



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 03:47 PM UTC

PDB ID : 9BLY / pdb_00009bly
EMDB ID : EMD-44681
Title : Composite structure of full-length human dynein-1 in phi-particle conformation
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.50 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:

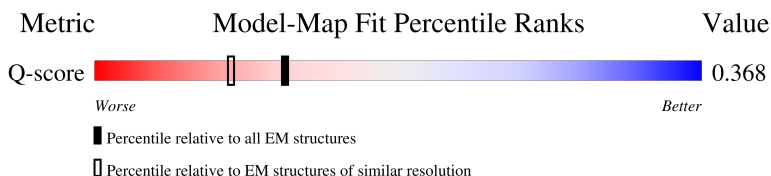
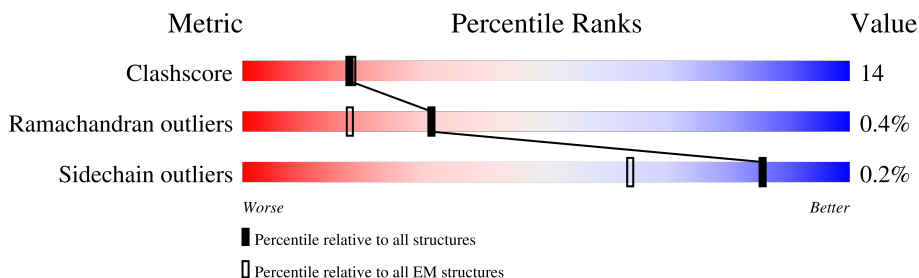
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	4646	<div> <div>5%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
1	B	4646	<div> <div>72%</div> <div>25%</div> <div>..</div> </div>
2	C	638	<div> <div>57%</div> <div>38%</div> </div>
2	D	638	<div> <div>35%</div> <div>27%</div> <div>38%</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	492	
3	F	492	
4	G	96	
4	H	96	
5	I	89	
5	J	89	
6	K	113	
6	L	113	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 89391 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4542	Total	C	N	O	S	0	0
			36692	23323	6381	6822	166		
1	B	4521	Total	C	N	O	S	0	0
			36527	23221	6349	6791	166		

- Molecule 2 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	394	Total	C	N	O	S	0	0
			3112	1962	541	594	15		
2	D	394	Total	C	N	O	S	0	0
			3112	1962	541	594	15		

- Molecule 3 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	311	Total	C	N	O	S	0	0
			2518	1614	425	468	11		
3	F	311	Total	C	N	O	S	0	0
			2518	1614	425	468	11		

- Molecule 4 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	93	Total	C	N	O	S	0	0
			742	468	128	143	3		
4	H	93	Total	C	N	O	S	0	0
			742	468	128	143	3		

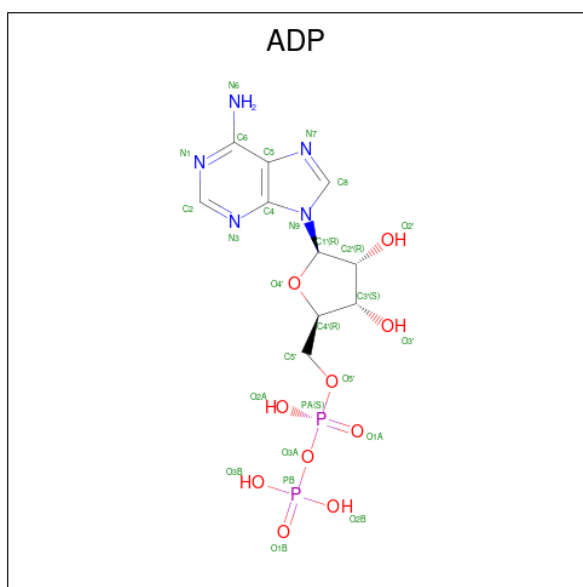
- Molecule 5 is a protein called Dynein light chain 1, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
5	J	89	Total	C	N	O	S	0	0
			728	465	122	135	6		

- Molecule 6 is a protein called Dynein light chain Tctex-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	113	Total	C	N	O	S	0	0
			872	548	142	175	7		
6	L	113	Total	C	N	O	S	0	0
			872	548	142	175	7		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



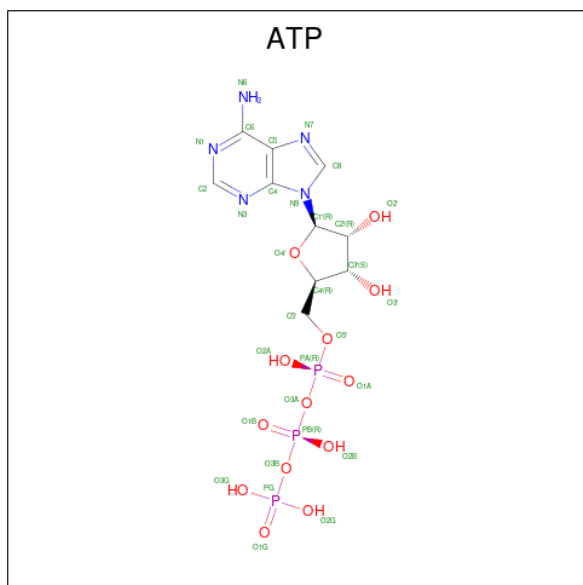
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

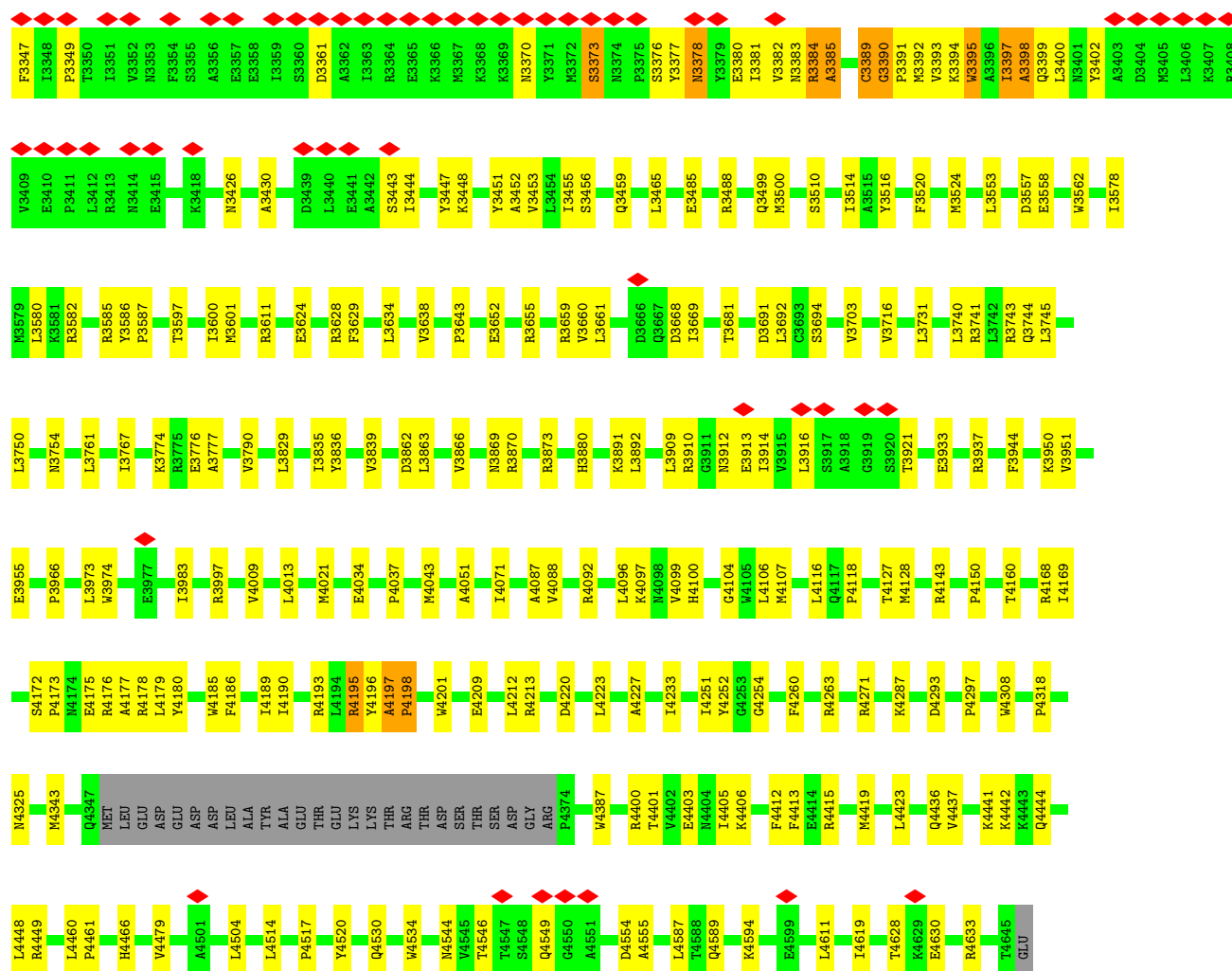


Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

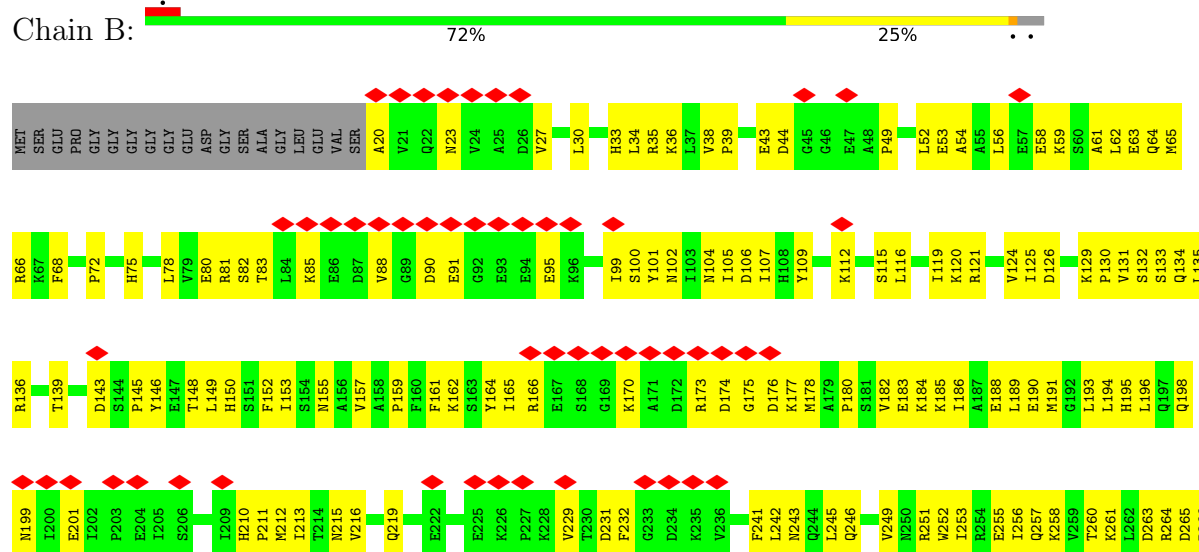
Mol	Chain	Residues	Atoms		AltConf
9	A	2	Total	Mg	0
			2	2	
9	B	2	Total	Mg	0
			2	2	

