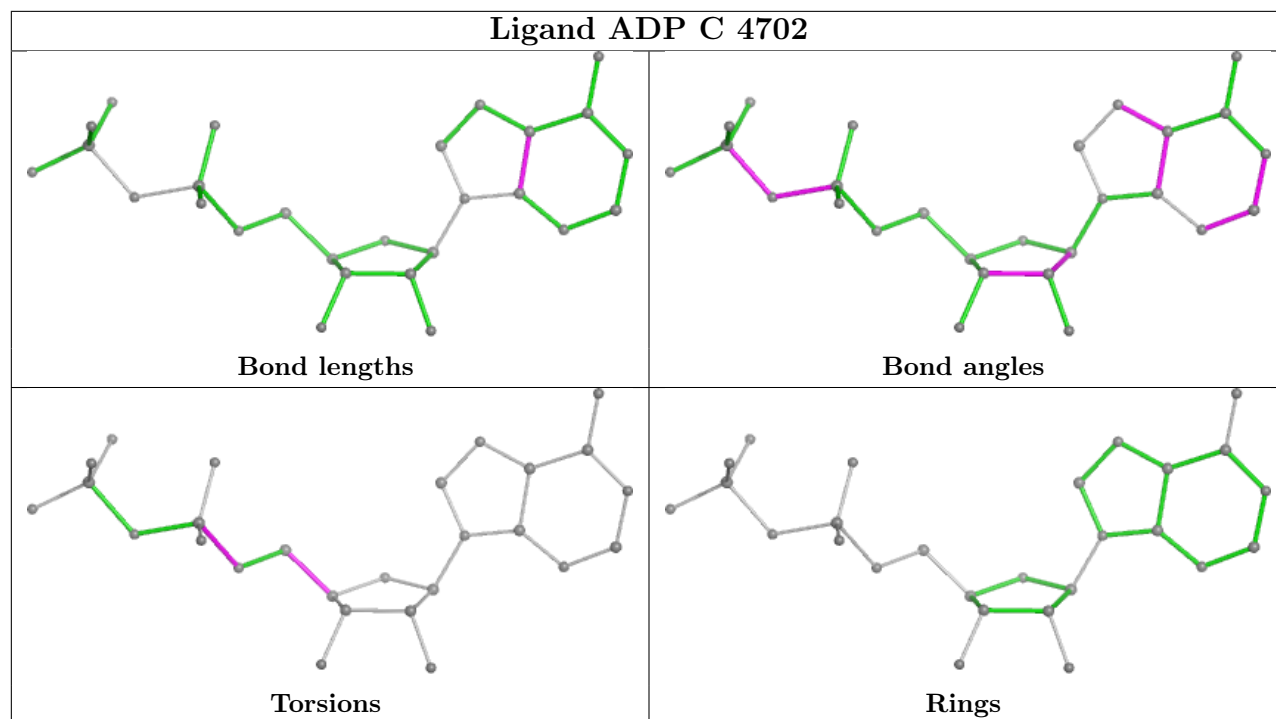
5 of 12 torsion outliers are listed below:

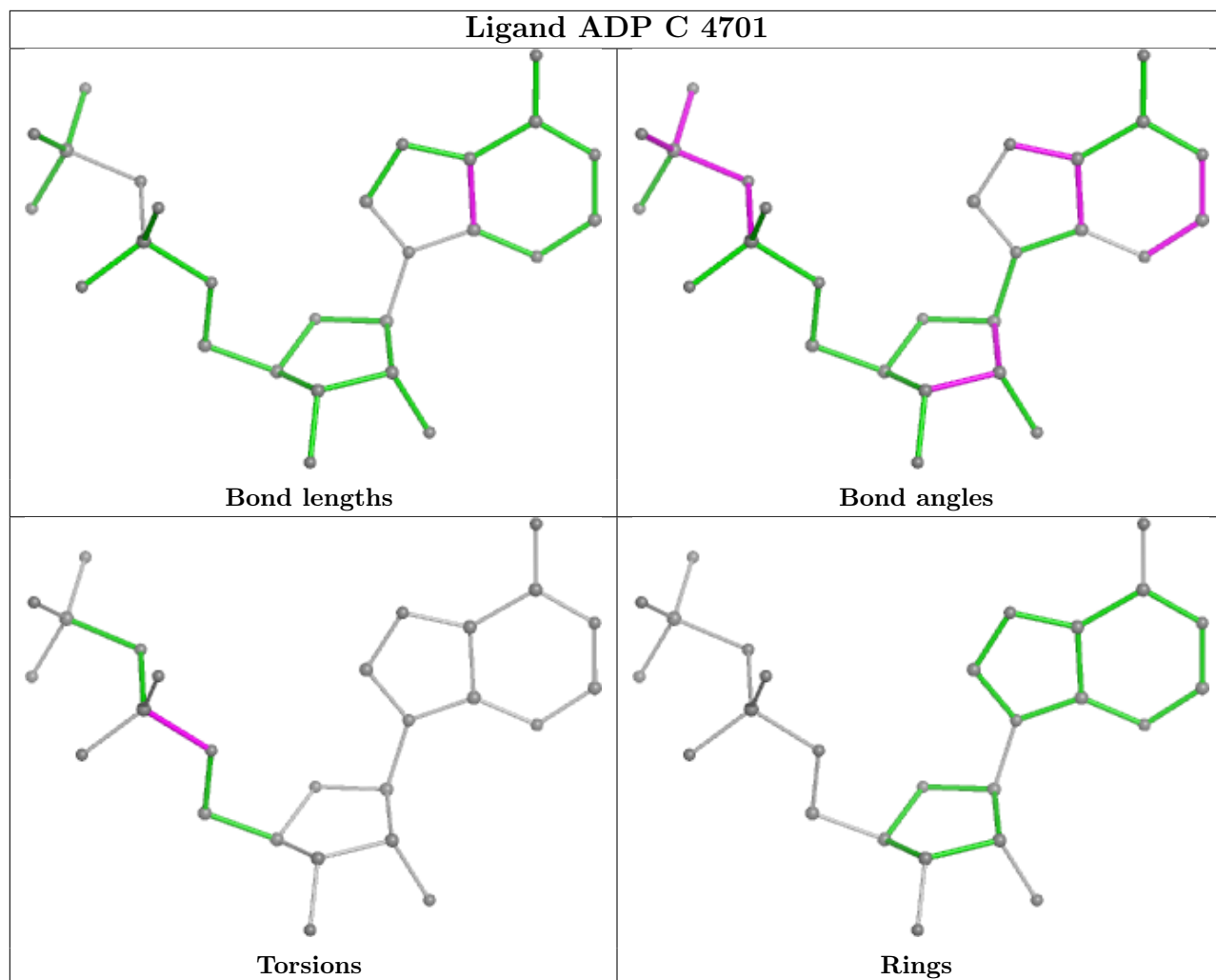
Mol	Chain	Res	Type	Atoms
19	C	4701	ADP	C5'-O5'-PA-O1A
19	C	4702	ADP	C5'-O5'-PA-O1A
19	C	4702	ADP	C5'-O5'-PA-O2A
20	C	4704	ATP	C5'-O5'-PA-O1A
20	C	4704	ATP	C5'-O5'-PA-O3A

