



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 07:22 PM EST

PDB ID : 7MOQ
EMDB ID : EMD-23926
Title : The structure of the Tetrahymena thermophila outer dynein arm on doublet microtubule
Authors : Kubo, S.; Yang, S.K.; Ichikawa, M.; Bui, K.H.
Deposited on : 2021-05-03
Resolution : 8.00 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:

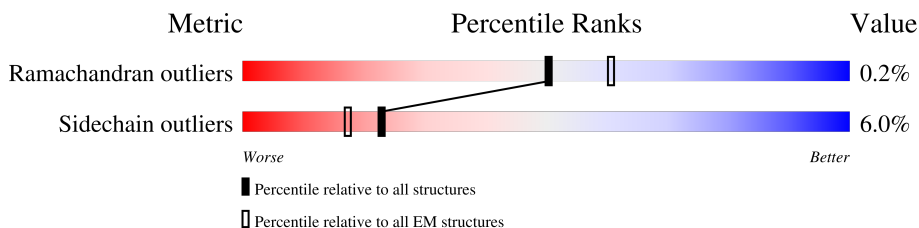
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 8.00 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)
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	8% 92%
2	B	4594	23% 87% 11%
3	C	4620	27% 89% 10%
4	D	667	50% 50%
4	d	667	19% 81%
5	E	670	9% 64% 35%
5	e	670	16% 84%
6	F	133	72% 26%
7	G	159	59% 40%


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Mol	Chain	Length	Quality of chain
8	H	92	91% 8%
9	I	110	81% 19%
10	J	93	90% 10%
11	K	111	86% 14%
12	L	111	87% 13%
13	M	87	99%
14	N	132	83% 17%
15	O	117	93% 5%
16	P	110	93% 6%
17	Q	443	79% 15% 5%
17	U	443	79% 15% 5%
17	Y	443	79% 15% 5%
17	q	443	79% 15% 5%
17	u	443	79% 15% 5%
17	y	443	79% 15% 5%
18	R	449	83% 12%
18	S	449	83% 12%
18	W	449	83% 12%
18	r	449	83% 12%
18	s	449	83% 12%
18	w	449	83% 12%
19	T	309	42% 58%
20	V	130	75% 25%
20	x	130	78% 22%
21	X	555	75% 25%

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Mol	Chain	Length	Quality of chain
22	Z	538	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '10%', a green segment in the middle labeled '21%', and a grey segment on the right labeled '78%'. The segments are stacked horizontally to total 100%.</p>

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 129847 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	340	2698	1720	458	508	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	4091	33080	21201	5547	6175	157	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	4159	33529	21421	5645	6289	174	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	331	2669	1719	439	493	18	0	0
4	d	128	957	597	170	187	3	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	436	3264	2059	565	621	19	0	0
5	e	109	684	414	132	138		0	0

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

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

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

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

- Molecule 8 is a protein called Dynein light chain.

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

- Molecule 9 is a protein called Dynein light chain.

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

- Molecule 10 is a protein called Dynein light chain.

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

- Molecule 11 is a protein called Dynein light chain.

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

- Molecule 12 is a protein called Dynein light chain.

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

- Molecule 13 is a protein called Dynein light chain.

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

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

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

- Molecule 16 is a protein called Thioredoxin.

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

- Molecule 17 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	420	3287	2068	563	628	28	0	0
17	U	420	3287	2068	563	628	28	0	0
17	Y	420	3287	2068	563	628	28	0	0
17	u	420	3287	2068	563	628	28	0	0
17	q	420	3287	2068	563	628	28	0	0
17	y	420	3287	2068	563	628	28	0	0

- Molecule 18 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	429	3342	2118	568	634	22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
18	W	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
18	s	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
18	r	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
18	w	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		

- Molecule 19 is a protein called Outer dynein arm docking complex protein oda protein.

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

- Molecule 20 is a protein called Docking complex 1/2 protein.

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

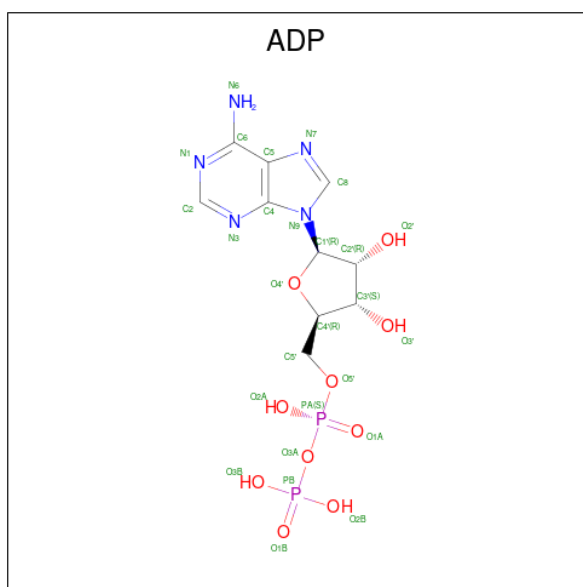
- Molecule 21 is a protein called Docking complex 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	140	Total	C	N	O	S	0	0
			1149	719	210	218	2		

- Molecule 22 is a protein called Outer dynein arm docking complex protein oda protein.

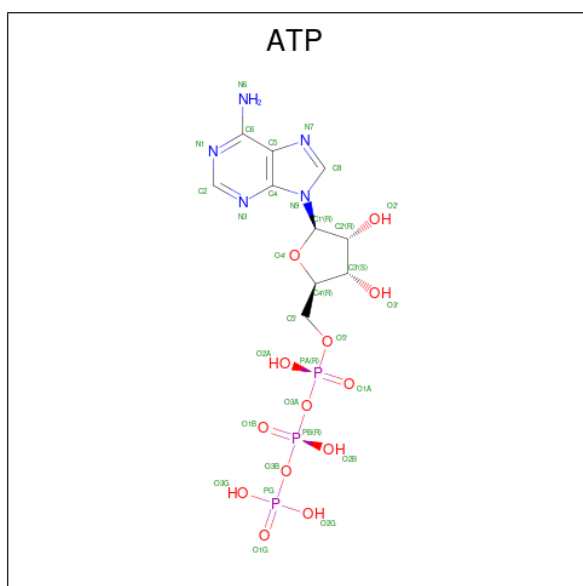
Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	117	Total	C	N	O	S	0	0
			993	614	191	186	2		

- Molecule 23 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



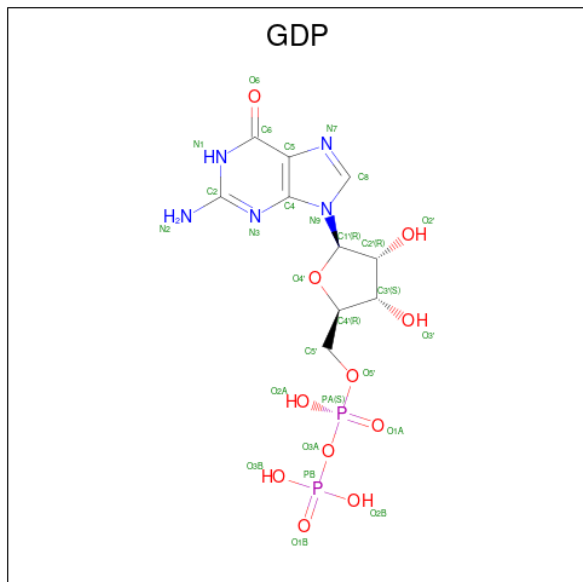
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
23	C	1	54	20	10	20	4	0
23	C	1	54	20	10	20	4	0

- Molecule 24 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



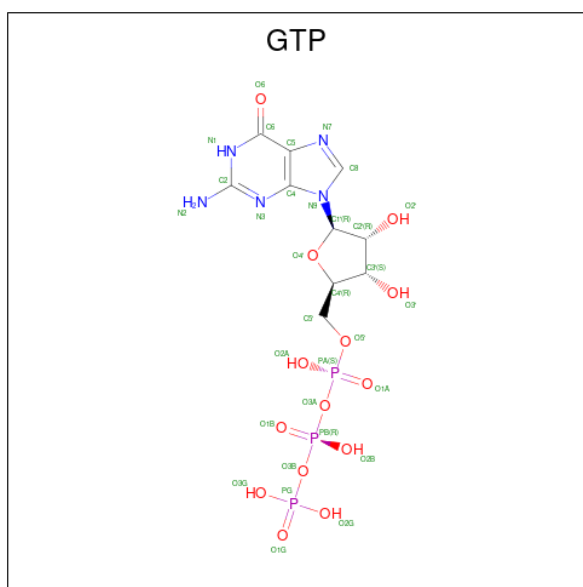
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
24	C	1	31	10	5	13	3	0

- Molecule 25 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
25	Q	1	Total	C	N	O	P	0
			28	10	5	11	2	
25	U	1	Total	C	N	O	P	0
			28	10	5	11	2	
25	Y	1	Total	C	N	O	P	0
			28	10	5	11	2	
25	u	1	Total	C	N	O	P	0
			28	10	5	11	2	
25	q	1	Total	C	N	O	P	0
			28	10	5	11	2	
25	y	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 26 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