E3269	S3138	R2921	M2755	D2573	ASP	V2907	L2028	R1623	G1455	M1346	S1175
V3270	H3139	Q2930	L2756	R2576	GLU	L2208	L2032	S1624	E1456	K1347	L1176
I3271	R3140	Q2930	R2757	R2576	GLU	Y2211	L2032	S1625	M1457	E1348	K1177
A3272	I3143	I2961	M2773	L2581	GLU	T2214	R2037	F1629	L1459	Q1349	R1178
D3273	K2962	K2962	V2774	Y2582	ALA	R2039	S2038	F1631	I1466	P1350	K1179
K3274	V2963	V2963	E2775	P2590	ALA	L2039	L2039	G1632	R1467	W1351	I1180
Q3275	Q3152	D2973	F2776	L2591	S2410	Q2047	Q2047	V1633	V1478	V1352	K1181
M3276	T3153	E2974	F2784	L2592	L2413	G2224	P2225	G1633	I1487	Q1182	Q1182
S3277	L3154	D2975	T2788	L2593	L2422	P2226	S2226	E1635	R1488	E1184	F1183
V3278	A3157	V2979	Q2789	P2596	V2433	K2230	K2230	L1638	L1486	K1185	K1185
K3279	R3160	M2994	P2789	T2604	L2437	L2279	L2279	V1647	I1487	Y1187	Y1187
E3280	K3163	M2998	H2791	L2612	L2437	L2279	L2279	L1666	R1488	P1374	E1188
D3281	T3172	D3001	M2799	L2612	L2443	S2290	S2290	L1666	W1490	R1378	L1189
D3283	H3175	S3002	W2802	L2620	E2444	E2294	E2294	N1670	H1500	Q1387	R1196
K3284	H3182	R3007	W2803	W2621	H2445	L2295	L2295	K1568	K1508	R1388	L1196
V3285	H3182	R3008	R2804	E2629	L2446	L2295	L2295	Y1672	L1390	L1389	L1197
E3286	H3182	M3008	F2807	L2631	L2449	N2316	N2316	V1673	Y1512	K1391	E1198
V3289	Y3183	N3014	F2807	L2631	T2450	S2317	S2317	K1687	Y1513	G1392	K1199
I3290	A3184	N3014	R2811	L2632	R2451	V2318	V2318	T1683	F1516	Y1401	Q1200
E3291	L3194	V3017	W2825	K2633	L2452	L2319	L2319	E1393	W1523	E1402	I1201
A3292	T3211	L3020	D2835	Y2638	R2453	R2332	R2332	K1697	W1523	I1396	F1202
Q3293	E3217	M3030	D2835	L2659	S2457	F2343	F2343	I1698	K1526	M1399	Q1203
V3296	R3297	M3043	E2841	L2664	M2461	Q2346	Q2346	E1700	I1530	V1400	F1204
K3297	R3297	M3043	E2841	E2665	E2487	L2353	L2353	E1700	F1534	I1401	P1205
S3298	L3044	L3044	W2844	L2666	R2488	L2136	L2136	T1712	W1537	E1402	W1208
I3299	L3229	D3045	W2845	L2667	E2488	A2354	A2354	T1721	R1411	L1408	D1212
K3300	K3232	I3059	T2846	L2668	Q2491	T2355	T2355	V1724	H1412	W1413	N1213
K3301	K3232	I3059	T2846	L2668	R2492	V2356	V2356	K1729	R1411	E1413	I1214
R3308	K3236	F3066	L2850	V2687	T2498	C2389	C2389	Y1738	D1556	N1423	G1219
S3309	N3237	E3073	D2851	E2688	D2360	M2361	M2361	K1744	P1562	N1222	N1222
M3310	D3238	E3073	A2854	H2689	D2360	M2361	M2361	Y1745	Q1566	M1225	M1225
A3311	L3240	K3076	H2857	R2694	D2505	F2364	F2364	V1751	R1567	R1226	R1226
N3312	K3242	K3076	M2867	D2697	E2513	P2366	P2366	S1753	I1571	R1227	R1227
P3313	K3243	N3092	S2868	Q2698	D2536	E2389	E2389	F1575	F1575	K1228	D1229
P3314	Q3247	D3096	R2869	A2711	E2538	GLU	GLU	N1761	M1579	T1430	I1232
L3319	Q3248	W3097	L2882	C2712	E2538	ASP	ASP	G1771	G1432	G1431	Q1233
L3328	E3249	T3110	P2883	R2720	W2548	GLU	GLU	G1772	Q1433	Q1433	P1266
G3329	S3257	M3113	L2905	R2729	V2548	ALA	ALA	G1772	W1435	W1435	E1305
E3330	I3260	E3114	D2906	H2730	V2557	GLN	GLN	G1773	D1436	D1436	E1305
S3331	L3116	L3116	F2912	V2731	V2731	ARG	ARG	D1774	V1437	V1437	G1310
T3332	Q3263	K3117	N2913	P2732	V2562	ARG	ARG	V1781	K1441	K1441	W1340
T3333	Q3264	K3117	N2913	Y2738	A2563	LYS	LYS	L1792	A1444	A1444	V1452
D3334	H3265	Q3135	E2914	F2751	A2564	GLY	GLY				
W3335	H3265	Q3135	D2917		V2567	LYS	LYS				
K3336	Q3268	P3137				GLU	GLU				
Q3337											
I3338											
R3339											
I3342											
M3343											
R3344											
E3345											
N3346											



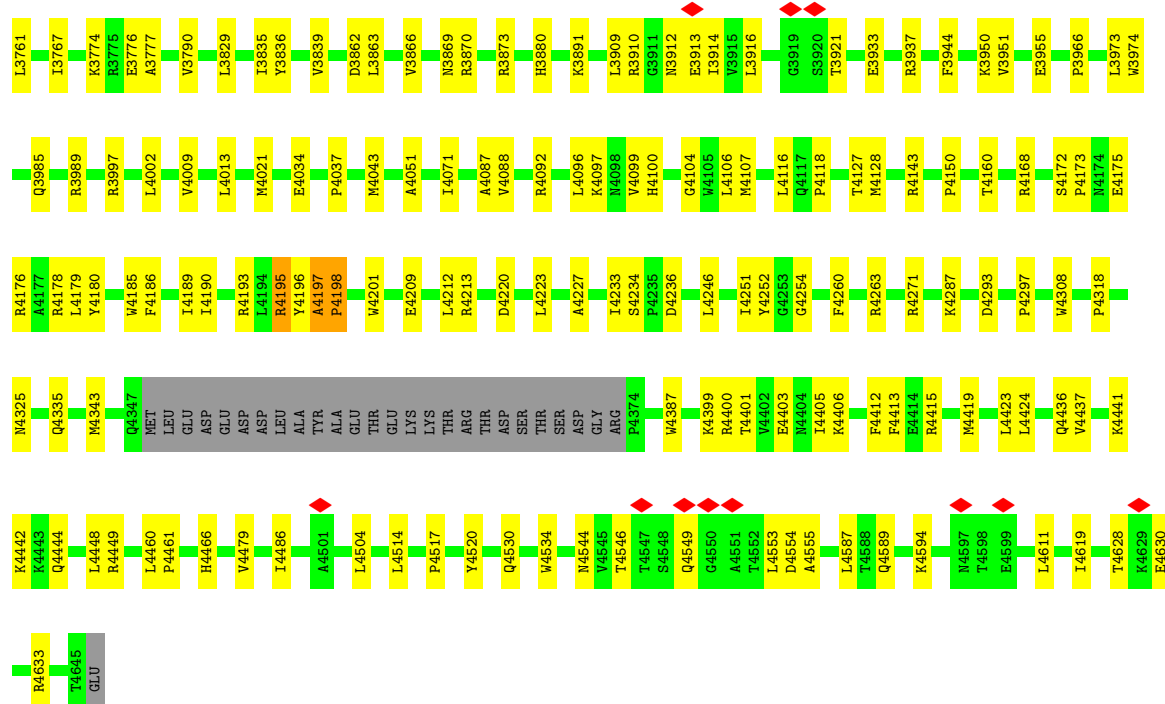
• Molecule 1: Cytoplasmic dynein 1 heavy chain 1

Chain B:



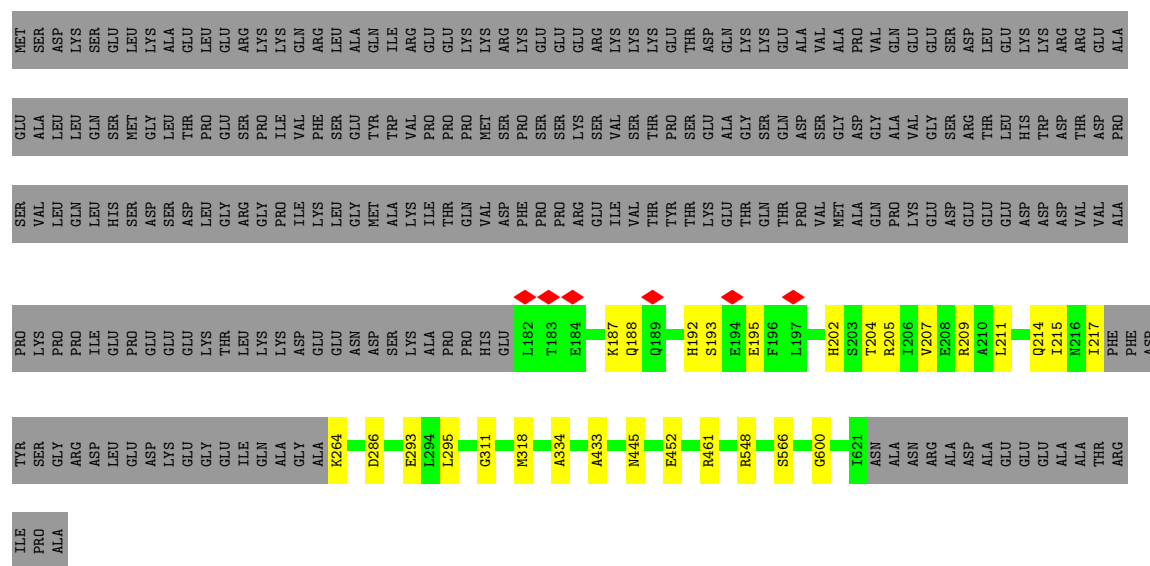
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E1305	Q1174	K1100	Q1019	VAL	E865	W782	W702	K613	S539	E408	E407	K337	G269
L1306	S1175	E1101	R1020	HIS	C867	E783	R704	D614	K540	F409	F409	D338	T270
G1310	L1176	F1102	L1023	LYS	M868	R786	Q707	L619	E541	E410	E274	P340	Q273
L1311	K1177	G1103	T1024	PRO	X869	R790	R716	K622	T543	F417	L341	E274	E274
L1312	R1178	P1104	T1025	GLY	D870	R793	I717	Y627	W546	M413	N342	F277	F277
W1340	I1180	V1106	M1026	GLU	T873	E793	F718	Y627	A549	V414	L344	L279	L279
E1348	K1181	I1107	G1029	P953	F874	R798	I719	Q631	R485	F417	L345	L280	L280
Q1349	Q1113	Q1113	L1033	K956	I877	I801	I720	A632	M550	Q421	T348	L281	L281
V1352	K1119	K1119	S1036	V959	R880	L804	E721	C633	R552	T422	E349	E282	E282
S1353	L1189	D1121	Y1037	H960	V881	W802	S722	M634	Y553	W423	L350	L285	L285
V1354	Y1190	E961	S1038	E961	Q882	V905	T723	S636	E555	D424	L351	Y286	Y286
R1357	H1124	H1124	A1039	E963	D887	G807	W725	R639	R556	D425	K352	R287	R287
R1388	K1125	K1125	V1040	E967	L888	L808	R726	D640	I557	E426	K353	T288	T288
L1389	E1126	E1126	M1041	Q967	N899	K809	G727	L641	V560	Y427	R354	Q289	Q289
L1390	Q1127	Q1127	G1042	V968	L890	K810	R728	P642	R563	L430	L357	E290	E290
L1391	L1128	L1128	I1043	P969	E811	E811	T729	G647	R563	Q431	I360	P295	P295
K1391	S1129	S1129	V1044	Y970	Y893	V812	G730	I648	R567	V432	F361	E296	E296
G1392	K1130	K1130	S1045	L971	S894	Q813	N731	I649	L568	L433	T362	V297	V297
Y1393	E1132	E1132	E1048	E977	W899	A817	L733	Q653	D570	L434	H363	L298	L298
M1394	Q1043	Q1043	Y1050	C978	Y899	E818	K734	I654	Q571	R435	L364	L299	L299
K1395	Y1050	Y1050	M1063	P987	K902	I820	L735	T659	L572	I437	K366	T300	T300
M1398	Q1058	Q1058	G1063	E985	L903	A821	V737	W659	K576	ASP	V438	L301	L301
L1399	C1069	C1069	Y1068	N986	I907	E822	N738	K663	N577	MET	K439	D302	D302
V1400	L1060	L1060	Y1069	F987	E908	W824	L740	R664	A578	LYS	R440	I303	I303
L1401	E1141	E1141	T1062	A988	E908	W824	L740	V665	N579	VAL	K441	I304	I304
E1402	S1207	S1207	L1072	W989	R914	K928	I743	E666	E580	ALA	R442	G307	G307
L1408	W1143	W1143	D1075	W989	L915	Q916	I744	D667	M581	GLU	E443	K308	K308
R1411	S1144	S1144	I1067	V982	Q916	A921	S747	V668	F582	VAL	E444	R309	R309
H1412	Q1145	Q1145	I1068	L993	Q916	Y832	E749	L669	I584	LEU	L446	F310	F310
W1413	I1211	I1211	Y1069	L994	A921	R835	W748	W673	A590	D516	W450	H311	H311
V1426	R1150	R1150	R1071	S995	Q924	E838	V750	N675	L591	A517	R451	A312	A312
S1427	L1153	L1153	L1072	P997	V925	E838	R751	H676	F592	N518	T452	T313	T313
E1428	L1156	L1156	D1075	P998	L926	N842	W755	V677	V593	A519	M453	V314	V314
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T1430	V1158	V1158	W1079	GLN	ALA	E845	G757	G679	E521	E522	L459	D319	D319
L1431	D1159	D1159	L1082	ARG	GLU	D848	R759	L682	I597	L525	Q460	T320	T320
D1436	T1160	T1160	Q1085	TVR	ASP	D849	V760	K683	G599	A526	G321	G321	G321
Q1440	S1162	S1162	I1086	GLN	LVS	L850	P761	F689	A600	Y527	L392	K323	K323
K1441	T1163	T1163	R1087	VAL	ALA	L851	I764	K692	I601	E528	L463	L326	L326
A1444	S1164	S1164	K1088	VAL	VAL	I853	V765	L693	E603	N529	D464	N330	N330
V1452	D1165	D1165	A1089	HIS	ASP	E854	Q770	N694	Y604	V530	M466	D331	D331
G1455	L1167	L1167	R1090	TVR	MET	E855	Q770	E897	Q605	E532	K468	Y332	Y332
E1456	A1166	A1166	R1090	ASP	ASP	E860	Q773	I698	L608	V533	R470	N333	N333
M1457	T1168	T1168	F1083	GLU	THR	V861	L774	P699	I609	D534	H403	P334	P334
	F1169	F1169	D1094	LEU	ALA	R862	I779		Q610	G535	V404		
	Q1233	Q1233		E1014									