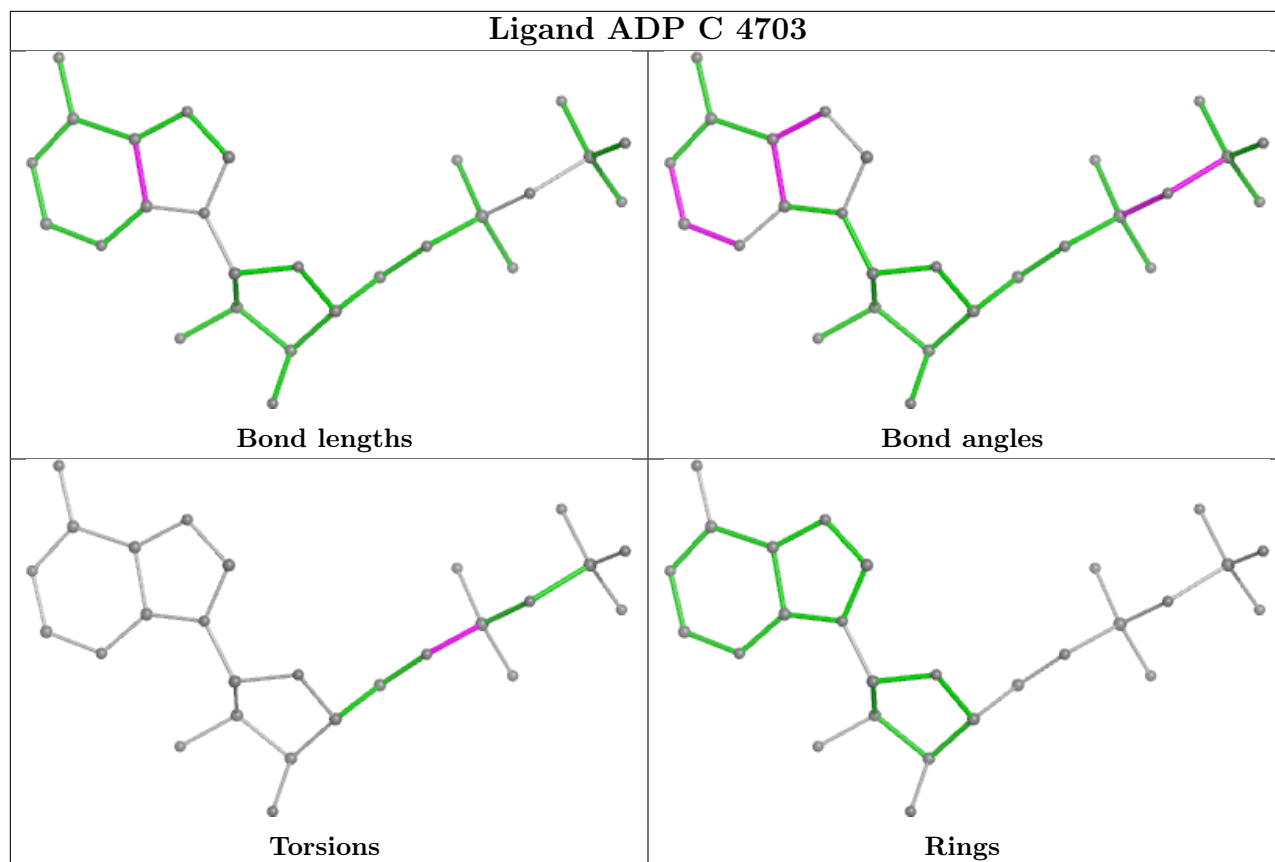
There are no ring outliers.

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	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

Continued on next page...

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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.

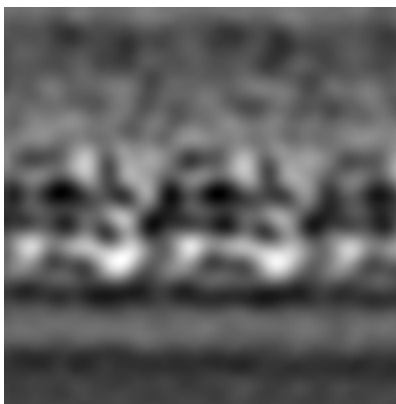
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

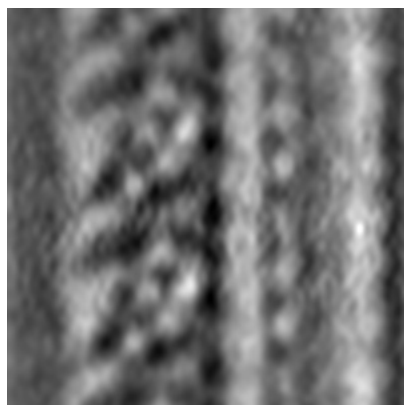


Y

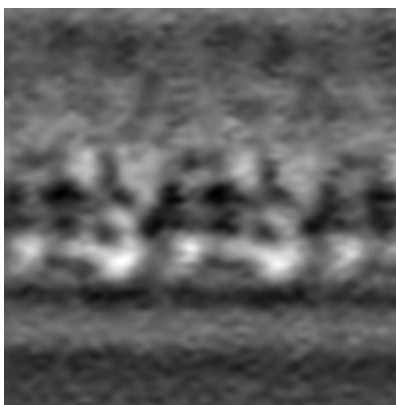


Z

6.1.2 Raw map



X



Y



Z

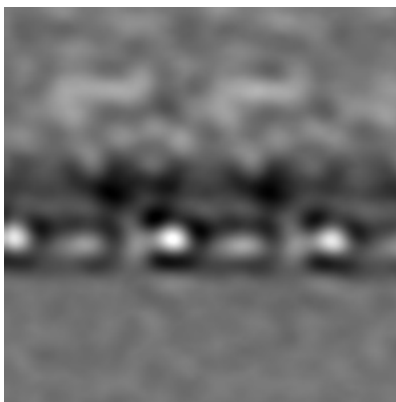
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 37