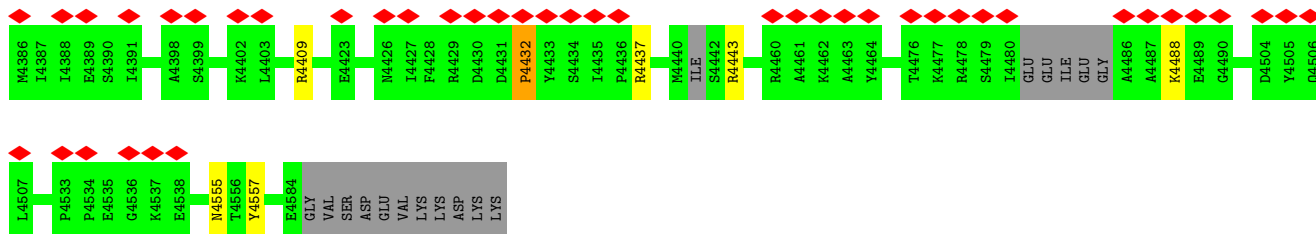


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
26	R	1	Total 32	C 10	N 5	O 14	P 3	0
26	S	1	Total 32	C 10	N 5	O 14	P 3	0
26	W	1	Total 32	C 10	N 5	O 14	P 3	0
26	s	1	Total 32	C 10	N 5	O 14	P 3	0
26	r	1	Total 32	C 10	N 5	O 14	P 3	0
26	w	1	Total 32	C 10	N 5	O 14	P 3	0

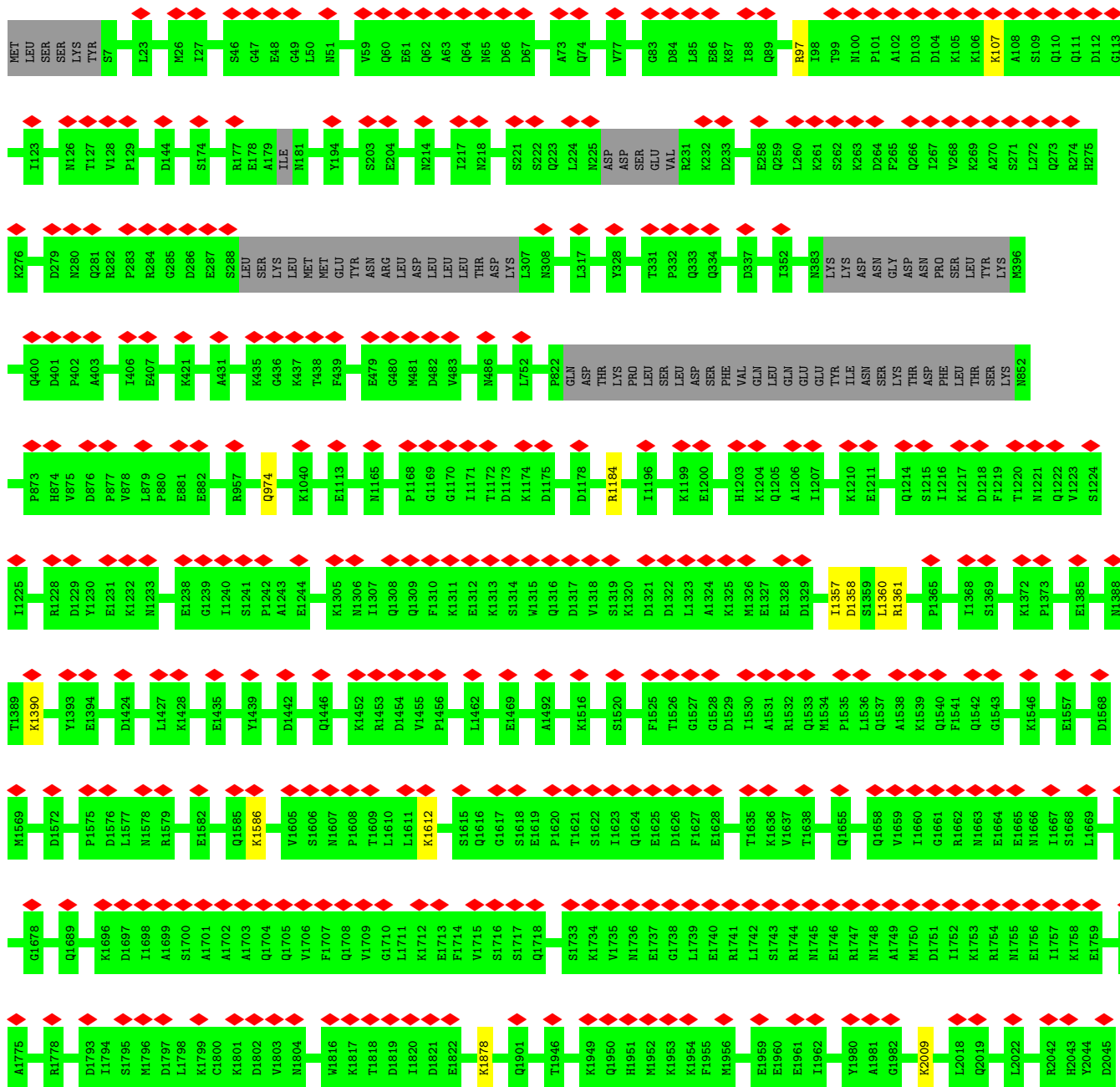
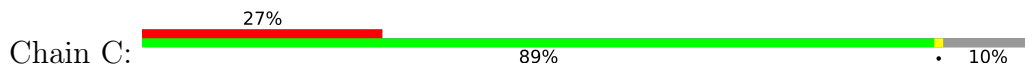
- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

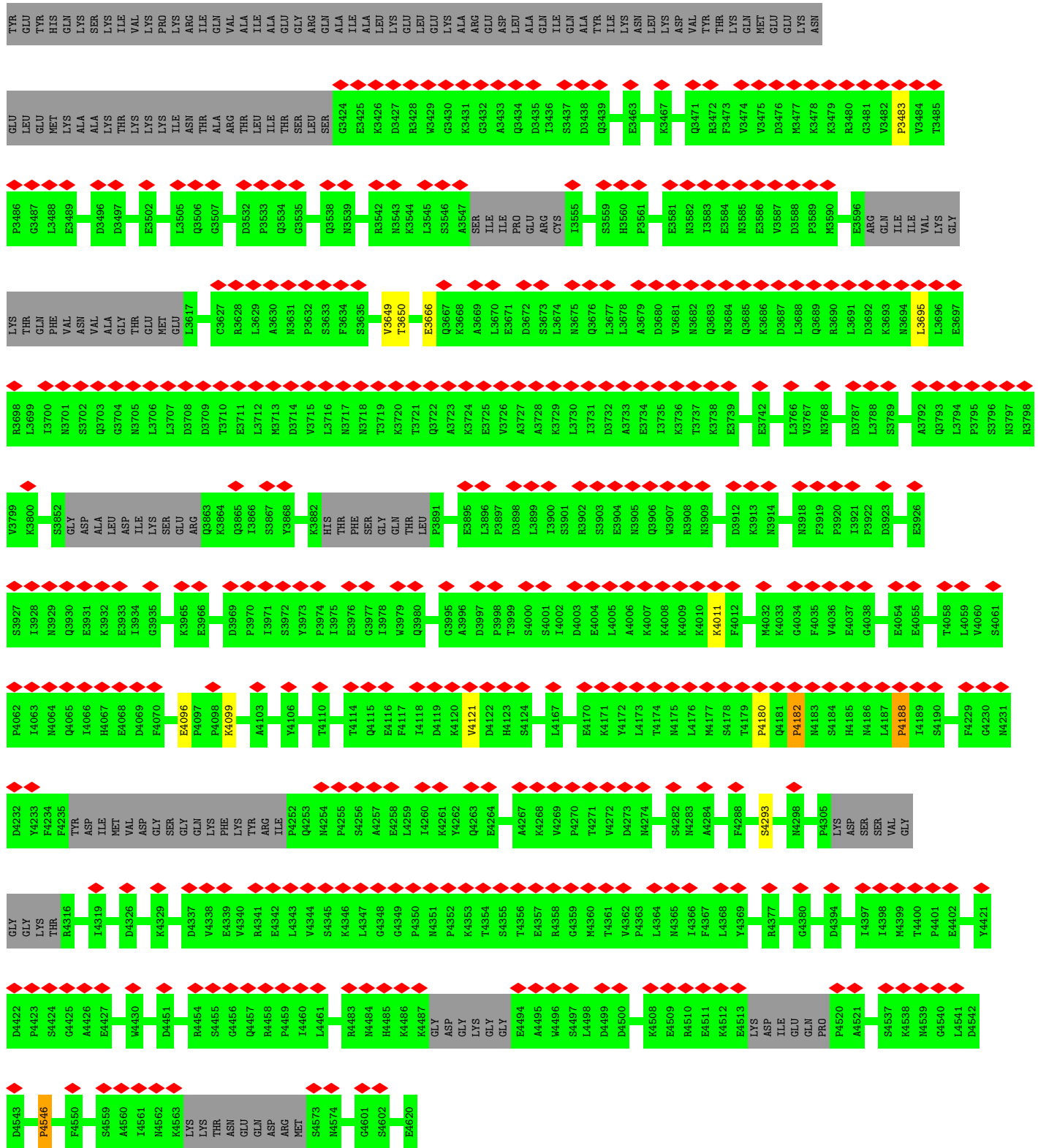
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
27	R	1	Total 1	Mg 1	0
27	S	1	Total 1	Mg 1	0
27	W	1	Total 1	Mg 1	0
27	s	1	Total 1	Mg 1	0
27	r	1	Total 1	Mg 1	0
27	w	1	Total 1	Mg 1	0