R3585	E3415	N3353	Q3275	V3148	F2776	P2596	L2422	S2226	K3060	K1865	E1635	L1458
L3588	K3418	F3354	M3276	Q3152	F2784	T2604	V2433	R2230	T2061	K1878	L1638	L1459
T3597	N3426	S3355	S3277	T3153	T2788	L2612	L2437	L2279	I2069	L1879	V1647	R1467
L3600	A3430	A3356	V3278	L3154	P2790	L2620	L2443	S2290	Q2079	R1887	L1666	I1487
M3601	A3430	E3357	D3281	A3157	H2791	N2621	E2444	E2294	L2080	A1895	N1670	V1490
R3611	D3439	E3358	L3282	R3160	Y2792	E2629	H2446	L2295	R2091	R1899	S1671	H1500
E3624	D3440	S3360	L3283	K3163	M2799	L2630	L2450	N2316	K2104	A1908	V1672	K1508
R3628	E3441	A3362	K3284	T3172	V2802	L2631	T2450	S2317	R2107	E1914	V1673	
F3629	A3442	I3363	V3285	H3175	V2803	L2632	R2451	V2318				
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L3634	E3365	E3366	V3289	H3182	F2807	Y2638	S2457	R2332	E2120	V1929	K1687	Y1512
V3638	I3290	Y3183	I3290	Y3183	R2811	T2644		F2343	F1930	T1693	T1693	Y1513
P3643	M3367	A3184	E3291	A3184	W2825	G2647	M2461	Q2346	N1931	K1697	K1697	F1516
R3651	K3368	L3194	A3292	L3194	W2835	L2659	E2487	Q2346	D1937	N1699	N1699	W1593
E3652	K3369	T3211	Q3293	T3211	D2835	L2659	R2488	L2353	D1958	E1700	E1700	K1526
R3655	N3370	E3217	V3296	E3217	E2841	D2664	Q2491	A2354	E1959	T1712	T1712	I1530
R3659	Y3371	R3220	K3297	R3220	R2844	E2665	R2492	T2355	R1962	V1721	V1721	F1584
V3660	P3375	L3229	I3299	L3229	W2845	N2667	I2498	C2359	E1965	V1724	V1724	W1537
L3661	S3376	K3300	K3300	K3300	T2846	L2668	D2505	Q2360	R1966	K1729	K1729	R1543
E3685	Y3377	K3301	K3301	K3301	I2850	V2687	M2510	M2361	E1967			
D3666	N3378	R3308	R3308	A3236	D2851	H2688	R2513	F2364	E1980	Y1738	Y1738	D1566
Q3667	Y3379	S3309	S3309	N3237	A2854	H2689	E2513	P2386	R1983	K1744	K1744	E1564
L3668	K3380	M3310	M3310	D3238	R2857	R2694	D2536	L2157	E1984	Y1745	Y1745	R1567
I3669	I3381	K3239	K3239	K3239	M2867	Q2698	E2538	L2161	V1751	V1751	V1751	I1571
T3681	V3382	L3240	A3311	L3240	S2868	Q2698	W2548	D2163	L1752	L1752	L1752	F1575
D3691	N3383	K3241	P3312	K3241	R2869	A2711	V2567	V2164	S1753	S1753	S1753	
L3692	R3384	M3243	P3313	M3243	T2882	C2712	V2567	F2165	M1761	M1761	M1761	
C3693	A3385	Q3247	P3314	Q3247	I2882	R2720	V2567	E2174	G1771	G1771	G1771	
S3694	C3389	Q3248	L3319	Q3248	P2883	R2720	V2567	M2175	G1772	G1772	G1772	
V3703	G3390	E3249	G3328	E3249	L2905	R2720	V2567	T2176	G1773	G1773	G1773	
M3524	M3392	S3257	G3329	S3257	D2906	H2730	A2564	R2179	D1774	D1774	D1774	
L3553	K3394	E3330	E3330	E3330	V2912	V2731	V2567	L2195	V1781	V1781	V1781	
D3557	W3395	S3331	S3331	I3260	N2913	P2732	V2567	D2195	S2026	S2026	S2026	
E3558	A3396	T3332	T3332	Q3263	Q2914	Y2738	D2573	GLY	N2027	N2027	N2027	
W3562	I3397	D3334	D3334	L3264	E2914	F2751	R2576	GLU	L2028	L2028	L2028	
L3740	Q3399	K3334	K3334	H3285	D2917	F2751	R2576	GLY	L2032	L2032	L2032	
L3742	L3400	W3335	W3335	Q3268	R2921	M2755	L2581	GLU	R2037	R2037	R2037	
R3743	R3401	K3336	K3336	E3289	R2921	L2756	Y2582	GLU	S2038	S2038	S2038	
Q3744	Y3402	I3337	I3337	E3289	Q2930	R2757	P2590	ALA	L2039	L2039	L2039	
L3745	A3403	K3338	K3338	I3271	Q2930	M2773	L2591	S2410	Q2047	Q2047	Q2047	
L3750	D3404	V3270	V3270	I3271	T2961	V2774	V2592		F2059	F2059	F2059	
N3754	N3405	R3339	R3339	A3272	K2962	E2775	L2593					
	L3406	I3342	I3342	D3273	V2963							
	K3407	M3343	M3343	K3274								
	R3408	R3344	R3344									
	V3409	E3345	E3345									
	E3410	N3346	N3346									
	P3411	F3347	F3347									
	L3412	I3348	I3348									
	R3413	P3349	P3349									
	N3414	T3350	T3350									
		I3351	I3351									
		V3352	V3352									



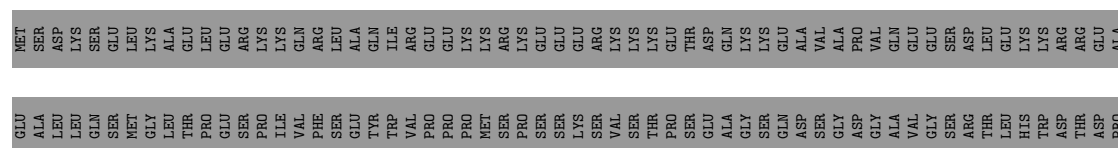
• Molecule 2: Cytoplasmic dynein 1 intermediate chain 2

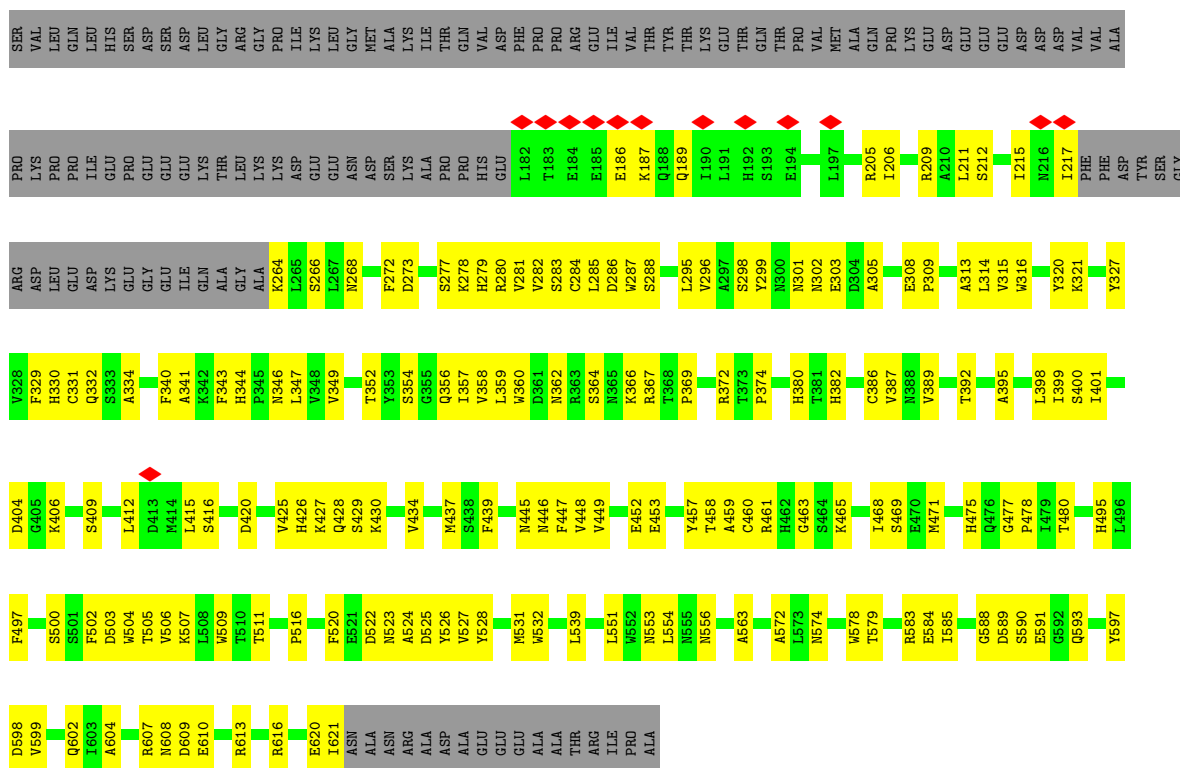
Chain C: 57% 38%



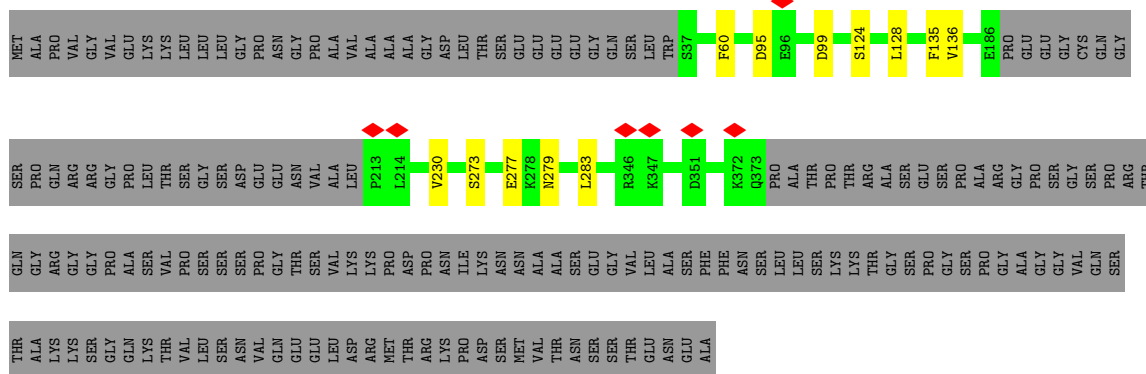
• Molecule 2: Cytoplasmic dynein 1 intermediate chain 2

Chain D: 35% 27% 38%

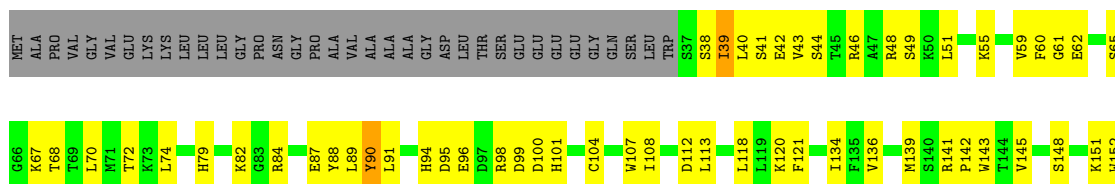


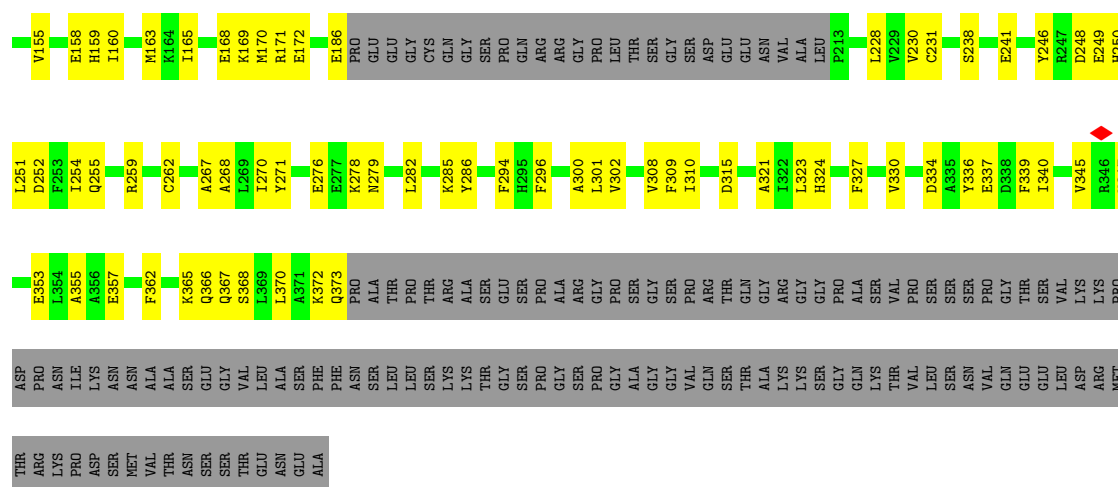


- Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2

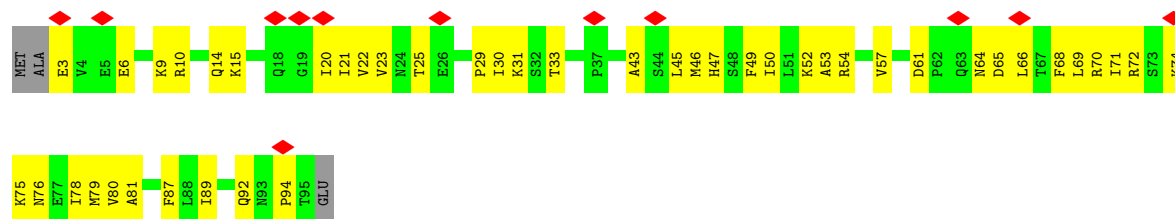


- Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2

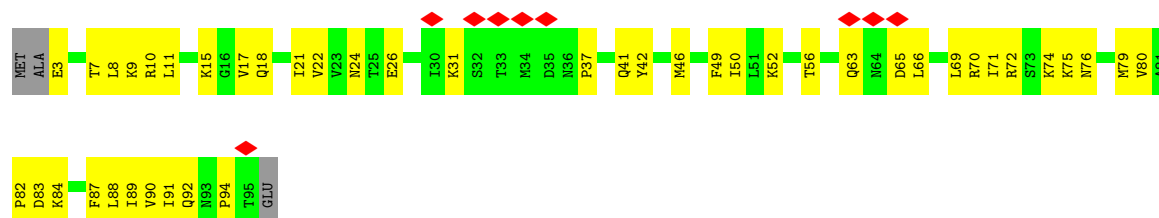




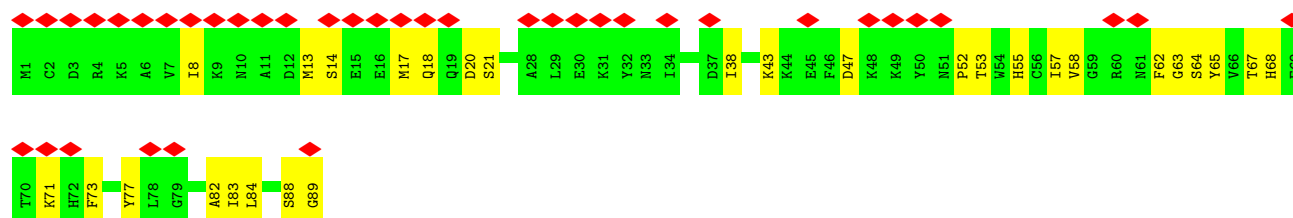
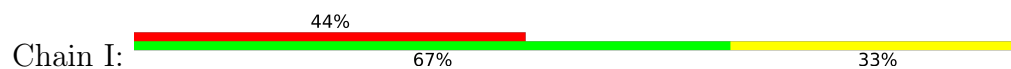
• Molecule 4: Dynein light chain roadblock-type 1