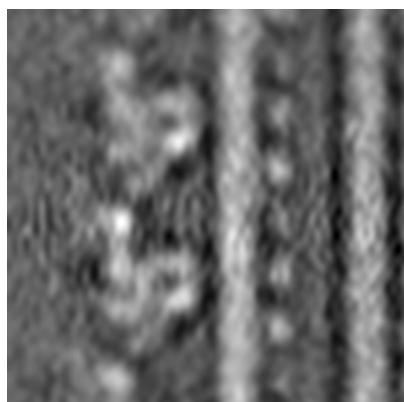


Y Index: 37

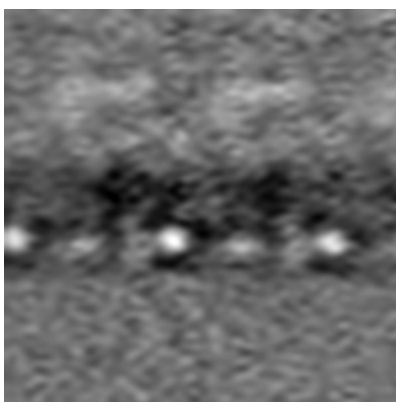


Z Index: 37

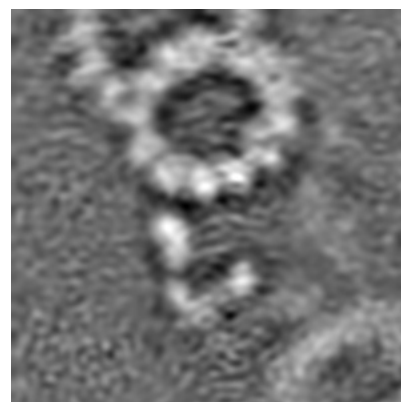
6.2.2 Raw map



X Index: 37



Y Index: 37



Z Index: 37

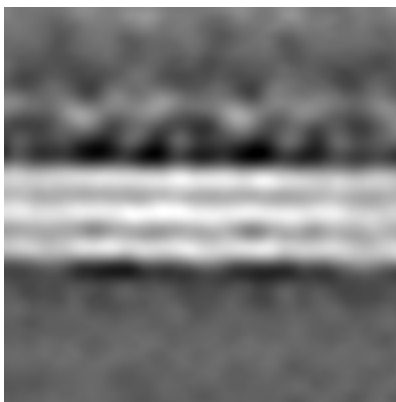
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 29