T1120	K1121	D1122	G1123	K1126	H1133	D1136	K1137	K1138	L1139	L1140	H1141	S1142	V1143	M1144	K1145	V1146	I1147	S1148	D1149	V1150	K1151	D1152	V1153	E1154	F1155	R1156	K1173	H1174	H1175	I1178	T1179	E1180	K1181	T1183	D1184	D1185	F1186	L1187	E1199	K1223	R1224	D1225	L1226	D1227	I1228	F1229	M1230	K1231	E1232	E1234				
S1236	F1236	R1237	K1238	E1239	F1240	M1241	Q1242	K1243	L1244	F1245	D1247	Y1248	T1249	S1250	S1251	M1252	G1253	Y1254	E1255	N1256	I1257	N1258	N1259	A1260	Y1261	T1263	I1264	M1265	V1266	Y1267	Y1268	H1269	K1270	G1276	R1277	A1278	L1279	E1280	N1283	L1284	E1285	K1286	L1287	F1288	E1289	L1290	Q1291	K1292	S1293	N1294	Y1295	W1330	R1331	
E1367	K1368	M1371	M1372	K1373	THR	VAL	LEU	PRO	LEU	VAL	SER	A1381	S1384	E1385	F1386	M1387	E1388	D1389	V1402	F1403	D1404	L1408	F1409	F1410	I1415	L1416	A1434	Q1435	K1436	E1437	A1438	K1439	I1440	E1441	K1442	K1443	L1444	K1445	M1446	Q1449	W1450	K1453	Q1479	L1482	D1483	G1486	K1492							
F1496	I1527	L1534	Q1586	K1589	K1590	K1604	SER	F1606	S1613	M1614	Q1615	S1616	L1617	L1618	T1619	S1622	M1623	P1628	K1629	V1630	C1631	E1632	Y1633	D1636	K1642	T1643	L1644	T1645	F1646	E1647	P1648	P1649	A1650	M1651	P1652	A1653	E1654	T1655	S1656	K1657	V1658	G1659	I1660	M1662	I1663	S1664	K1665							
D1666	D1667	E1668	K1669	P1670	F1672	S1673	S1674	K1675	F1676	I1677	C1678	E1679	A1681	H1684	I1700	A1704	K1705	N1706	T1707	A1708	D1709	L1710	S1713	G1714	D1715	K1716	P1717	R1718	E1719	E1720	W1721	V1722	E1723	G1724	Y1725	M1726	G1743	R1744	A1745	F1746	D1748	L1749	A1750	G1751	G1752	S1753	E1754	T1755	A1756	M1757	K1758			
E1759	C1760	Q1761	K1762	L1763	H1770	K1773	PRO	K1774	W1775	ARG	G1777	D1778	L1779	H1780	I1781	L1782	H1785	V1801	E1802	V1806	I1806	Q1807	K1808	V1809	S1810	E1811	A1812	E1813	K1828	PRO	ASP	SER	ASP	ASP	ASP	HIS	LEU	ARG	GLN	THR	LEU	ARG	PHE	TRP	TRP	GLU	LYS	ASP	LYS	ASN	LYS	M1850	I1872	
C1883	G1901	P1902	A1903	G1904	T1905	S1928	D1929	Q1930	R1957	Q1969	E1979	K1980	K1981	T1982	K1983	F1986	VAL	E1988	N2005	P2006	G2007	Y2008	A2009	G2010	R2011	R2023	M2027	V2028	V2029	P2030	D2031	L2032	R2084	Q2085	A2086	G2087	K2088	L2089	K2090	R2091	G2092	D2093	P2094	D2095	M2096	P2097	E2098	D2099	P2100					
L2101	R2104	T2116	D2117	G2127	P2131	K2132	L2133	D2134	P2135	F2136	T2137	K2138	Q2139	N2140	P2141	E2142	L2143	K2144	K2145	I2146	D2149	K2153	D2154	E2161	T2202	N2203	S2204	G2205	E2206	K2229	T2230	K2231	K2247	ASN	GLU	GLU	LYS	LYS	TYR	K2253	H2256	S2289	N2290	L2347	K2348	Q2349	Q2350							
K2351	E2352	M2353	A2354	ASN	MET	PRO	GLU	TYR	PRO	VAL	ILE	ASP	VAL	A2386	K2387	S2388	V2389	F2370	Y2371	R2372	Q2375	S2376	E2379	Q2380	N2381	I2382	D2383	V2384	D2386	K2387	N2388	R2389	VAL	ARG	HIS	ILE	C2394	F2395	H2416	L2417	PRO	LYS	LEU	LYS	LYS	MET	LYS	GLU	GLU	ASP	GLU	GLN	ALA	
LEU	E2433	A2434	F2435	I2437	F2438	L2441	I2444	G2445	D2454	S2455	LYS	ASP	MET	LYS	GLU	F2461	N2462	T2463	V2464	W2465	K2466	G2467	A2468	A2469	K2470	V2471	K2472	F2473	F2474	E2475	Q2476	G2477	L2478	C2479	Y2480	D2481	Y2484	D2485	I2486	N2487	E2488	N2489	K2490	W2491	N2492	T2493	W2494	K2495	V2496	E2497	D2498	Y2499	L2500	P2501
M2502	D2503	Q2504	R2521	Y2522	D2525	R2531	L2552	N2553	S2554	T2555	R2556	P2557	E2558	Q2559	V2560	M2583	V2584	E2585	K2586	K2587	N2588	G2589	Y2592	K2614	R2642	S2680	S2681	D2682	T2686	N2689	A2694	S2697	T2698	I2699	D2700	D2701	K2702	A2703	Q2704	K2705	V2841	E2855	E2856	Q2857	F2708	K2709	E2712	F2716						
N2724	THR	THR	ALA	F2728	A2732	Y2759	S2760	G2761	G2762	D2763	Y2795	E2798	A2799	I2800	S2801	K2802	C2803	I2804	G2805	E2806	F2807	P2808	E2809	T2810	E2811	F2820	T2821	G2822	F2823	V2824	A2825	A2826	H2827	GLN	GLY	LEU	ASP	GLN	GLN	TYR	T2835	Q2836	T2838	I2839	P2840	L2841	L2842	K2843	R2844	V2845	L2846	D2847		
D2848	K2849	L2850	E2851	E2852	E2855	F2905	I2906	N2907	G2908	F2909	E2910	I2911	D2912	Q2913	L2914	V2915	V2916	T2917	A2918	S2919	F2920	T2921	I2922	N2923	D2924	L2925	R2926	N2927	N2928	E2931	K2934	K2935	I2936	A2937	K2938	F2939	N2940	S2941	I2942	A2943	R2944	V2945	F2946	N2947	K2954	E2955	E2956	Q2957	F2958	L2959	I2960	F2976	K2977	



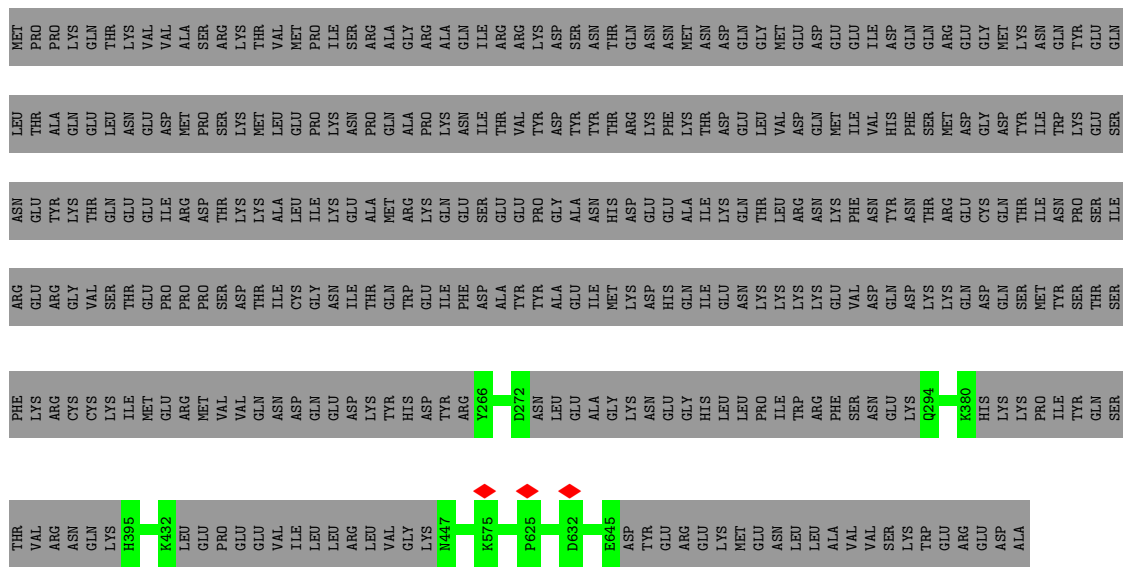
• Molecule 3: Dynein heavy chain, outer arm protein