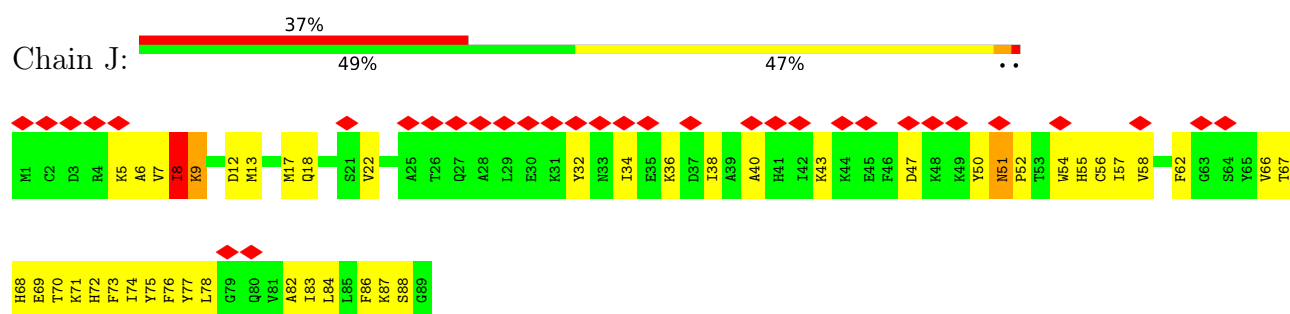
• Molecule 4: Dynein light chain roadblock-type 1



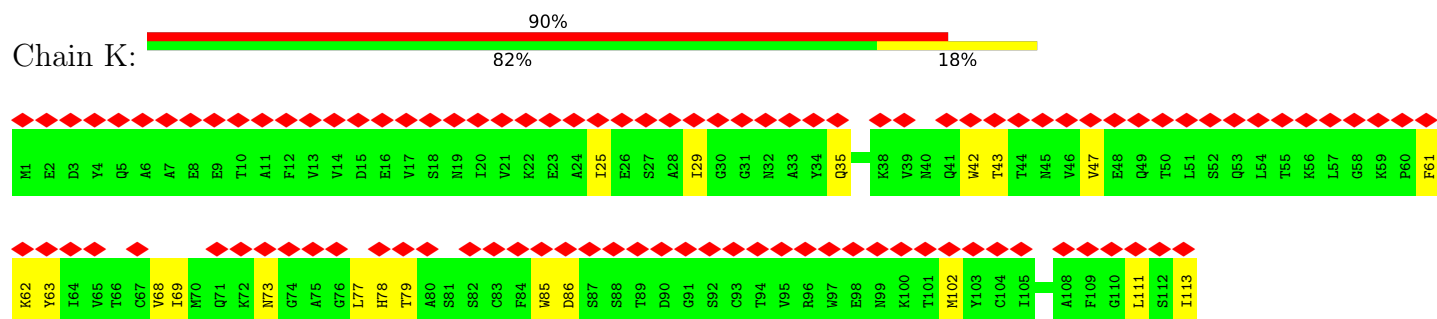
• Molecule 5: Dynein light chain 1, cytoplasmic



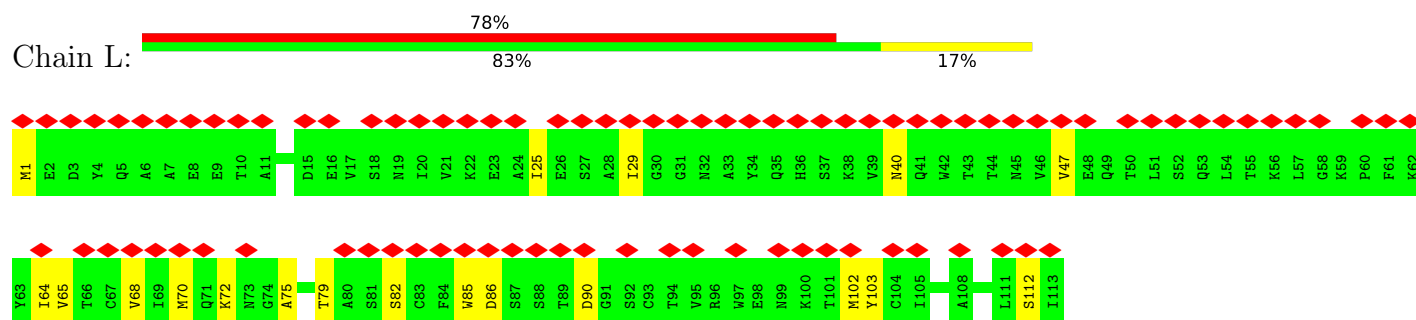
• Molecule 5: Dynein light chain 1, cytoplasmic



- Molecule 6: Dynein light chain Tctex-type 1



- Molecule 6: Dynein light chain Tctex-type 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57816	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.250	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	851.968, 851.968, 851.968	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.664, 1.664, 1.664	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: ATP, ADP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	1/37420 (0.0%)	0.53	15/50628 (0.0%)
1	B	0.31	1/37249 (0.0%)	0.52	12/50395 (0.0%)
2	C	0.32	0/3195	0.45	0/4351
2	D	0.29	0/3195	0.45	0/4351
3	E	0.28	0/2573	0.40	0/3473
3	F	0.27	0/2573	0.41	0/3473
4	G	0.17	0/752	0.36	0/1017
4	H	0.18	0/752	0.41	0/1017
5	I	0.16	0/744	0.43	0/997
5	J	0.34	0/744	0.56	0/997
6	K	0.12	0/888	0.33	0/1203
6	L	0.13	0/888	0.35	0/1203
All	All	0.30	2/90973 (0.0%)	0.51	27/123105 (0.0%)

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	7
1	B	0	6
3	F	0	1
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3242	LYS	C-O	-6.03	1.16	1.24
1	B	3242	LYS	C-O	-6.03	1.16	1.24

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1352	VAL	N-CA-C	-10.62	103.01	113.20
1	B	3242	LYS	O-C-N	-9.93	110.61	122.22
1	A	3242	LYS	O-C-N	-9.92	110.62	122.22
1	A	3361	ASP	CA-CB-CG	-9.67	102.93	112.60
1	B	3361	ASP	CA-CB-CG	-9.66	102.94	112.60

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1076	LEU	Peptide
1	A	1388	ARG	Sidechain
1	A	2453	ARG	Sidechain
1	A	2729	ARG	Sidechain
1	A	3242	LYS	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	36692	0	36960	767	0
1	B	36527	0	36807	1072	0
2	C	3112	0	2964	20	0
2	D	3112	0	2964	152	0
3	E	2518	0	2525	6	0
3	F	2518	0	2525	116	0
4	G	742	0	768	48	0
4	H	742	0	768	41	0
5	I	728	0	714	28	0
5	J	728	0	714	56	0
6	K	872	0	846	17	0
6	L	872	0	846	18	0
7	A	81	0	36	3	0
7	B	81	0	36	3	0
8	A	31	0	12	3	0
8	B	31	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	2	0	0	0	0
9	B	2	0	0	0	0
All	All	89391	0	89497	2178	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 14.

The worst 5 of 2178 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)
1:B:3381:ILE:CG2	1:B:3390:GLY:HA2	1.30	1.58
1:A:3381:ILE:CG2	1:A:3390:GLY:HA2	1.30	1.57
1:B:3381:ILE:CG2	1:B:3390:GLY:CA	1.94	1.46
1:A:3381:ILE:HG21	1:A:3390:GLY:CA	1.49	1.42
1:A:3381:ILE:CG2	1:A:3390:GLY:CA	1.94	1.41

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	4532/4646 (98%)	4352 (96%)	163 (4%)	17 (0%)	30	62
1	B	4509/4646 (97%)	4356 (97%)	132 (3%)	21 (0%)	24	57
2	C	390/638 (61%)	354 (91%)	36 (9%)	0	100	100
2	D	390/638 (61%)	359 (92%)	31 (8%)	0	100	100
3	E	307/492 (62%)	287 (94%)	20 (6%)	0	100	100
3	F	307/492 (62%)	286 (93%)	19 (6%)	2 (1%)	18	51
4	G	91/96 (95%)	84 (92%)	7 (8%)	0	100	100
4	H	91/96 (95%)	83 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
5	J	87/89 (98%)	80 (92%)	4 (5%)	3 (3%)	3	23
6	K	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
6	L	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
All	All	11013/12148 (91%)	10541 (96%)	429 (4%)	43 (0%)	31	62

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	589	ASN
1	A	1400	VAL
1	A	1401	ILE
1	A	3384	ARG
1	B	540	LYS

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	4044/4125 (98%)	4034 (100%)	10 (0%)	87	85
1	B	4028/4125 (98%)	4015 (100%)	13 (0%)	86	83
2	C	344/557 (62%)	344 (100%)	0	100	100
2	D	344/557 (62%)	344 (100%)	0	100	100
3	E	279/422 (66%)	279 (100%)	0	100	100
3	F	279/422 (66%)	279 (100%)	0	100	100
4	G	87/89 (98%)	87 (100%)	0	100	100
4	H	87/89 (98%)	87 (100%)	0	100	100
5	I	78/78 (100%)	78 (100%)	0	100	100
5	J	78/78 (100%)	77 (99%)	1 (1%)	61	72
6	K	97/97 (100%)	97 (100%)	0	100	100
6	L	97/97 (100%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9842/10736 (92%)	9818 (100%)	24 (0%)	85 85

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1354	VAL
1	B	1452	VAL
1	B	1395	LYS
1	B	2729	ARG
1	A	3373	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 122 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	607	GLN
1	B	4532	ASN
1	B	1855	GLN
1	B	4453	ASN
3	F	159	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	ADP	A	4703	-	28,29,29	0.47	0	43,45,45	0.47	0
7	ADP	A	4704	-	28,29,29	0.46	0	43,45,45	0.47	0
7	ADP	B	4704	-	28,29,29	0.46	0	43,45,45	0.47	0
8	ATP	B	4702	9	32,33,33	0.55	0	48,52,52	0.58	0
7	ADP	B	4703	-	28,29,29	0.47	0	43,45,45	0.47	0
8	ATP	A	4702	9	32,33,33	0.55	0	48,52,52	0.58	0
7	ADP	A	4701	9	28,29,29	0.46	0	43,45,45	0.49	0
7	ADP	B	4701	9	28,29,29	0.45	0	43,45,45	0.50	0

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
7	ADP	A	4703	-	-	0/16/32/32	0/3/3/3
7	ADP	A	4704	-	-	2/16/32/32	0/3/3/3
7	ADP	B	4704	-	-	2/16/32/32	0/3/3/3
8	ATP	B	4702	9	-	2/22/38/38	0/3/3/3
7	ADP	B	4703	-	-	0/16/32/32	0/3/3/3
8	ATP	A	4702	9	-	2/22/38/38	0/3/3/3
7	ADP	A	4701	9	-	0/16/32/32	0/3/3/3
7	ADP	B	4701	9	-	0/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