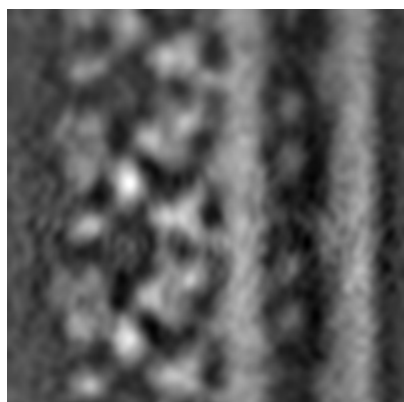


Y Index: 42

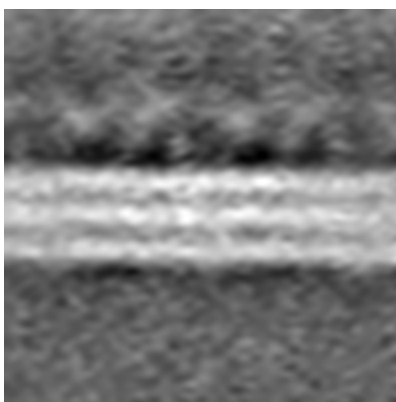


Z Index: 22

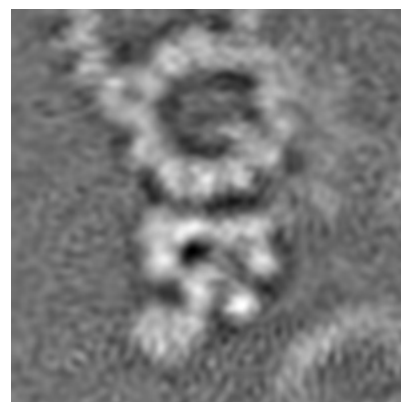
6.3.2 Raw map



X Index: 29



Y Index: 42

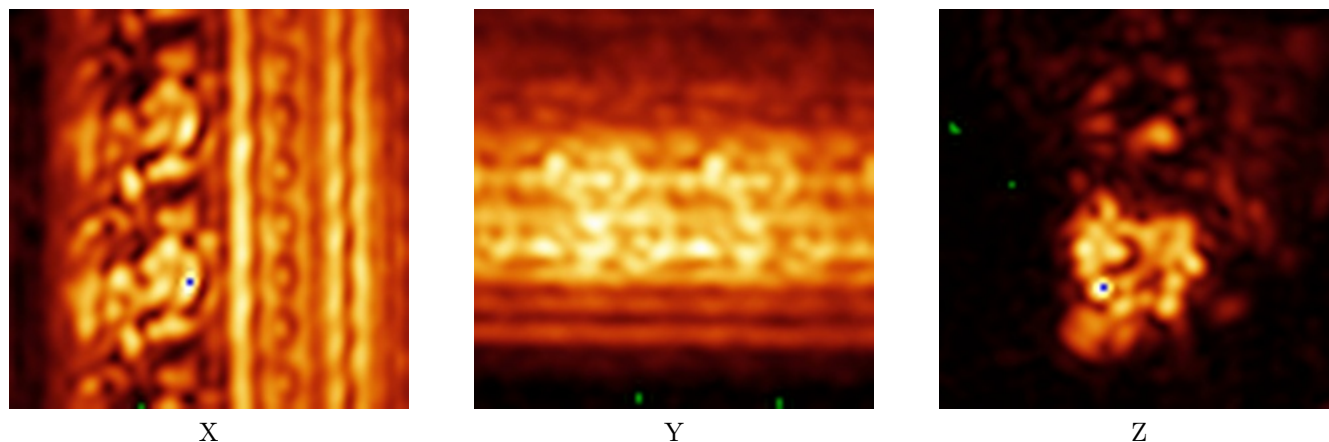


Z Index: 22

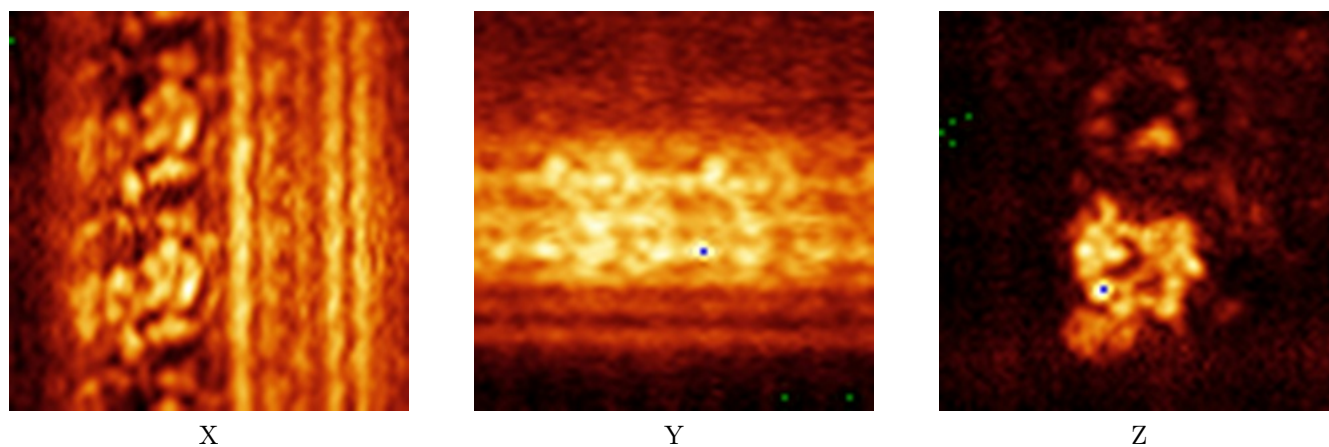
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



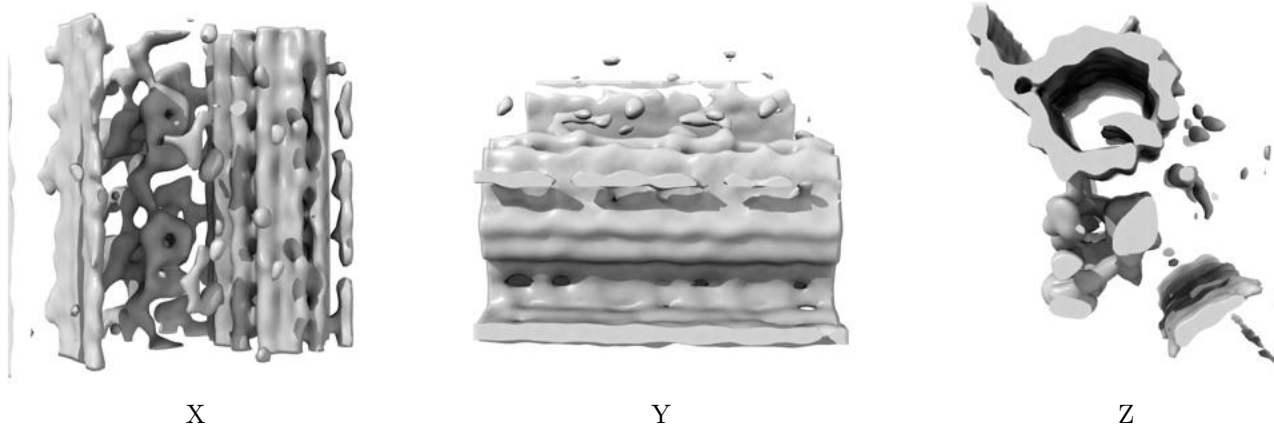
6.4.2 Raw map



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.

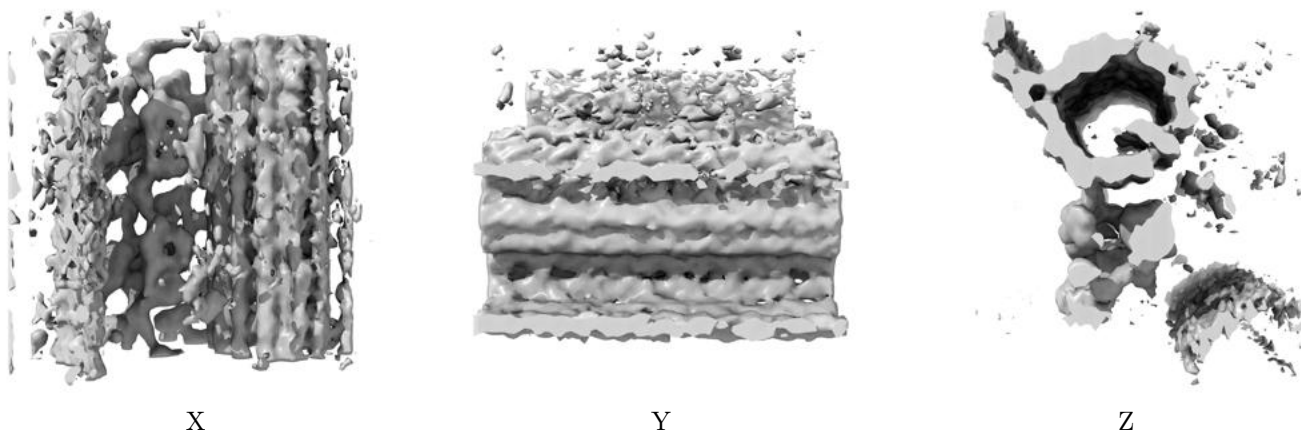
6.5 Orthogonal surface views [i](#)

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.