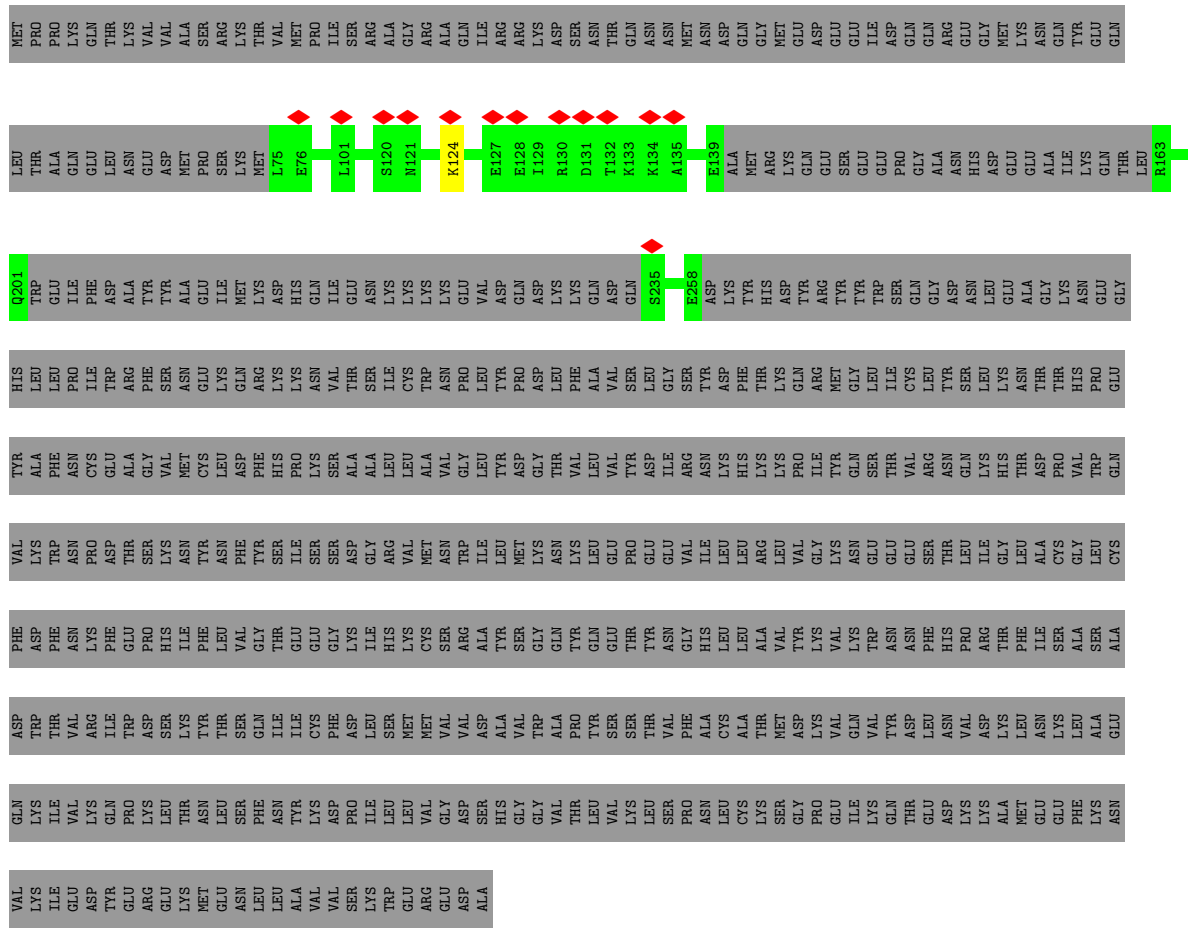


• Molecule 4: Dynein intermediate chain 2



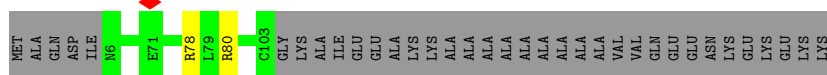


● Molecule 4: Dynein intermediate chain 2

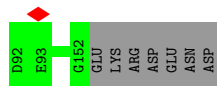
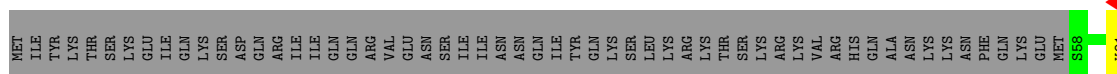


● Molecule 5: Flagellar outer dynein arm intermediate protein, putative

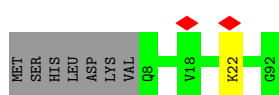
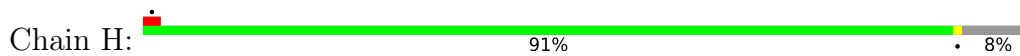




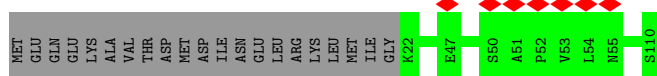
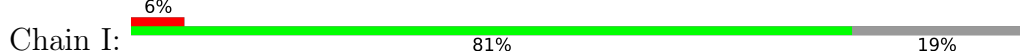
• Molecule 7: Dynein light chain roadblock-type 2 protein



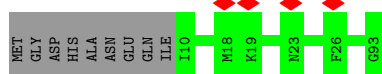
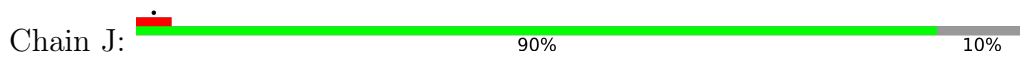
• Molecule 8: Dynein light chain



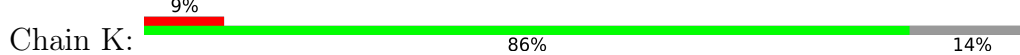
• Molecule 9: Dynein light chain



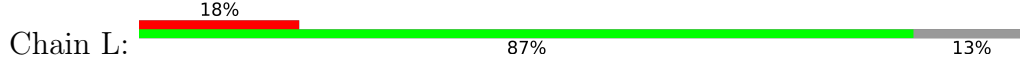
• Molecule 10: Dynein light chain



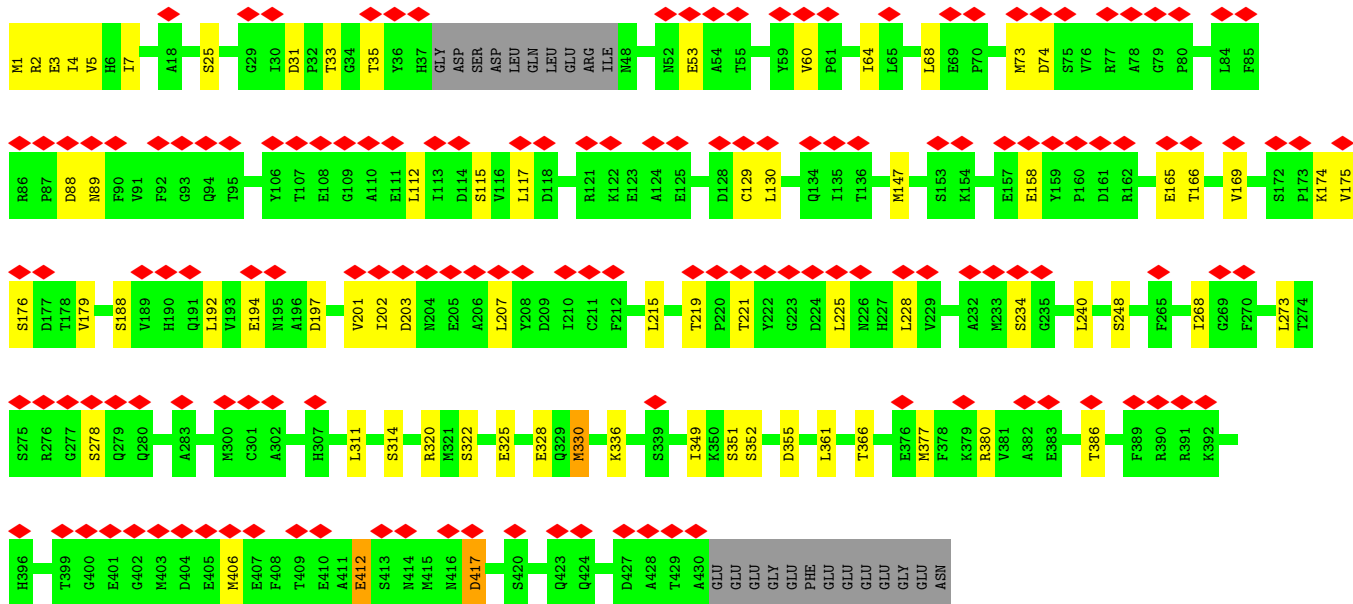
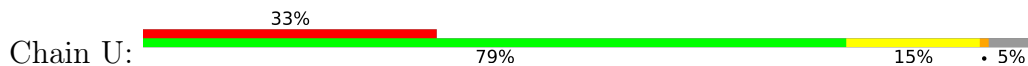
• Molecule 11: Dynein light chain