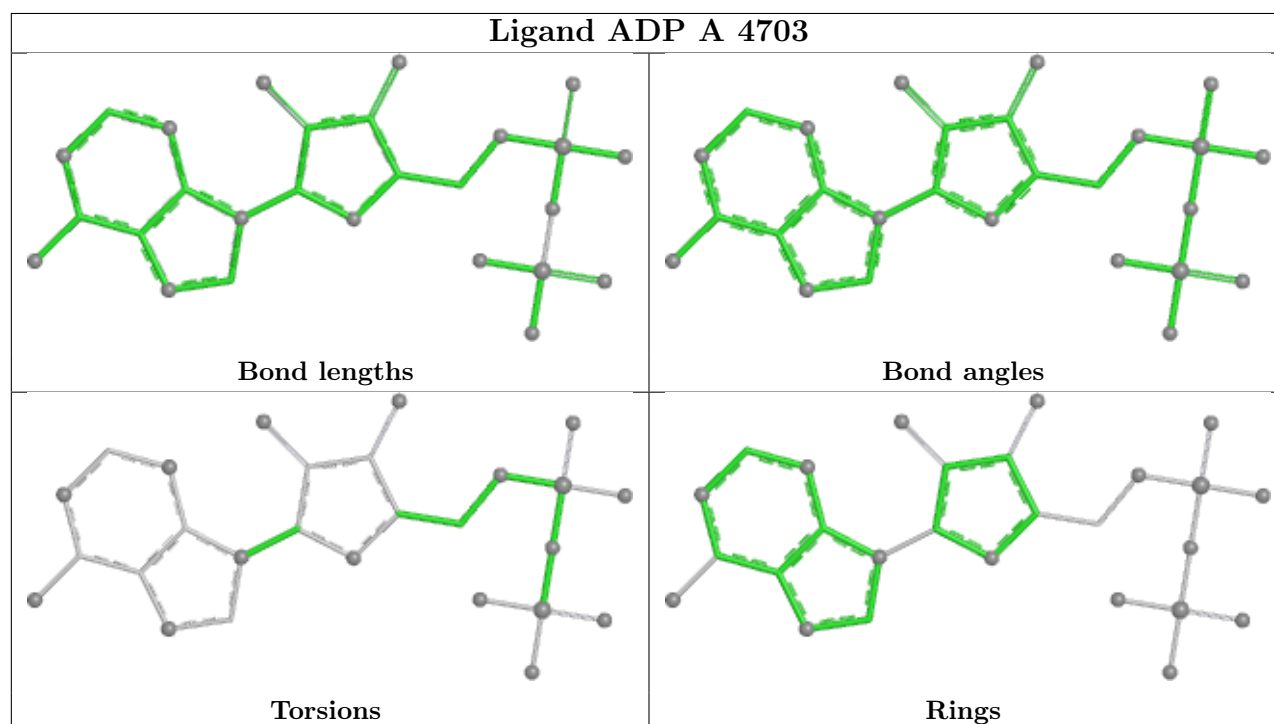
Mol	Chain	Res	Type	Atoms
7	A	4704	ADP	PA-O3A-PB-O2B
7	B	4704	ADP	PA-O3A-PB-O2B
8	A	4702	ATP	O4'-C4'-C5'-O5'
8	B	4702	ATP	O4'-C4'-C5'-O5'
7	A	4704	ADP	PA-O3A-PB-O1B

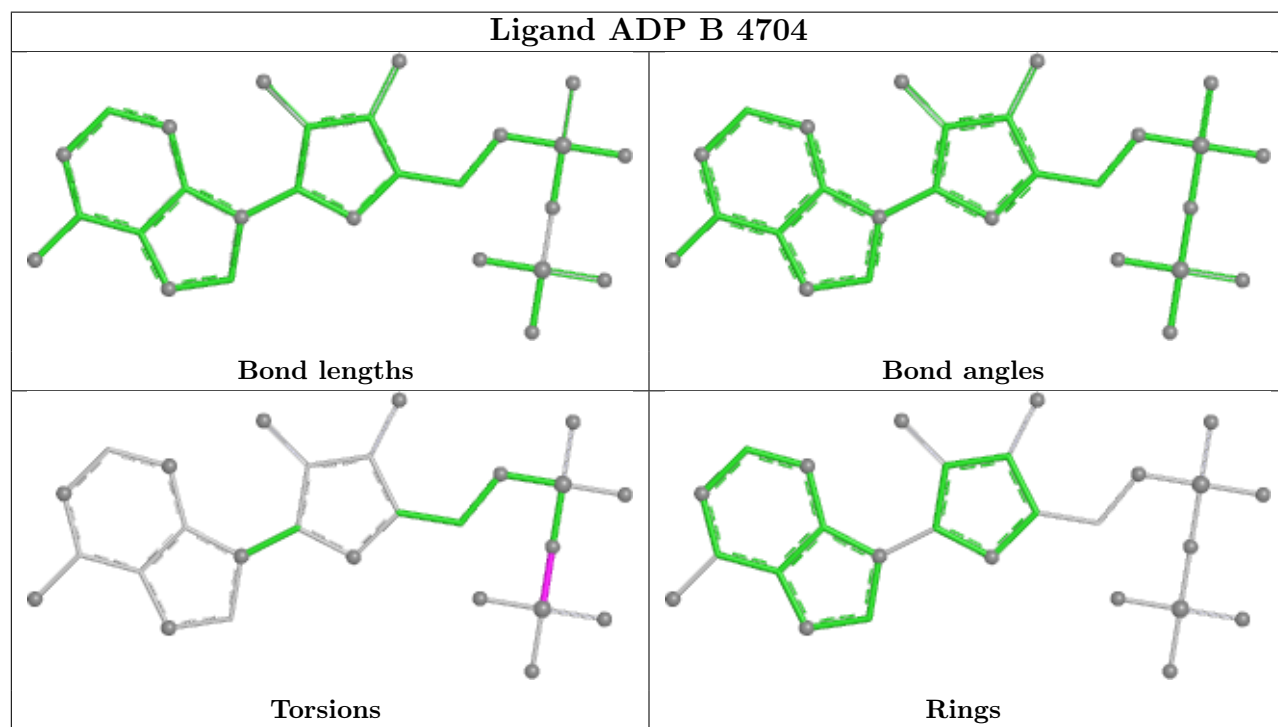
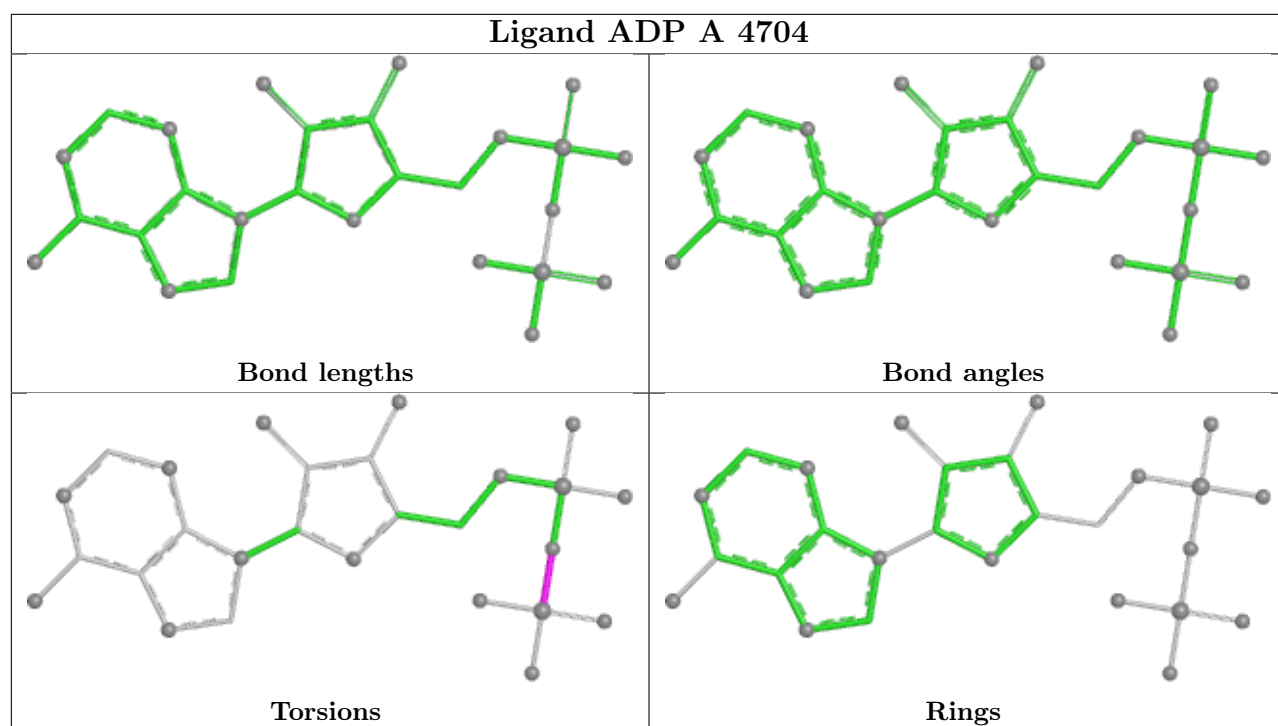
There are no ring outliers.

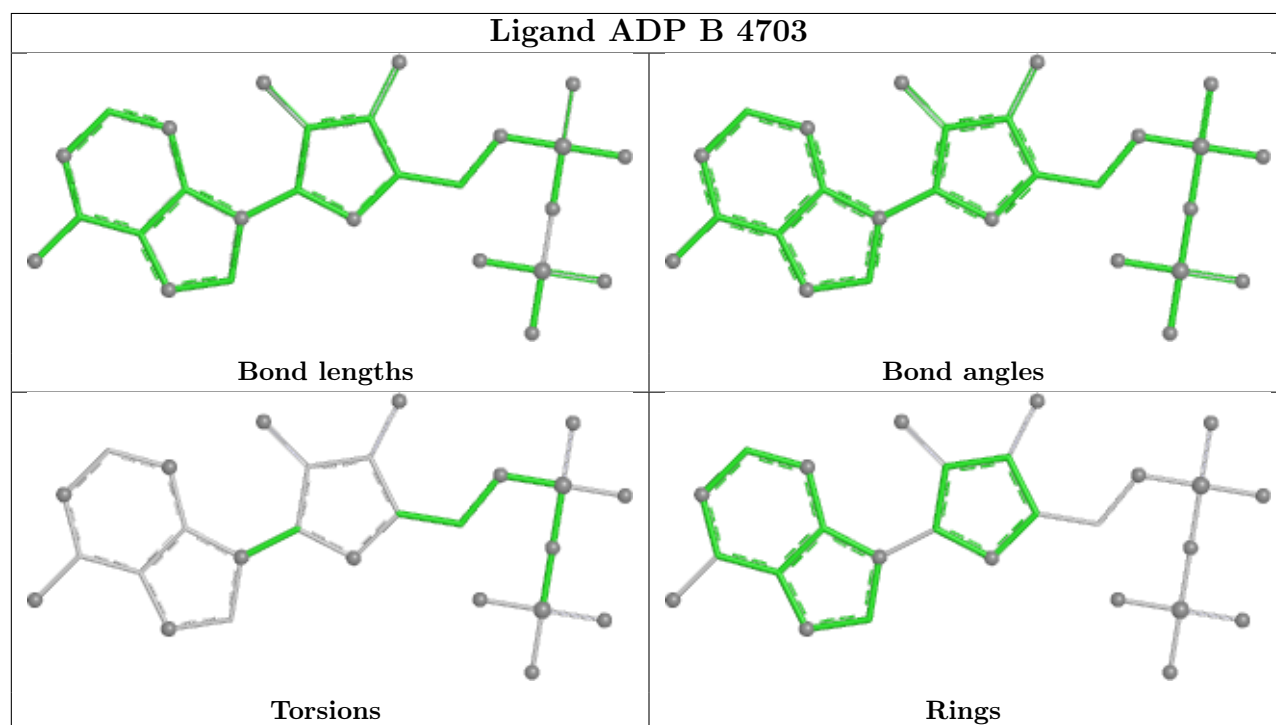
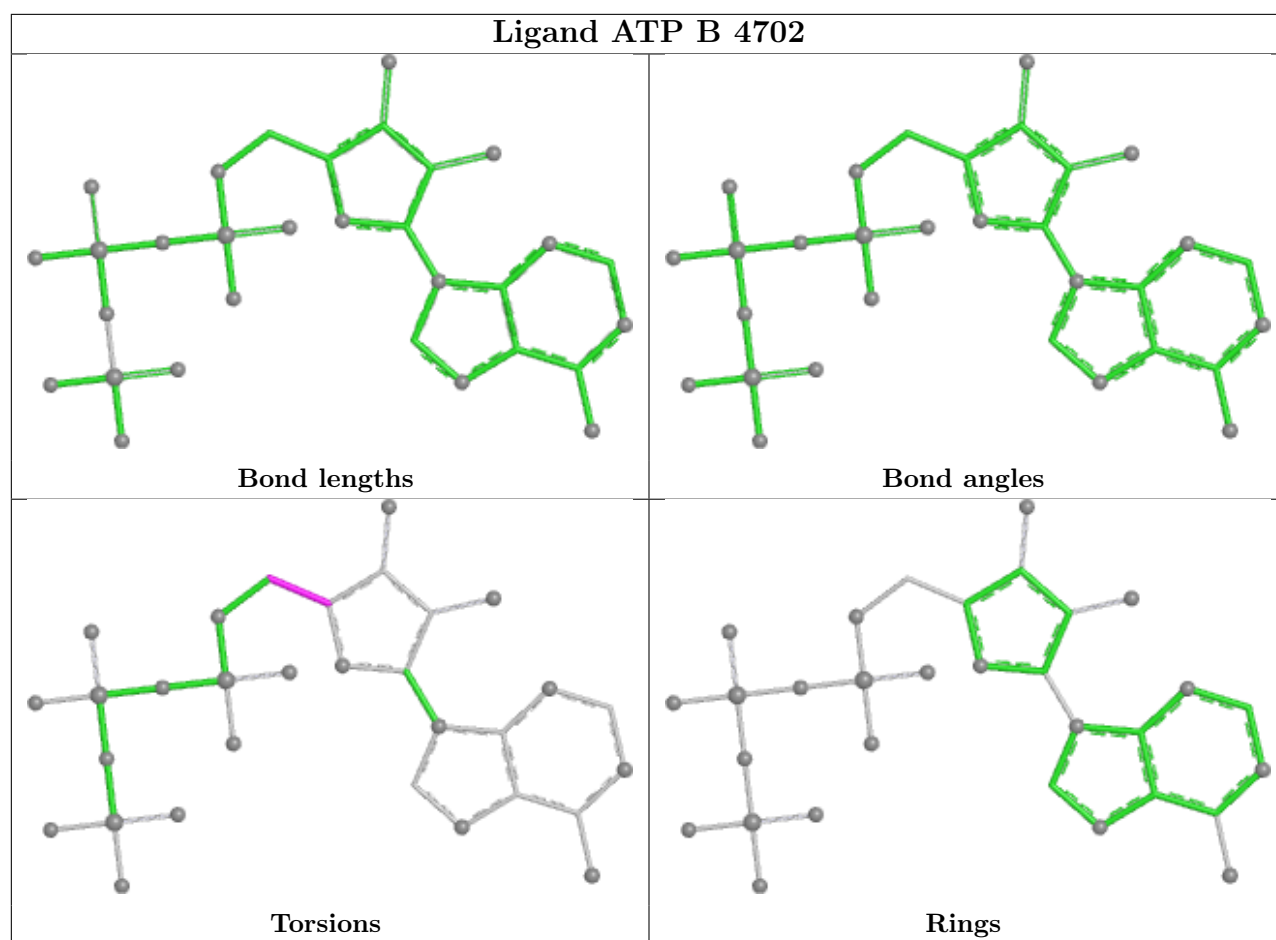
4 monomers are involved in 12 short contacts:

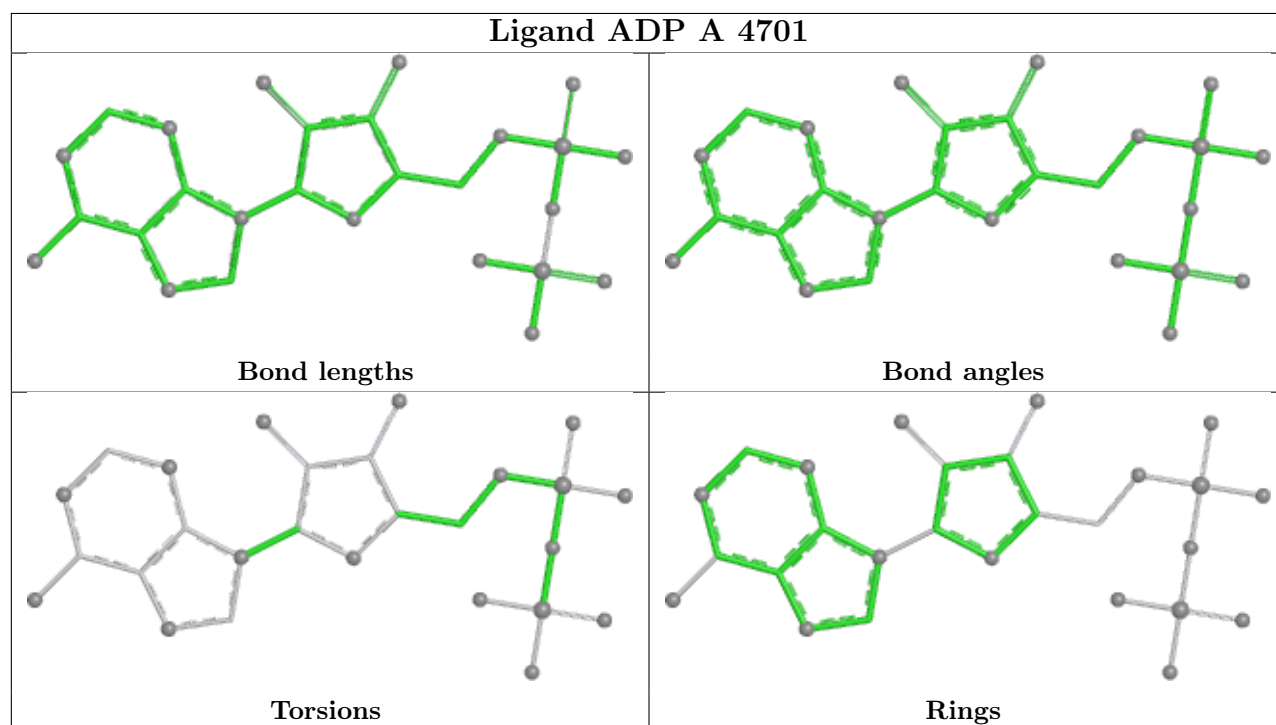
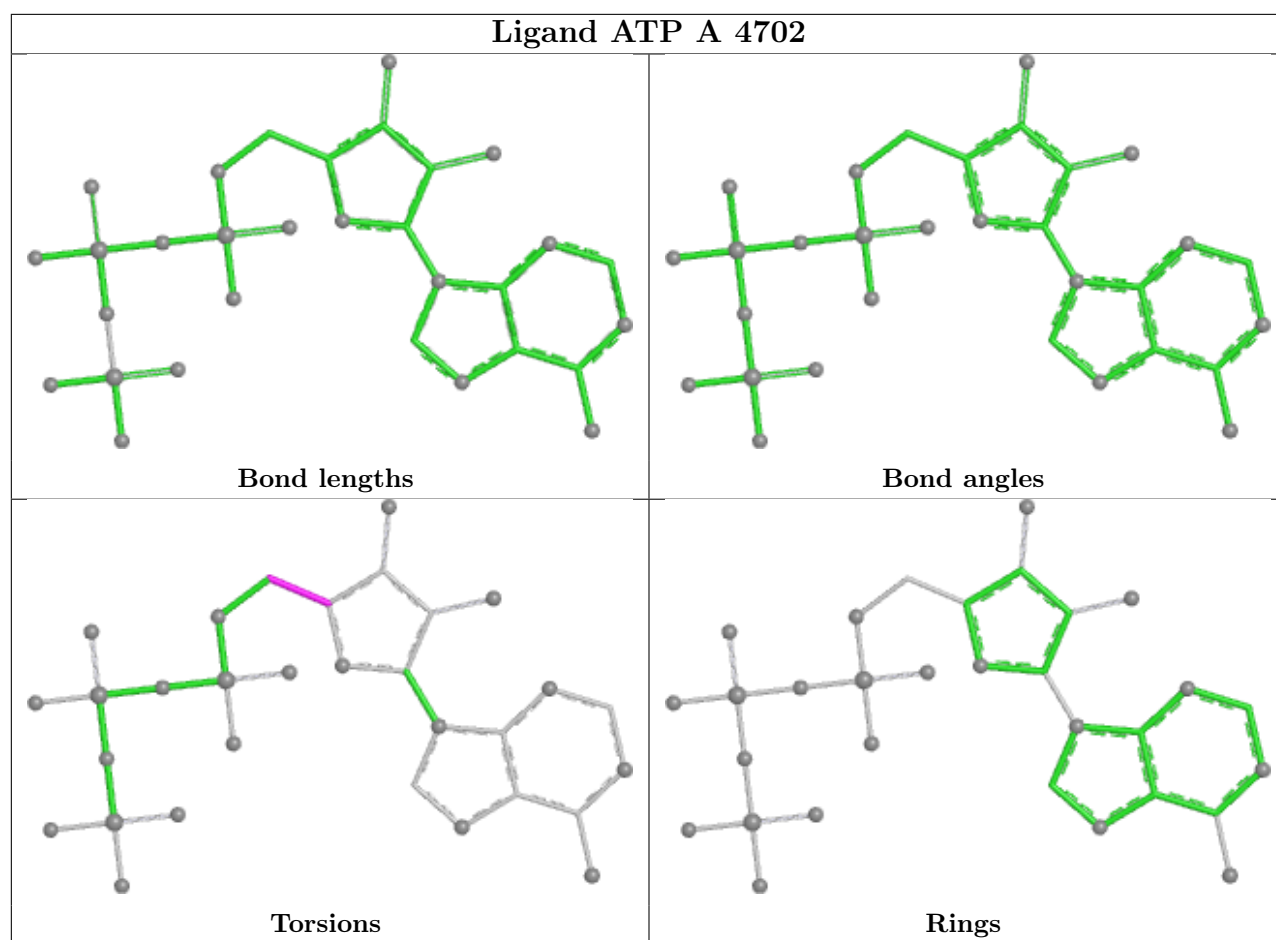
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	4702	ATP	3	0
8	A	4702	ATP	3	0
7	A	4701	ADP	3	0
7	B	4701	ADP	3	0

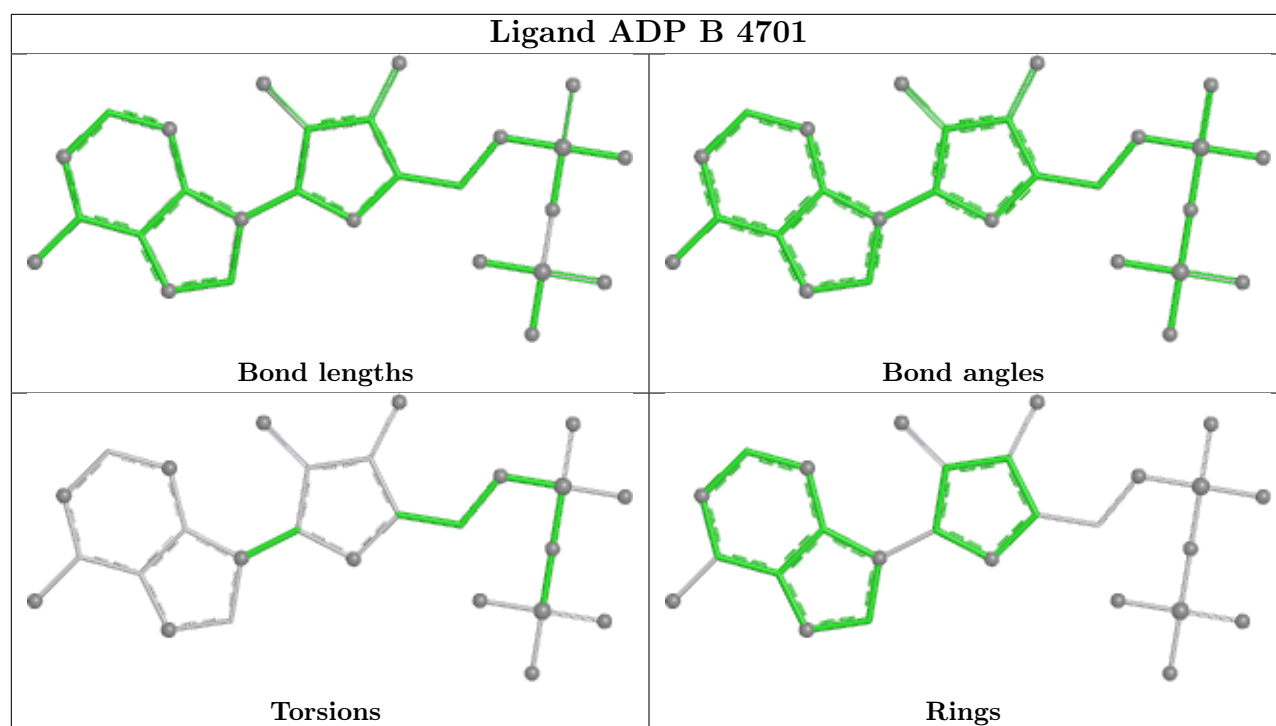
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

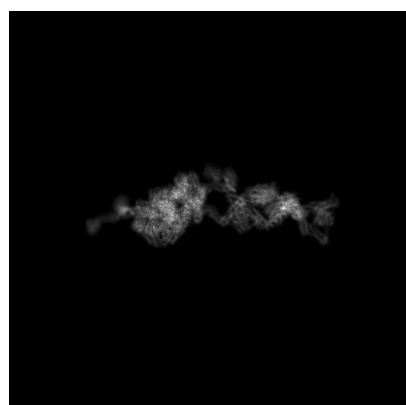
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44681. These allow visual inspection of the internal detail of the map and identification of artifacts.

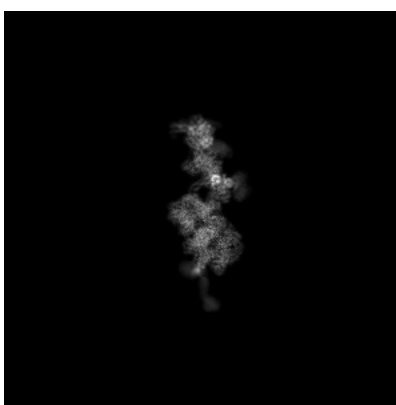
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

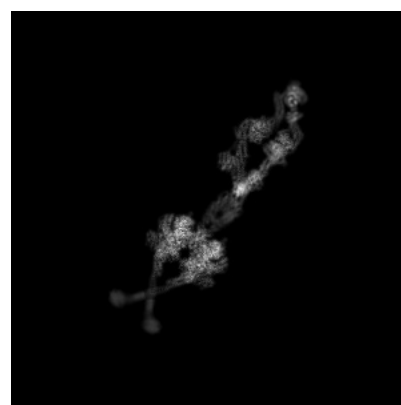
6.1.1 Primary map



X



Y



Z

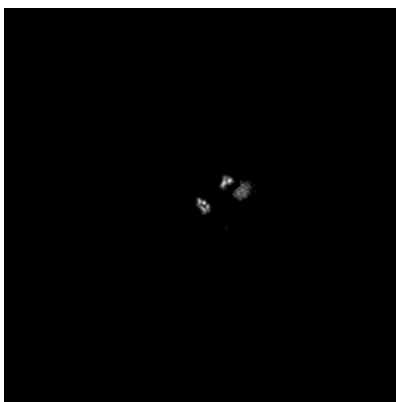
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

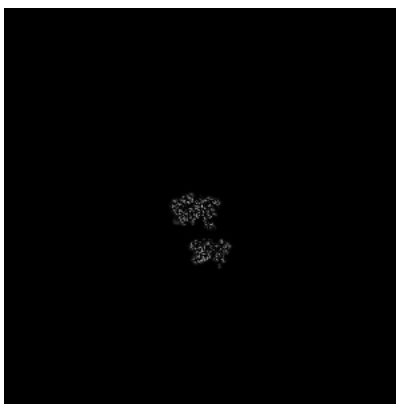
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 228



Y Index: 204

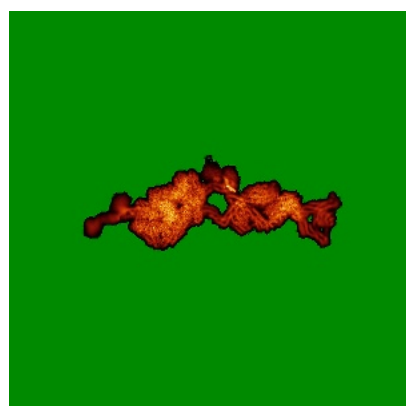


Z Index: 258

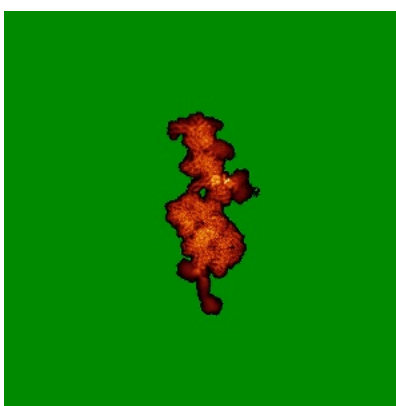
The images above show the largest variance slices of the map in three orthogonal directions.