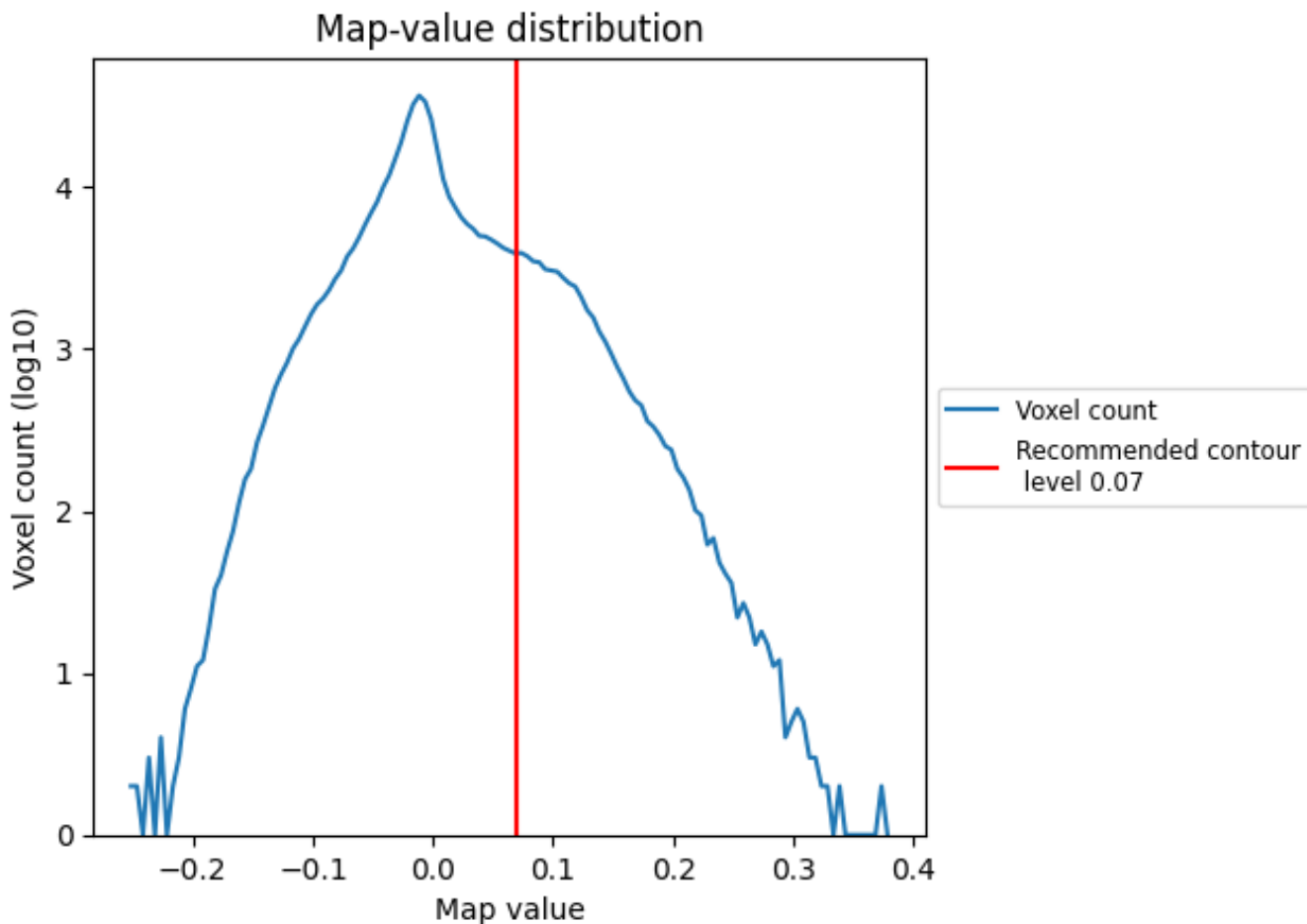
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

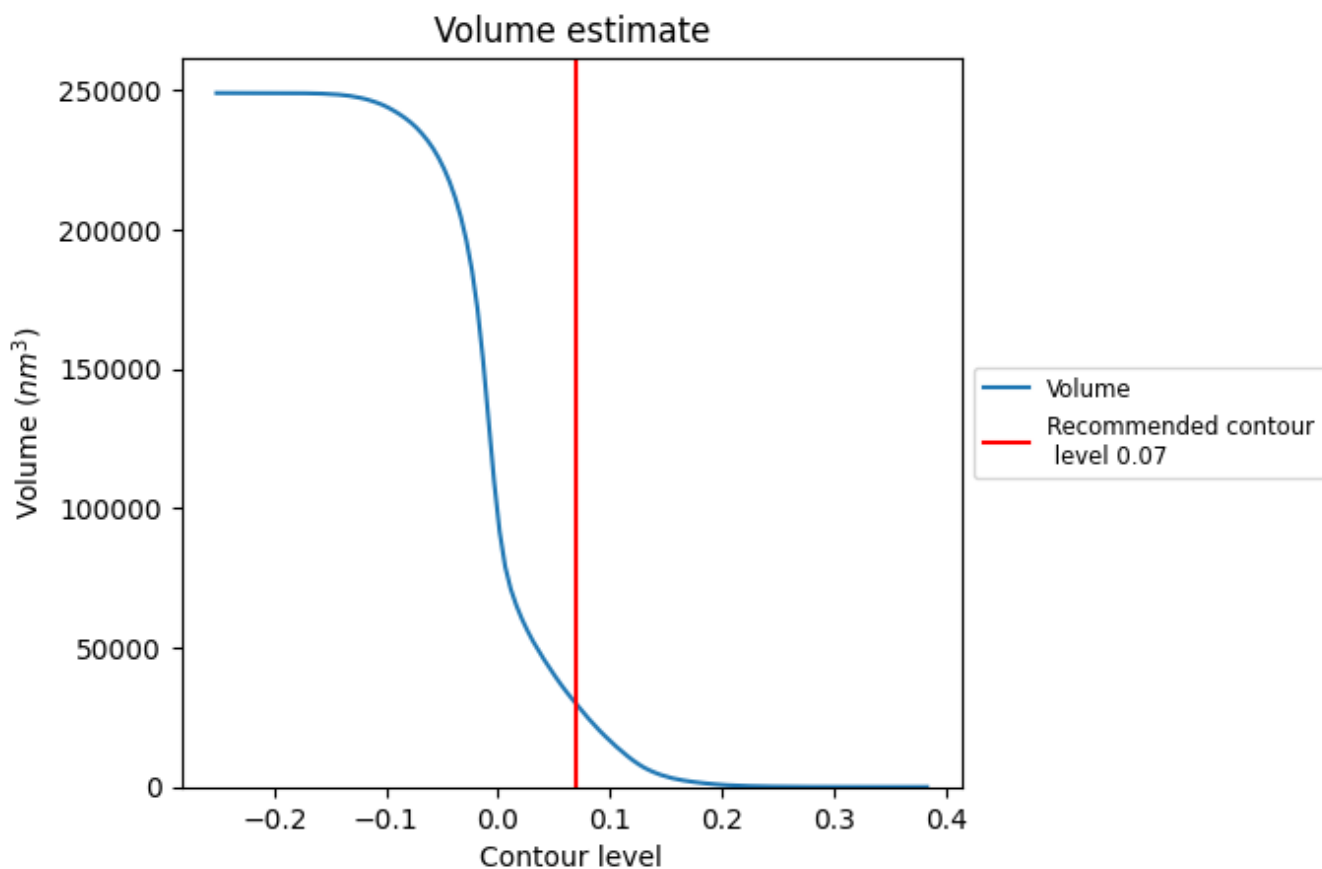
This section contains the results of statistical analysis of the map.