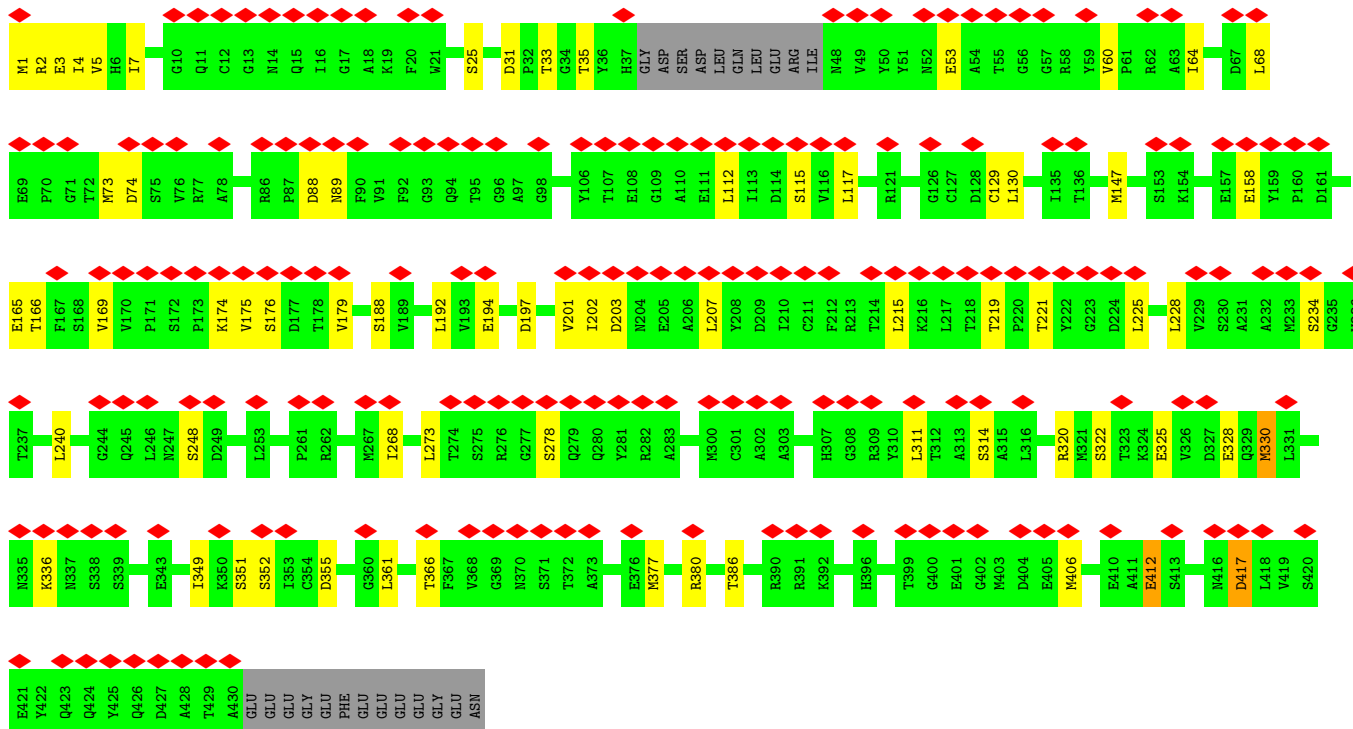
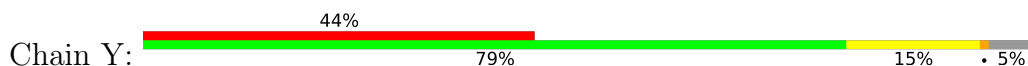
• Molecule 12: Dynein light chain



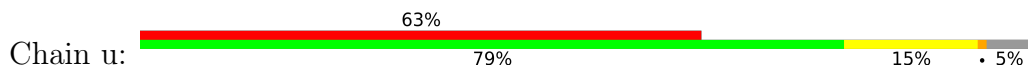
• Molecule 17: Tubulin beta chain

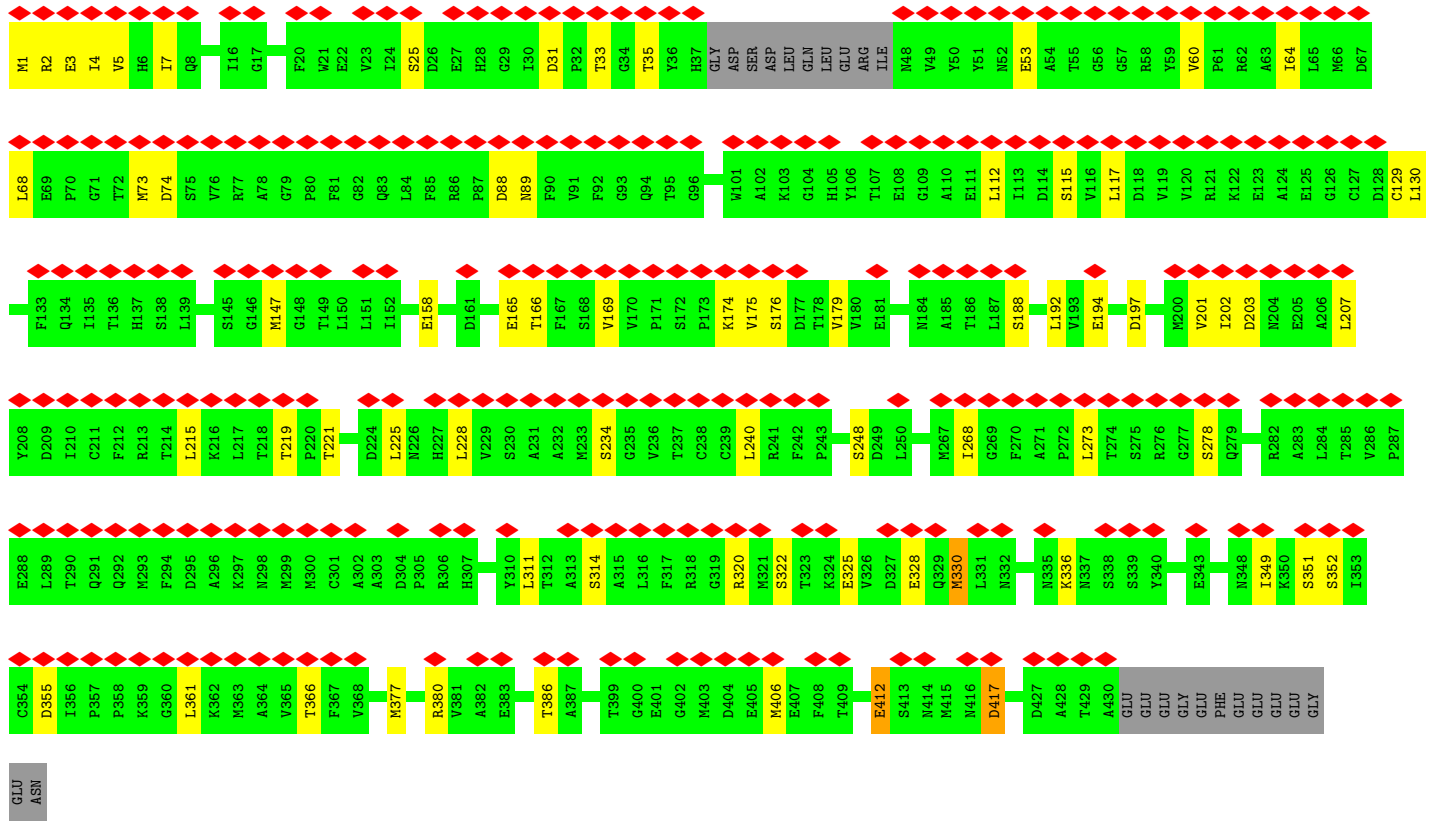


• Molecule 17: Tubulin beta chain

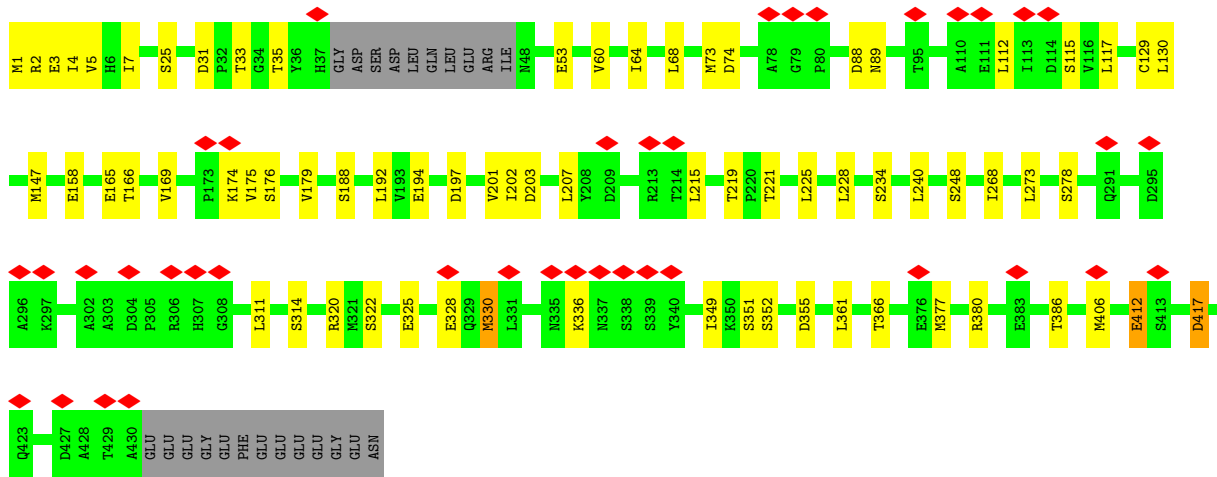
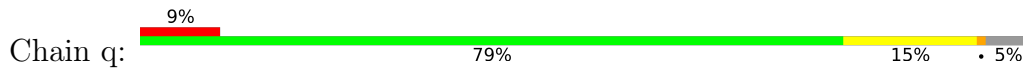