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

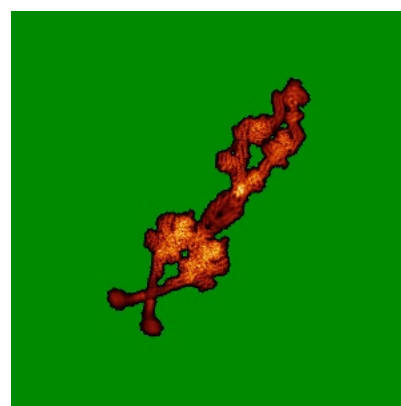
6.4.1 Primary map



X



Y



Z

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 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

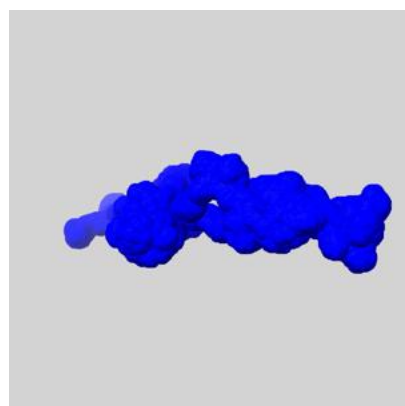
6.6 Mask visualisation [i](#)

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

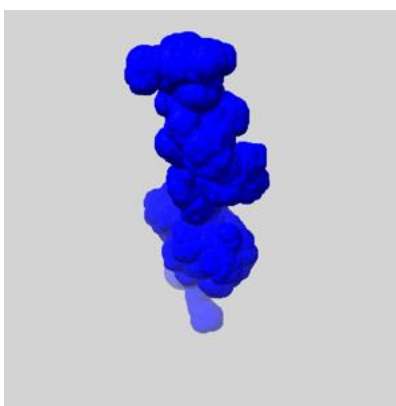
A mask typically either:

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

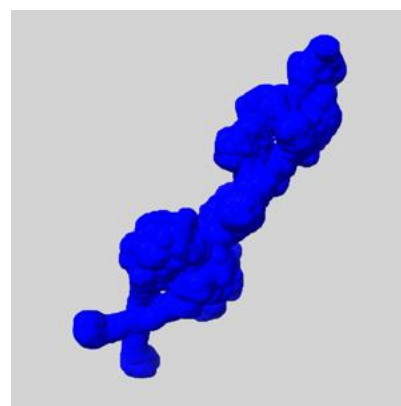
6.6.1 emd_44681_msk_1.map [i](#)



X



Y

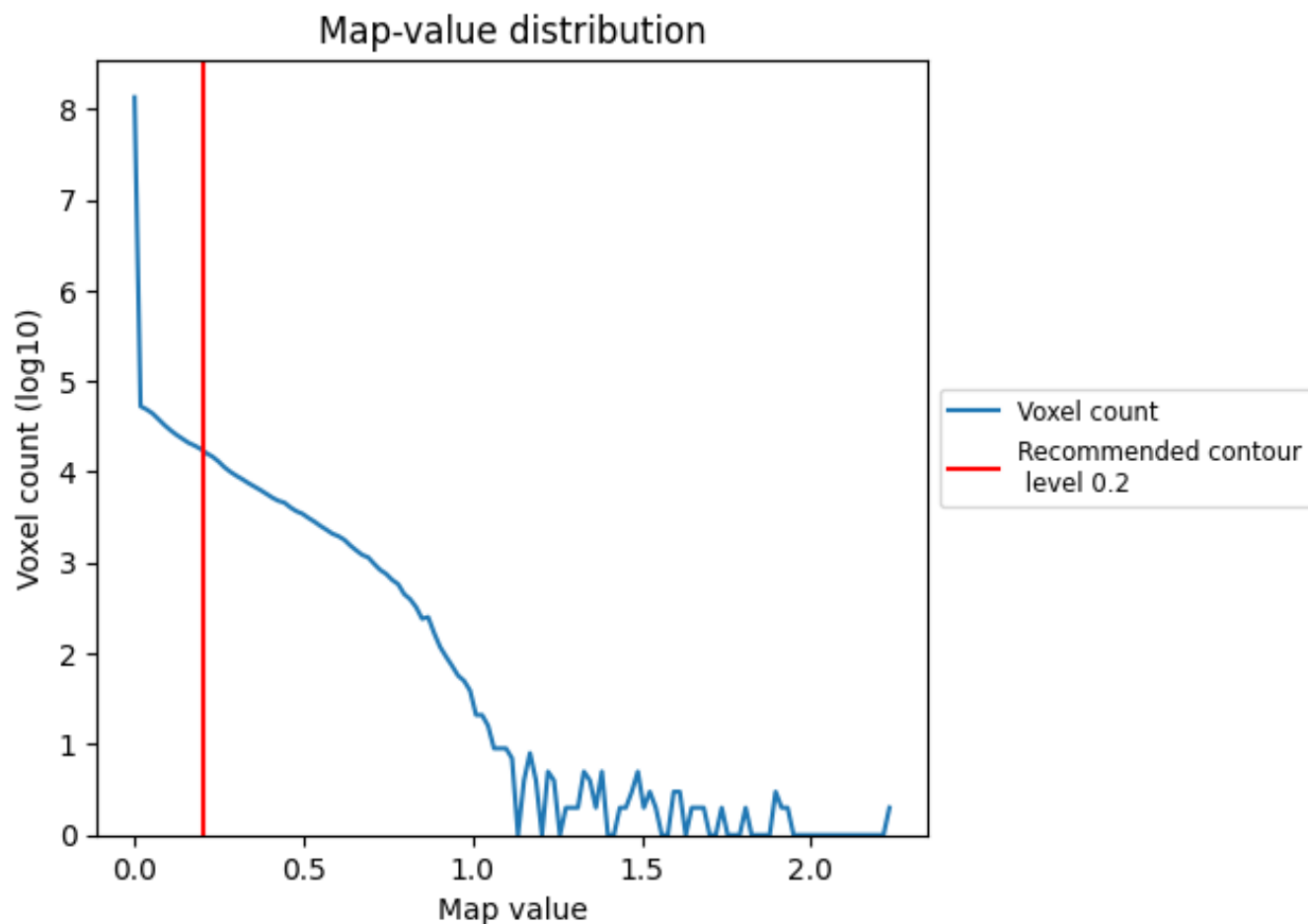


Z

7 Map analysis ⓘ

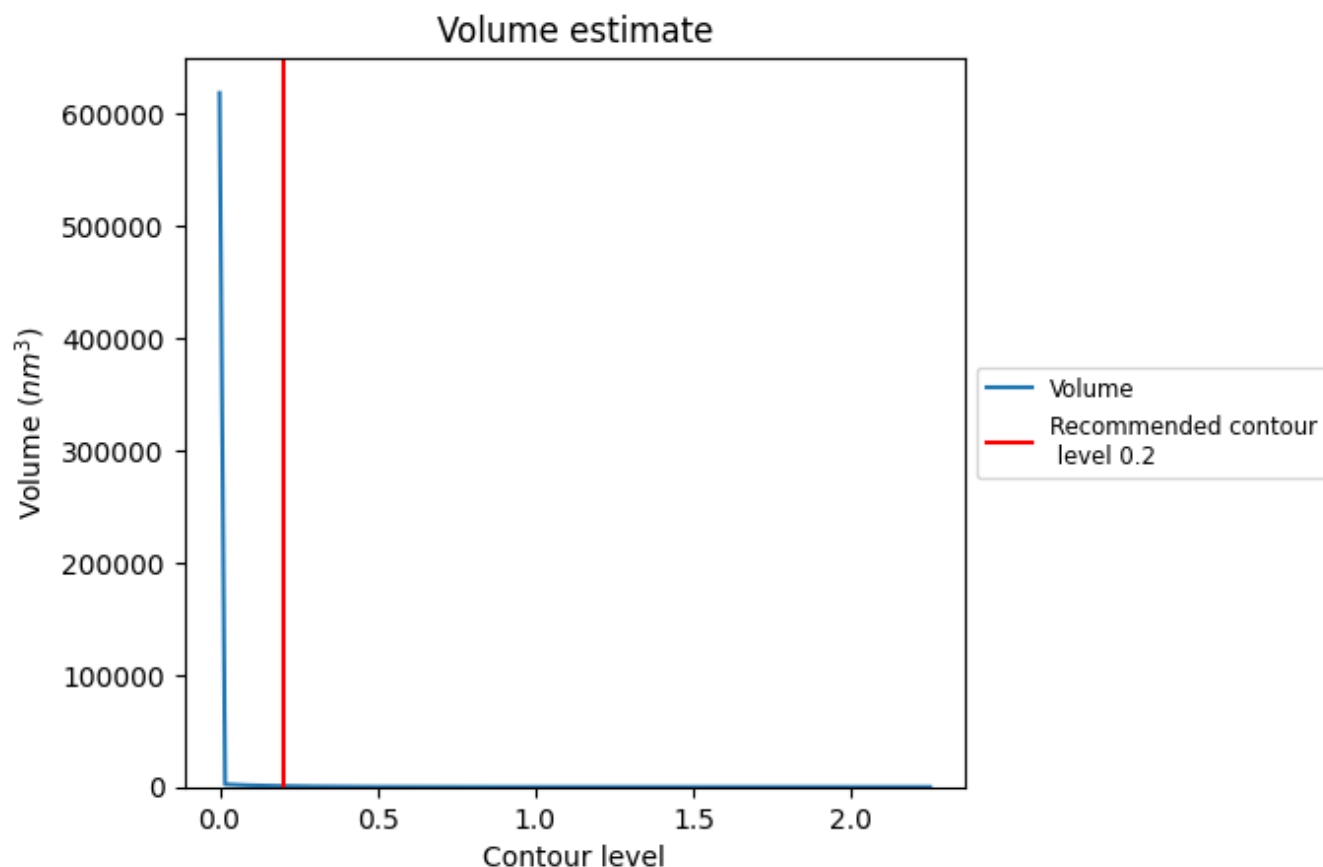
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

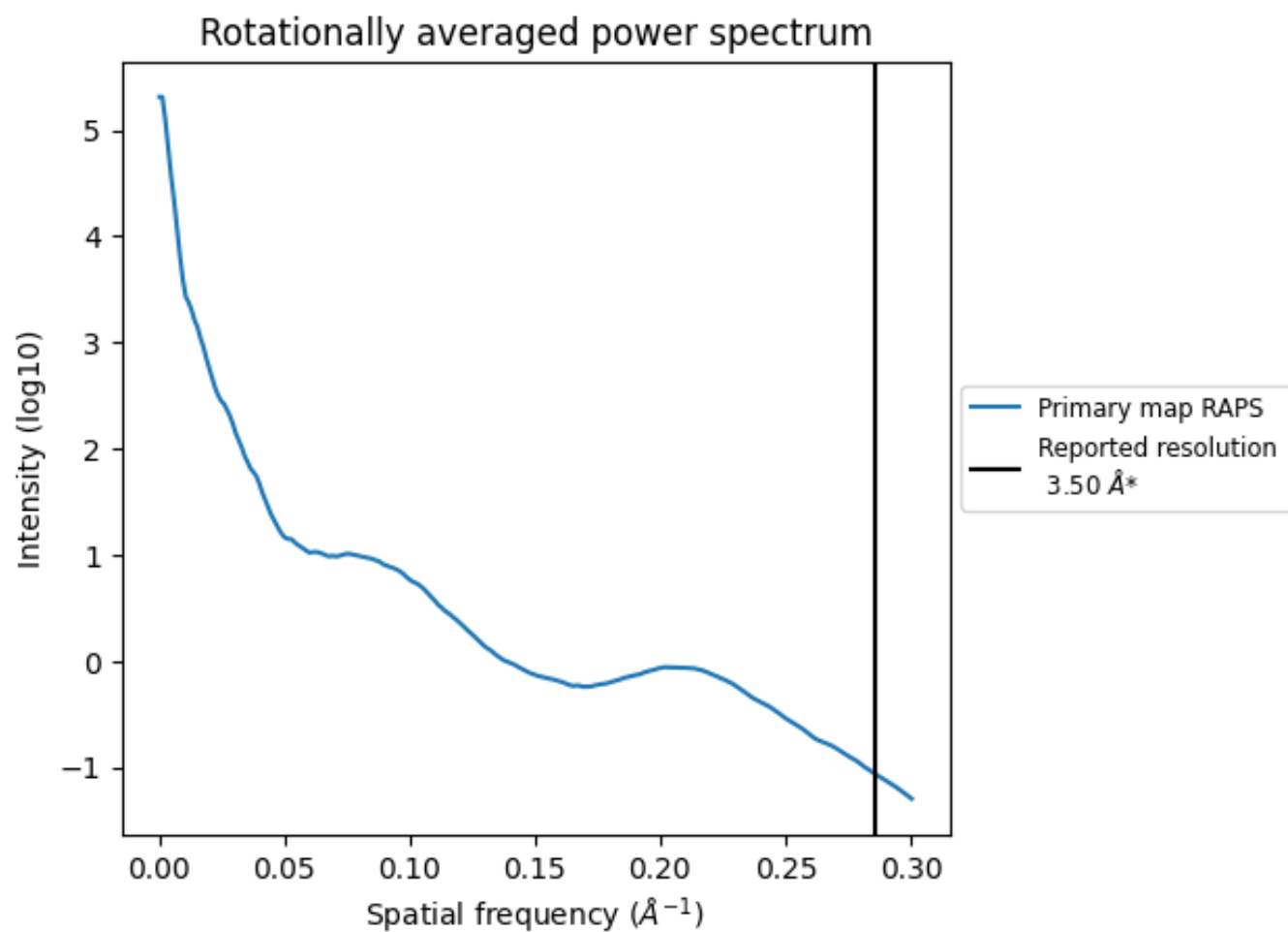
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 810 nm^3 ; this corresponds to an approximate mass of 731 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 ⓘ