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.

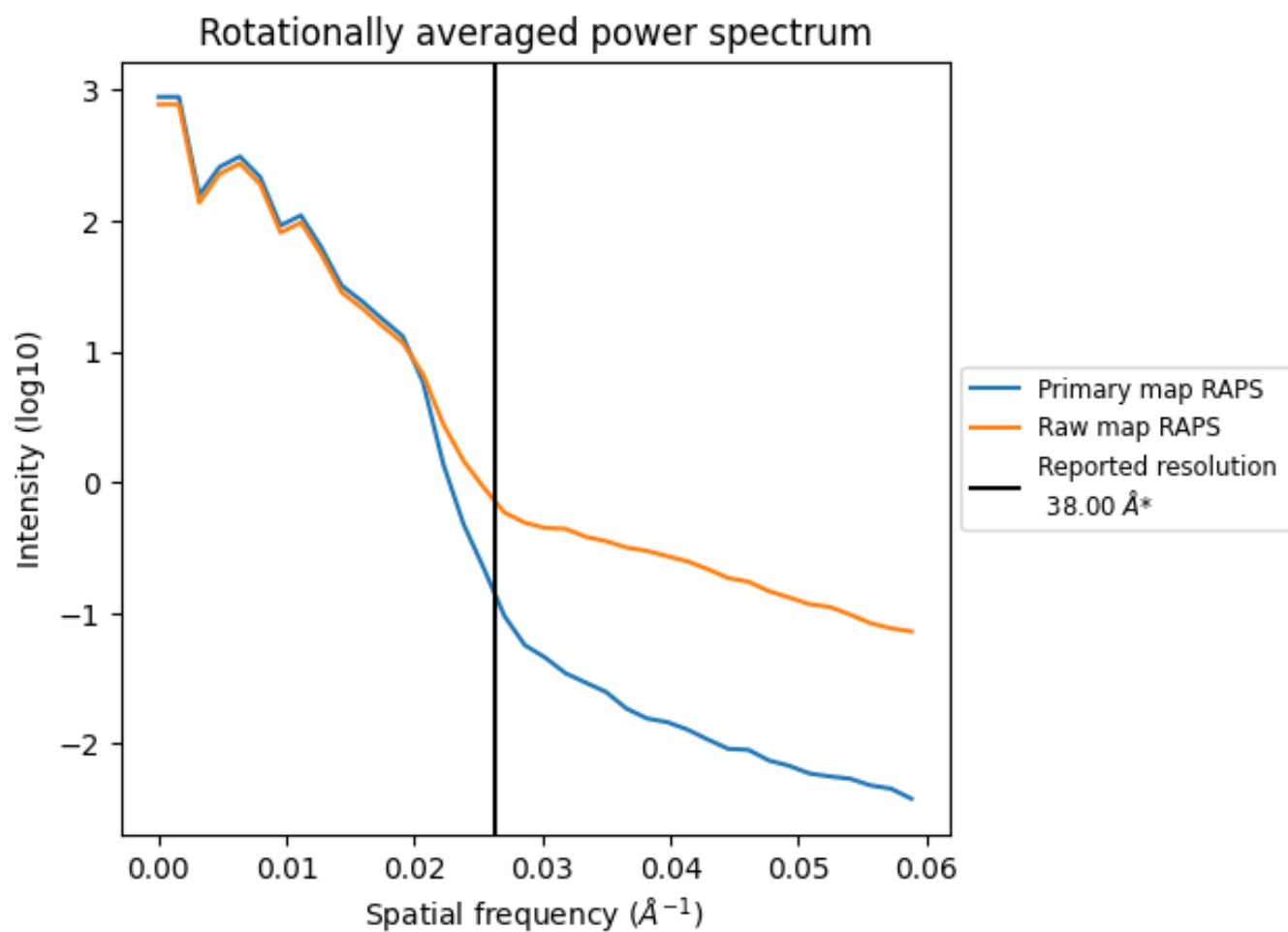
7.2 Volume estimate [i](#)



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 [i](#)