• Molecule 17: Tubulin beta chain

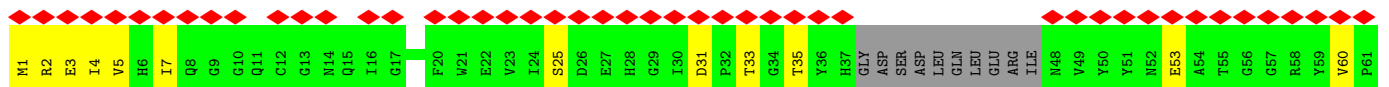
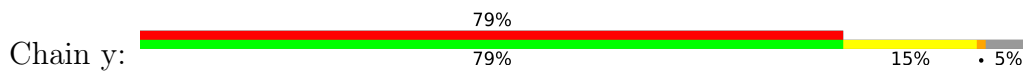


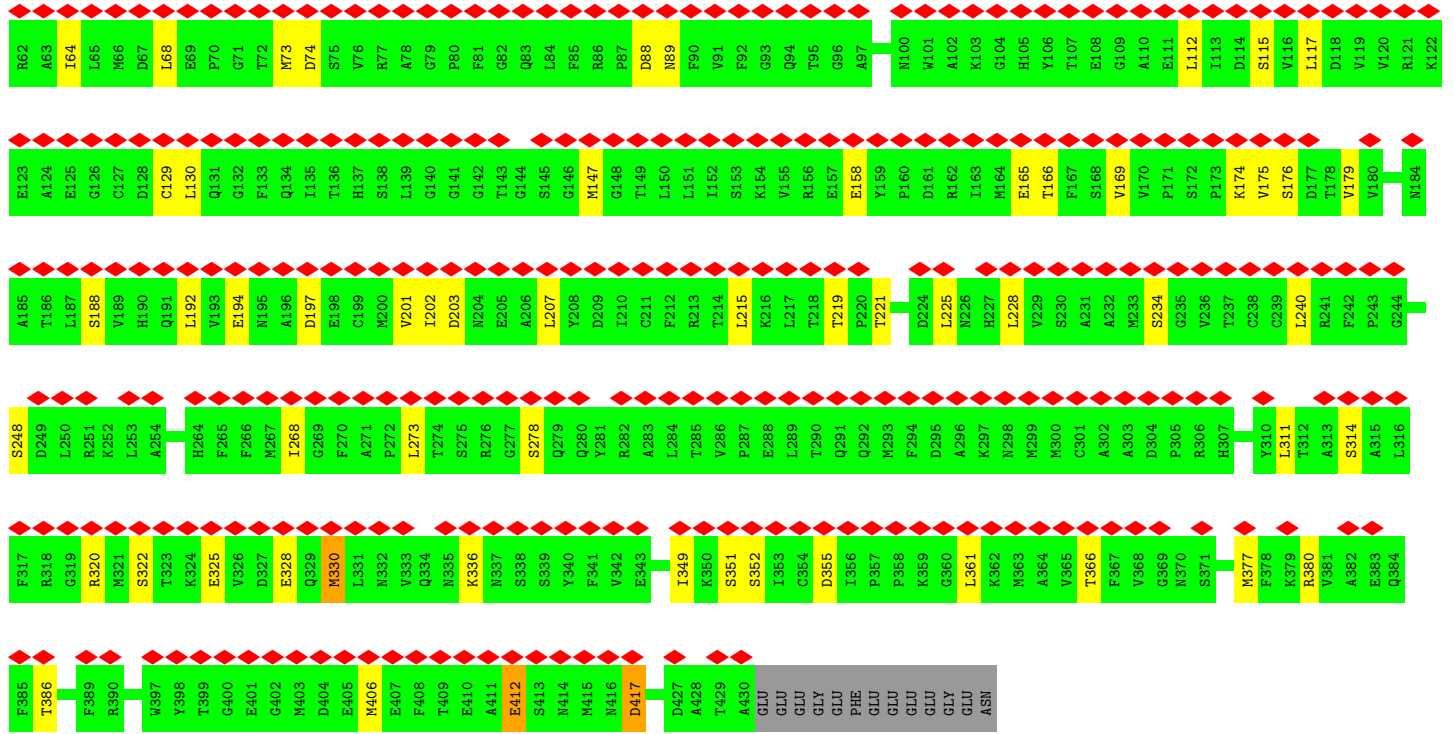


• Molecule 17: Tubulin beta chain

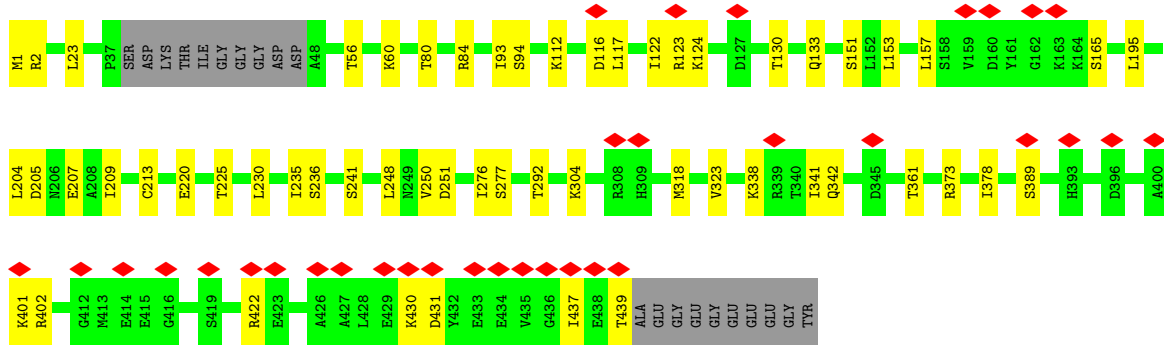
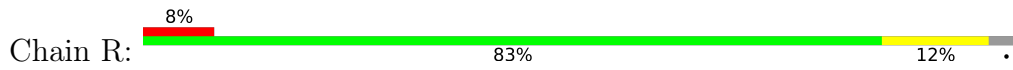


• Molecule 17: Tubulin beta chain

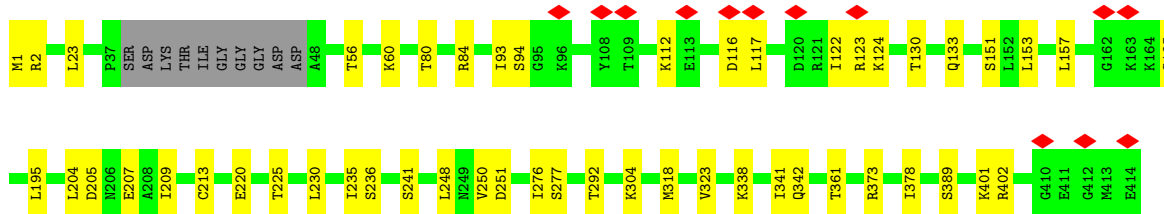
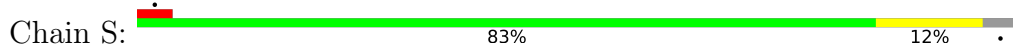