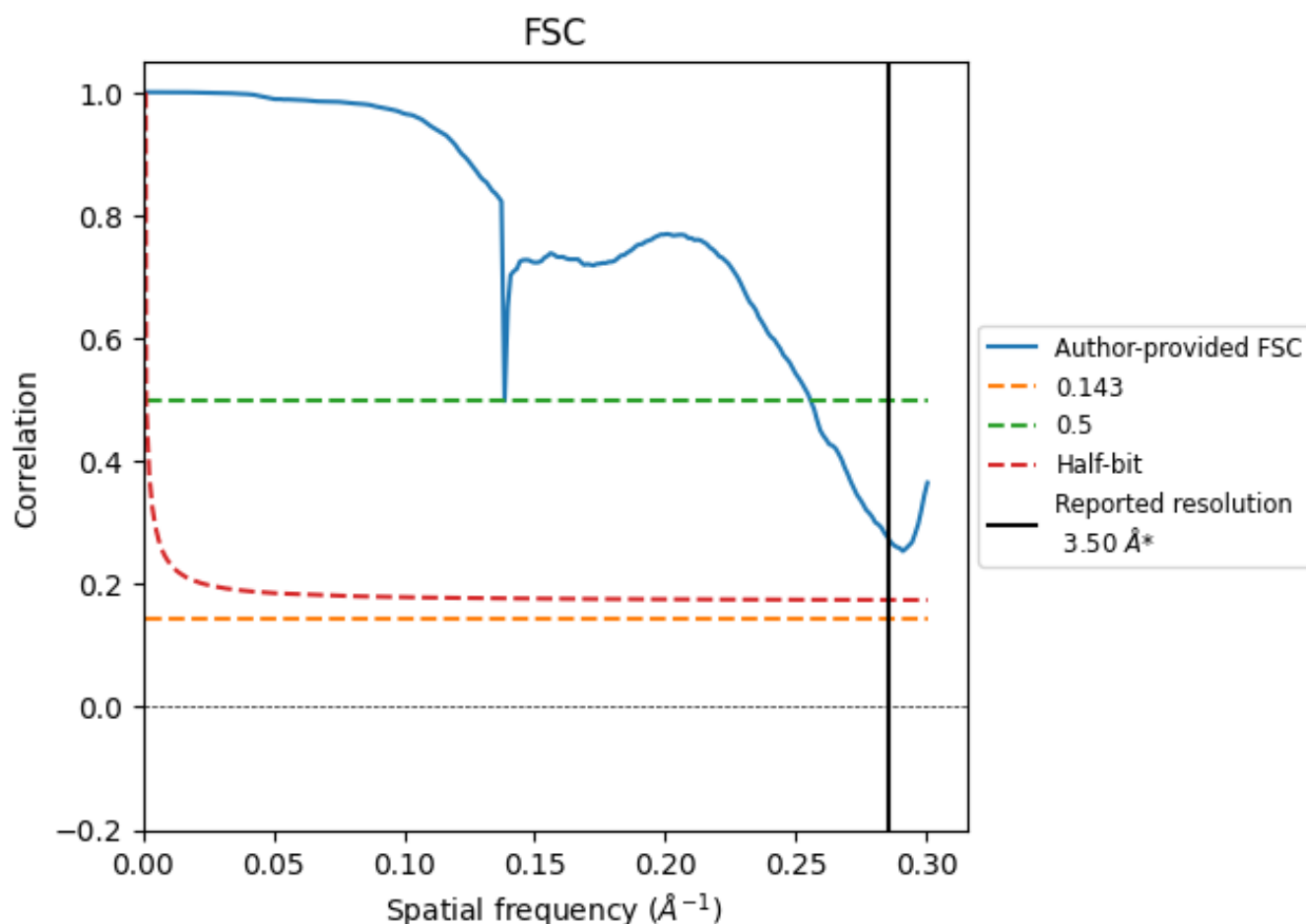


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

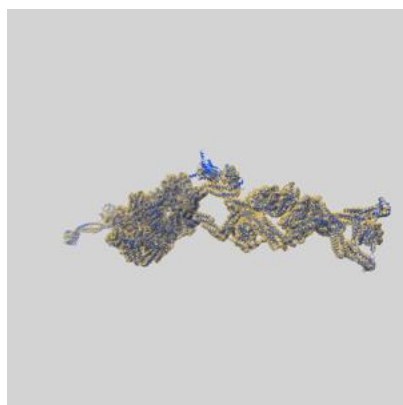
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	7.22	-
Unmasked-calculated*	-	-	-

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

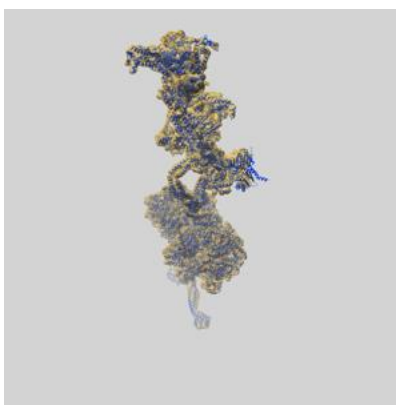
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44681 and PDB model 9BLY. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

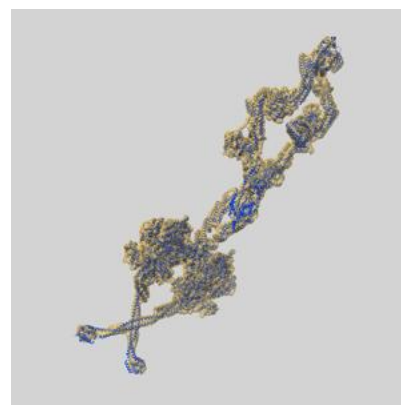
9.1 Map-model overlay [i](#)



X



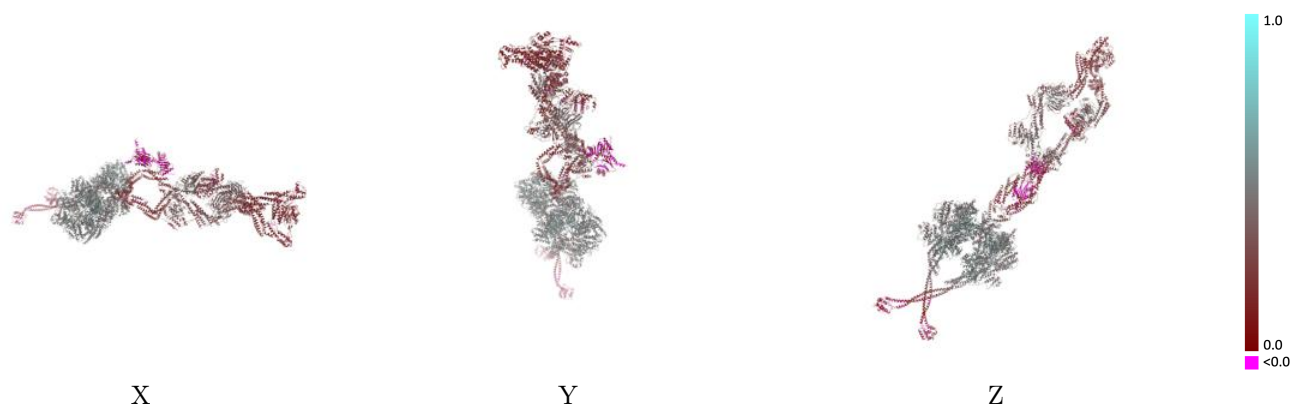
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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](#)

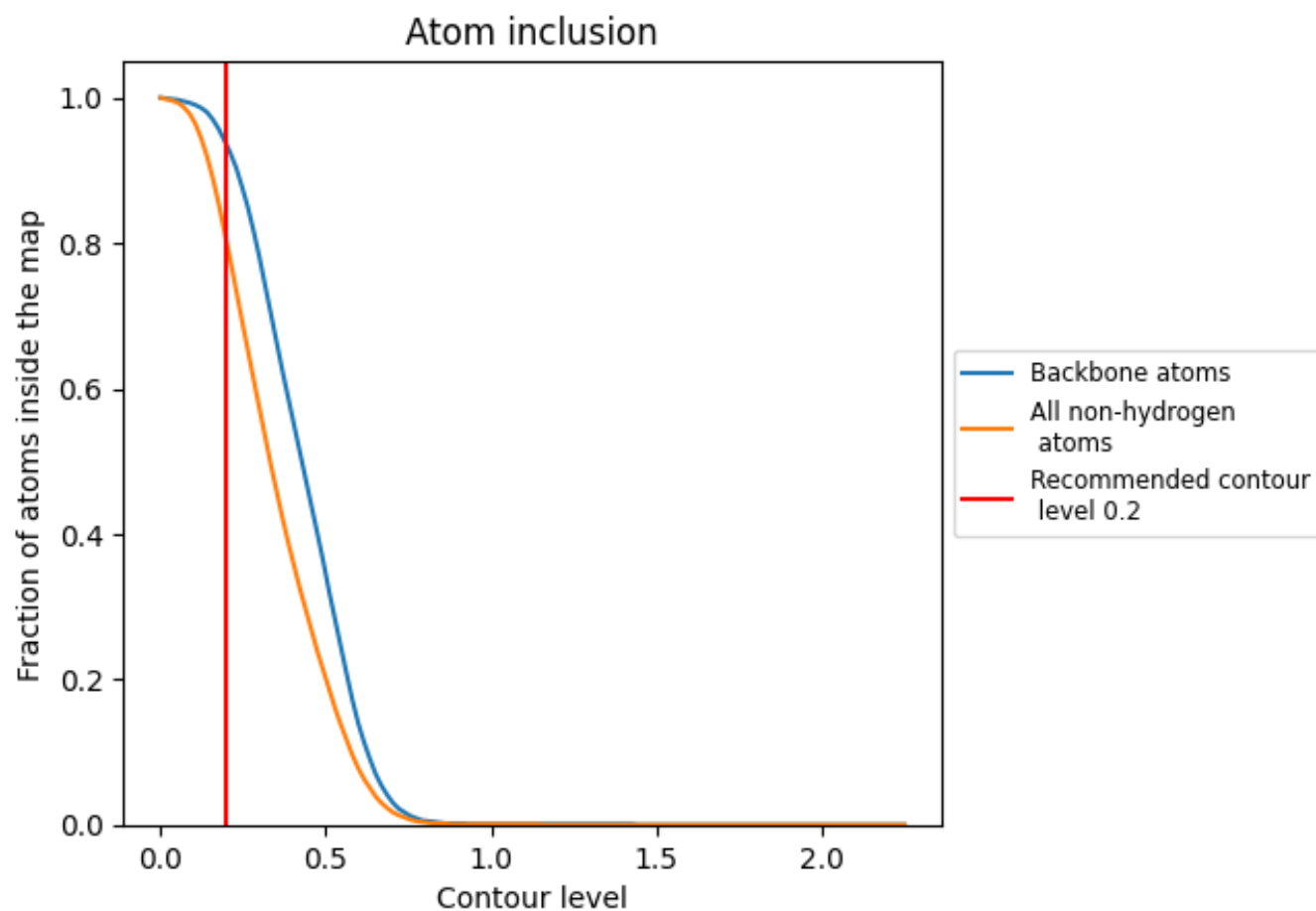


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 80% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8020	<div></div> 0.3680
A	<div></div> 0.8120	<div></div> 0.3890
B	<div></div> 0.8190	<div></div> 0.3860
C	<div></div> 0.8850	<div></div> 0.3810
D	<div></div> 0.8570	<div></div> 0.3470
E	<div></div> 0.8340	<div></div> 0.3510
F	<div></div> 0.8580	<div></div> 0.3310
G	<div></div> 0.6840	<div></div> 0.1860
H	<div></div> 0.7400	<div></div> 0.1990
I	<div></div> 0.5190	<div></div> 0.0560
J	<div></div> 0.5850	<div></div> 0.0370
K	<div></div> 0.1050	<div></div> 0.0280
L	<div></div> 0.1960	<div></div> 0.0710