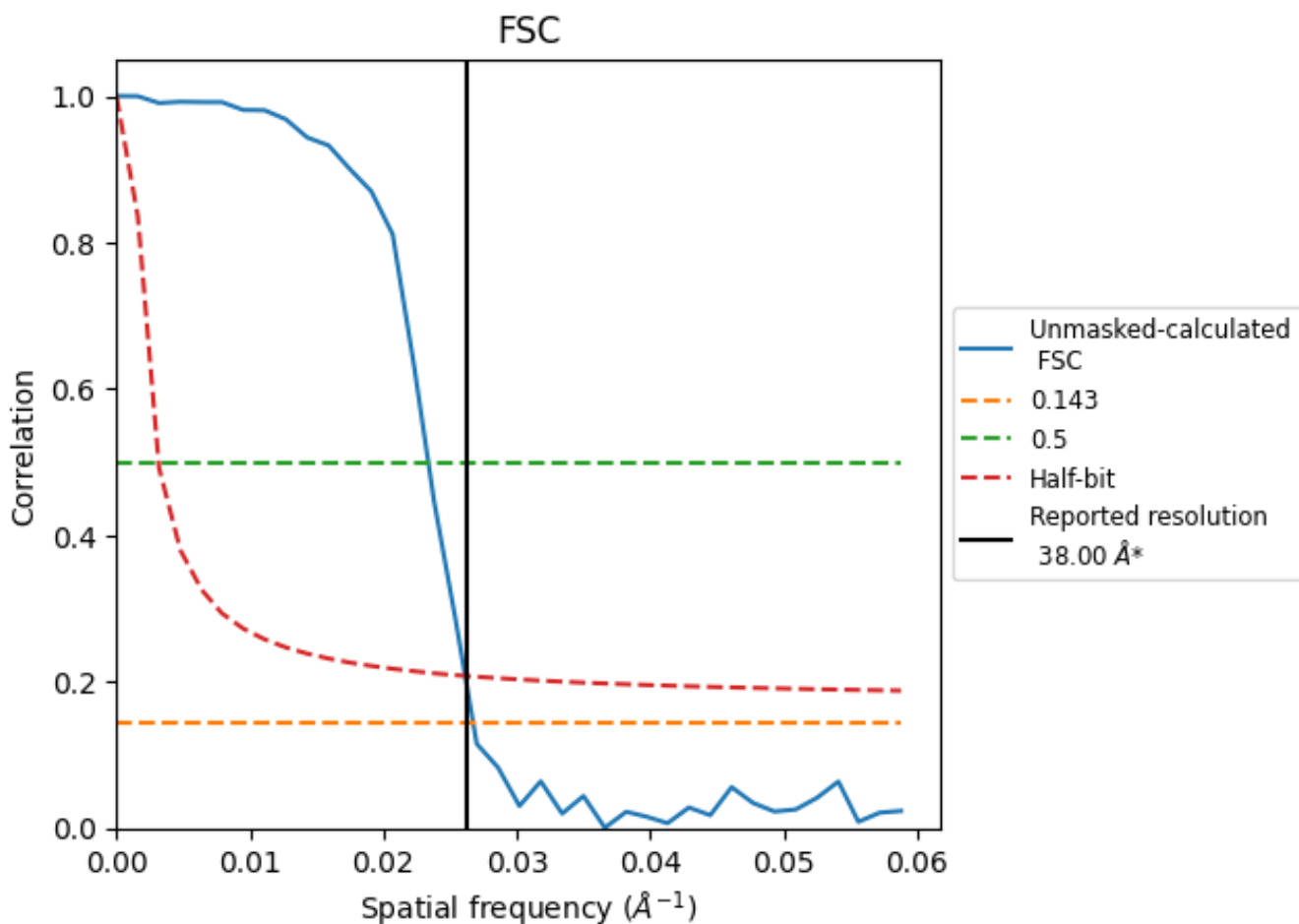


*Reported resolution corresponds to spatial frequency of 0.026 Å⁻¹

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 0.026 Å⁻¹

8.2 Resolution estimates [i](#)

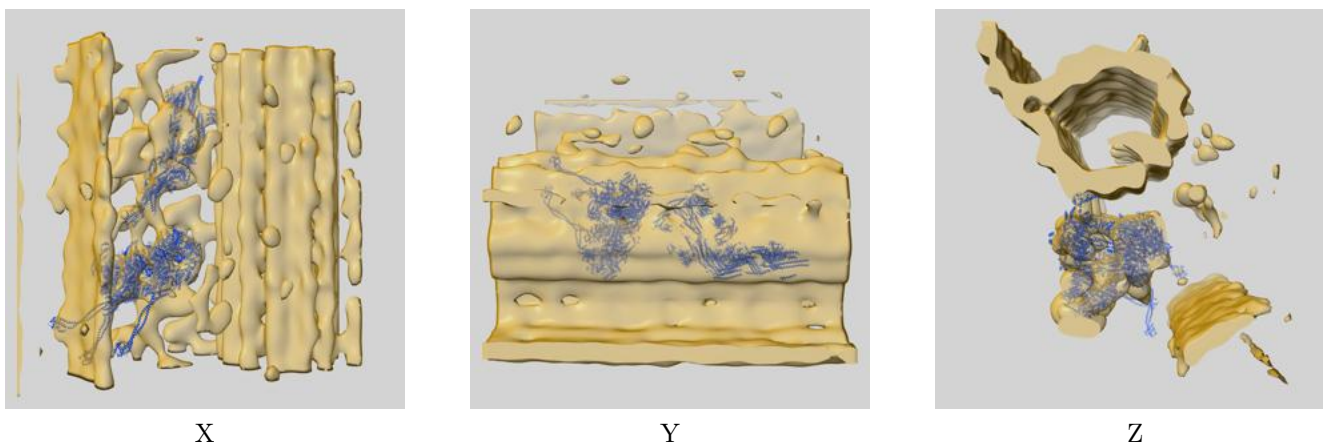
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	38.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	37.31	42.74	38.17

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

9 Map-model fit [i](#)

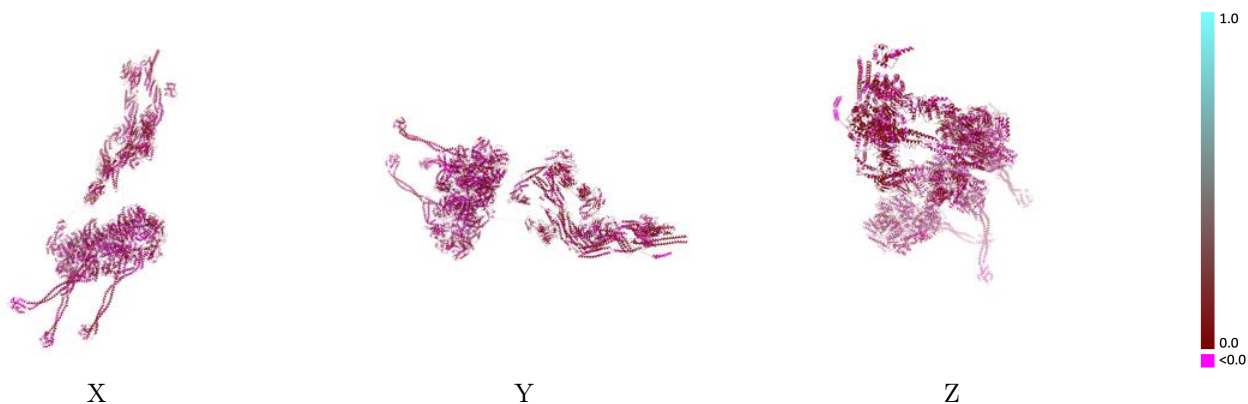
This section contains information regarding the fit between EMDB map EMD-16304 and PDB model 8BWY. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