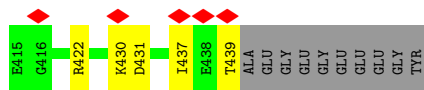


• Molecule 18: Tubulin alpha chain

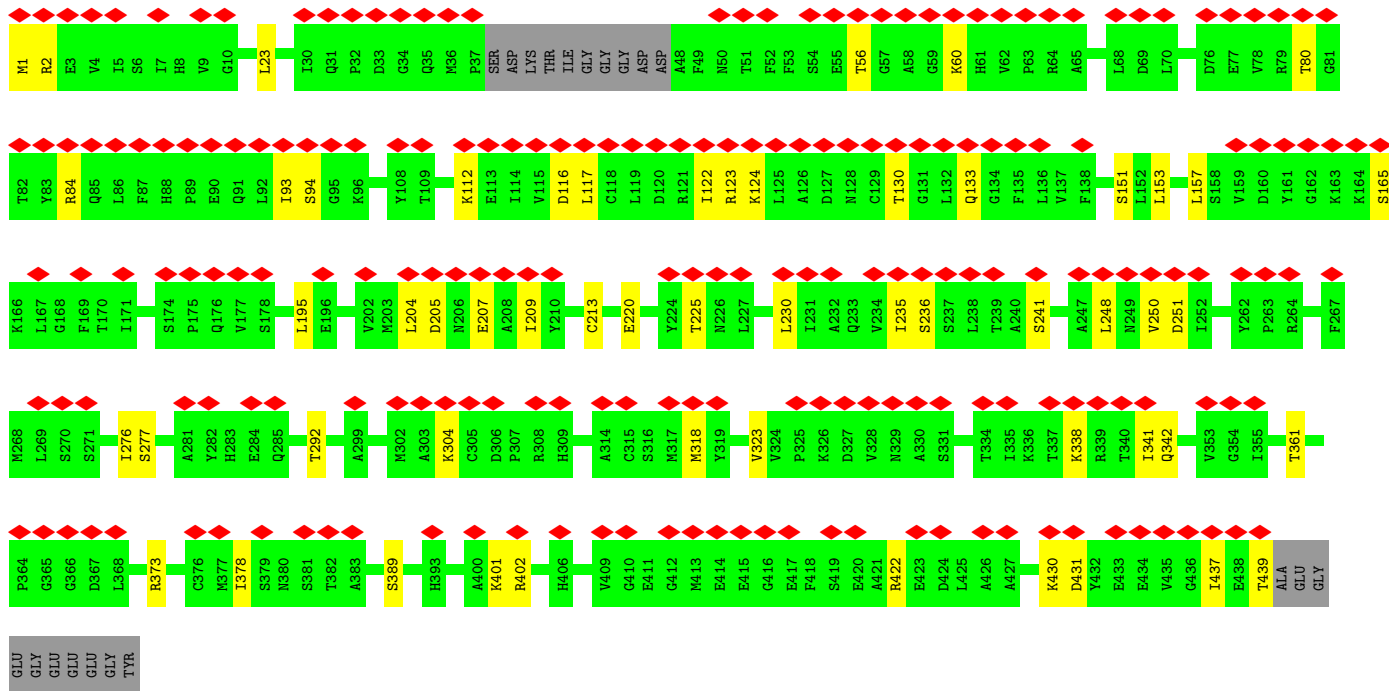
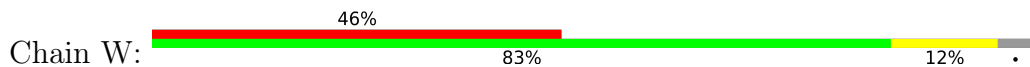


• Molecule 18: Tubulin alpha chain

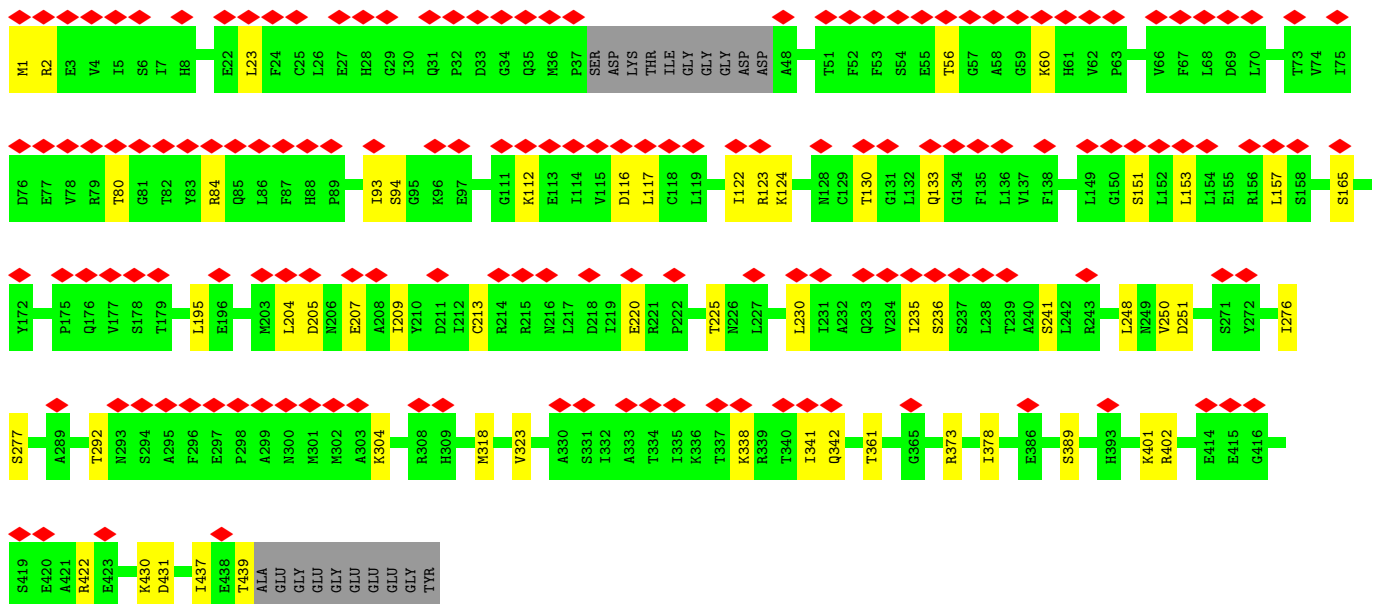
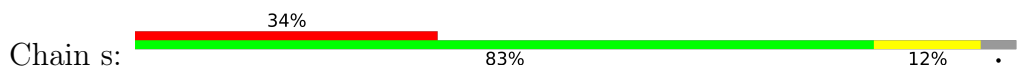




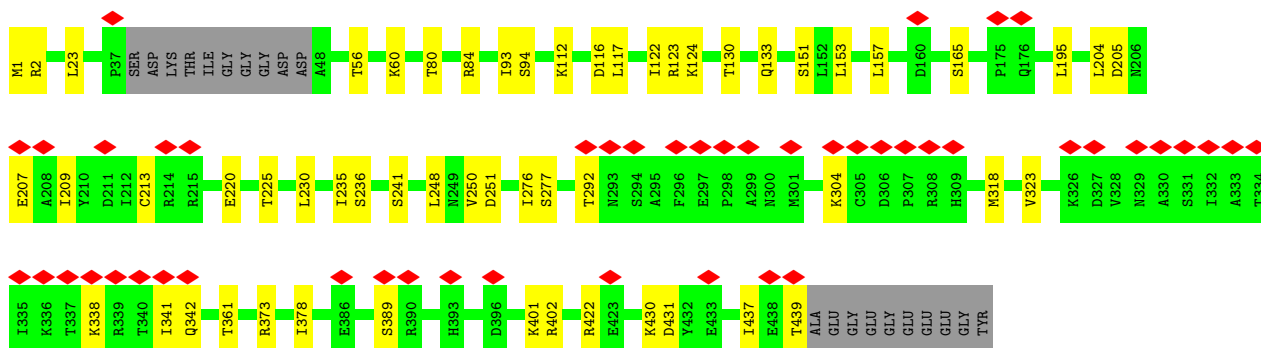
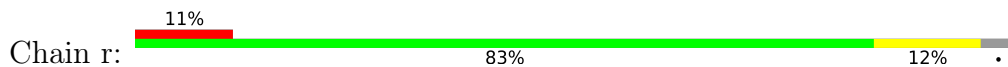
• Molecule 18: Tubulin alpha chain



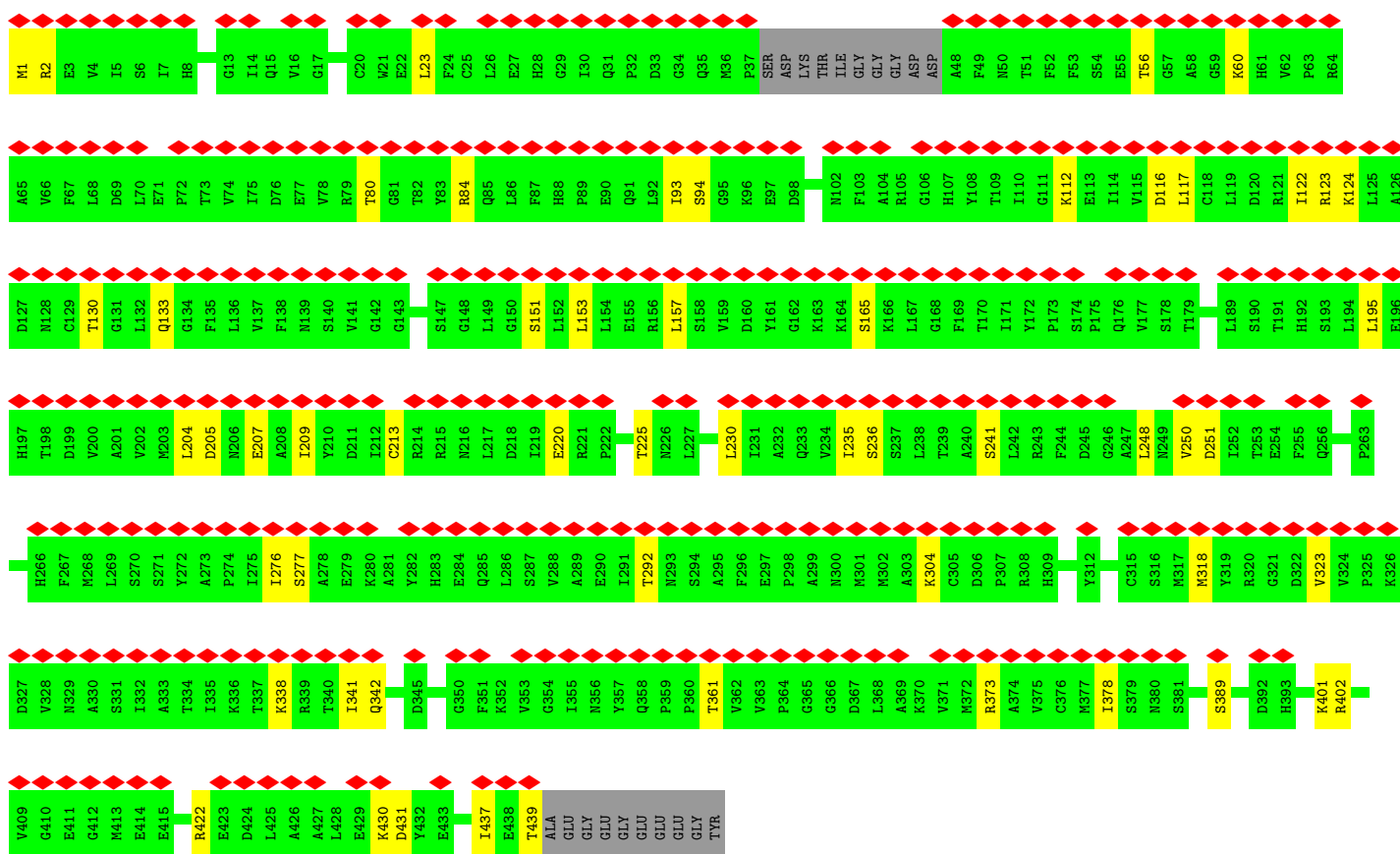
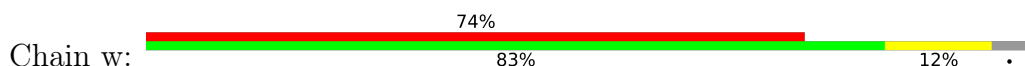
• Molecule 18: Tubulin alpha chain