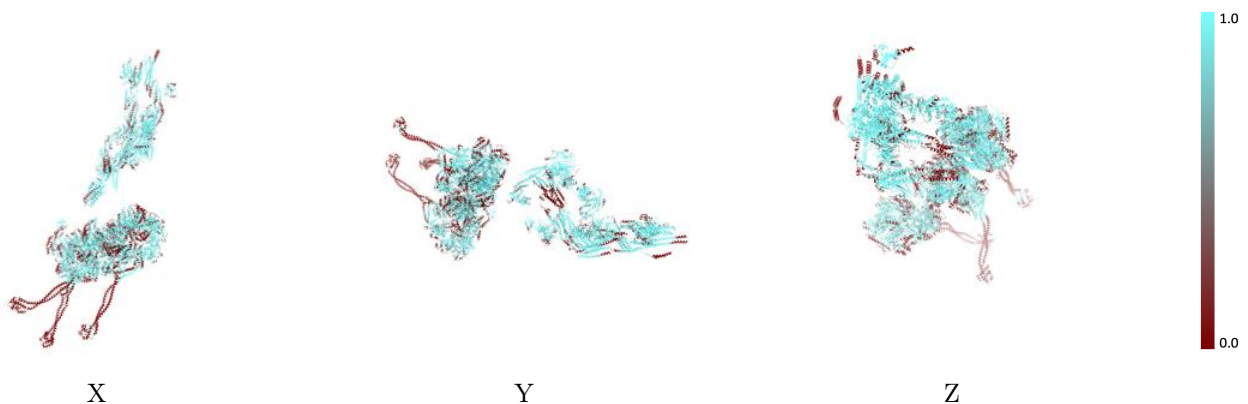
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



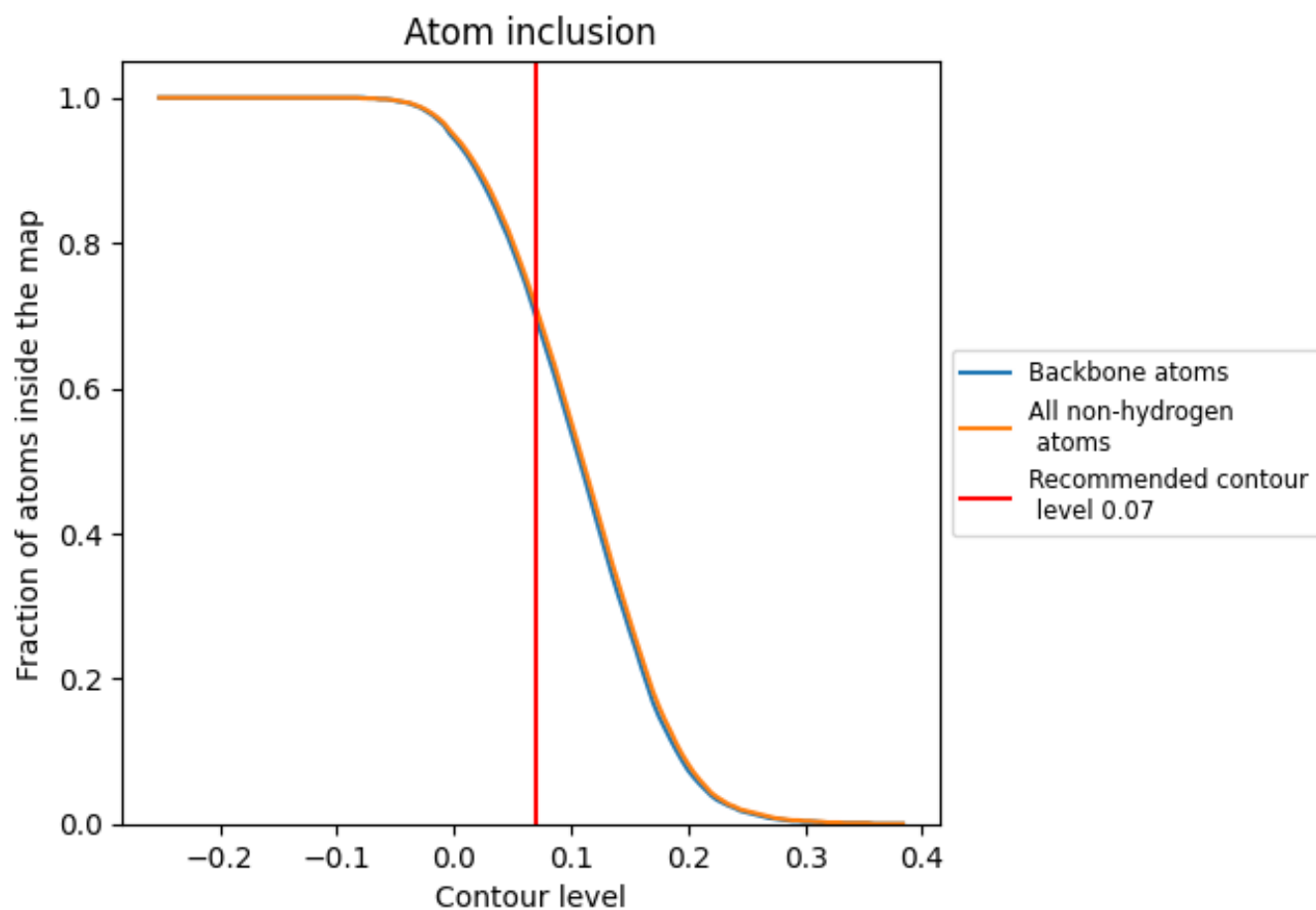
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.0390
A	 0.6750	 0.0370
B	 0.6630	 0.0380
C	 0.7000	 0.0390
F	 0.8470	 0.0450
G	 0.8310	 0.0380
H	 0.9050	 0.0530
I	 0.8240	 0.0560
J	 0.9210	 0.0690
K	 0.7370	 0.0400
L	 0.7260	 0.0150
M	 0.9820	 0.0700
N	 0.9300	 0.0450
O	 0.8320	 0.0260
P	 0.9330	 0.0590
T	 0.6940	 0.0350
V	 0.7880	 0.0600
d	 0.9190	 0.0420
e	 0.7580	 0.0260
x	 0.6910	 0.0510