• Molecule 18: Tubulin alpha chain

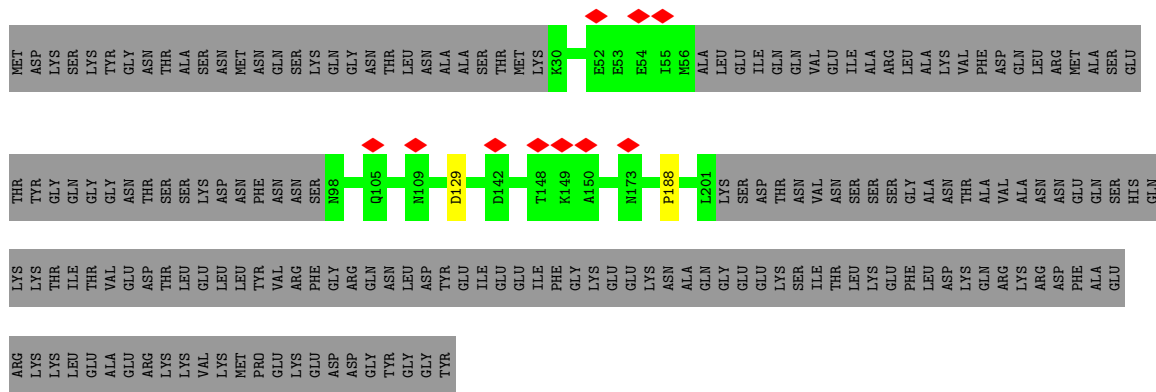


• Molecule 18: Tubulin alpha chain

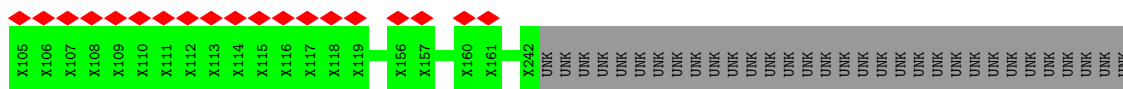
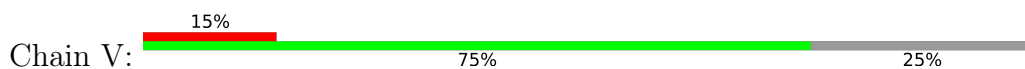


• Molecule 19: Outer dynein arm docking complex protein oda protein

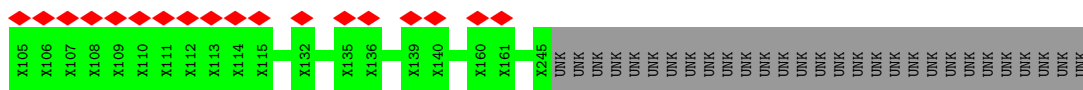
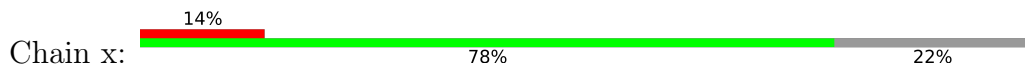




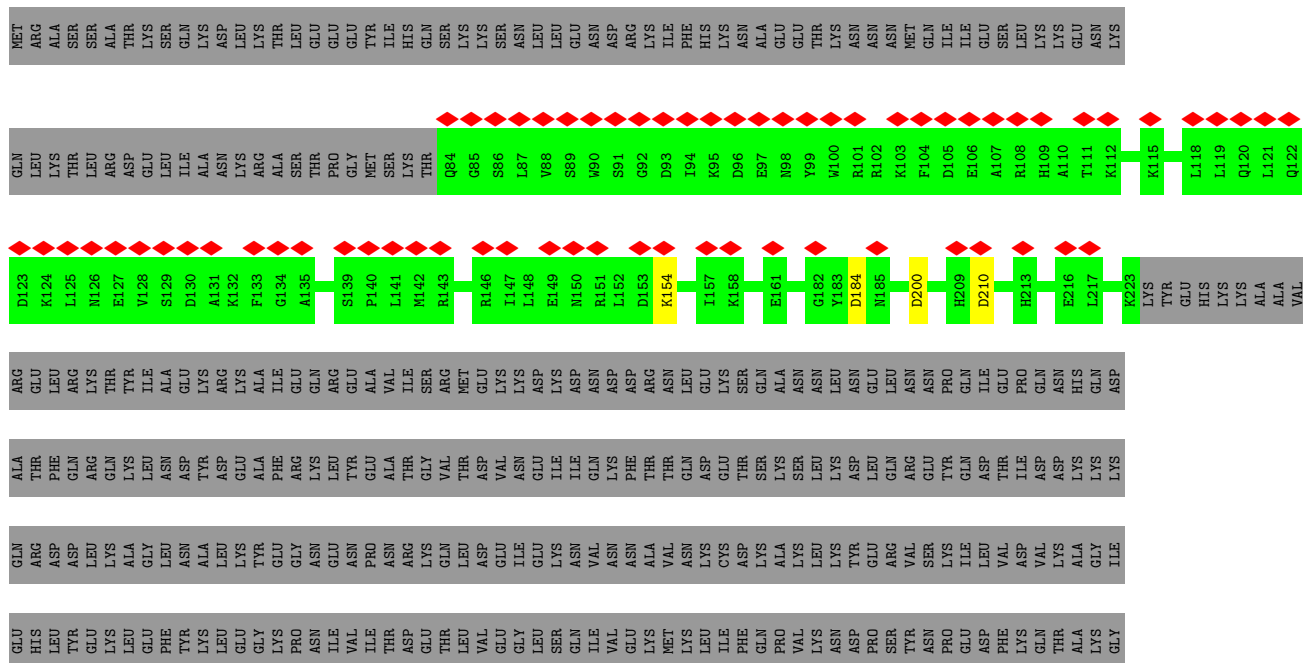
• Molecule 20: Docking complex 1/2 protein



• Molecule 20: Docking complex 1/2 protein



• Molecule 21: Docking complex 1 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	139548	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	14.861	Depositor
Minimum map value	-5.362	Depositor
Average map value	0.626	Depositor
Map value standard deviation	2.312	Depositor
Recommended contour level	3.1	Depositor
Map size (\AA)	313.95, 232.05, 461.37	wwPDB
Map dimensions	169, 85, 115	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.73, 2.73, 2.73	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: MG, ADP, GDP, GTP, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/2778	0.57	0/3776
2	B	0.31	3/33725 (0.0%)	0.52	11/45530 (0.0%)
3	C	0.28	0/34189	0.49	11/46162 (0.0%)
4	D	0.32	0/2737	0.52	0/3707
4	d	0.34	0/973	0.50	0/1319
5	E	0.31	0/3334	0.55	4/4523 (0.1%)
5	e	0.27	0/687	0.57	2/940 (0.2%)
6	F	0.28	0/793	0.51	0/1070
7	G	0.27	0/751	0.52	0/1014
8	H	0.28	0/718	0.46	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	0.28	0/790	0.50	0/1063
13	M	0.27	0/743	0.45	0/996
14	N	0.31	0/915	0.55	0/1229
15	O	0.28	0/891	0.47	0/1209
16	P	0.30	0/866	0.49	0/1171
17	Q	0.32	0/3359	0.63	4/4546 (0.1%)
17	U	0.32	0/3359	0.63	4/4546 (0.1%)
17	Y	0.32	0/3359	0.63	4/4546 (0.1%)
17	q	0.32	0/3359	0.63	4/4546 (0.1%)
17	u	0.32	0/3359	0.63	4/4546 (0.1%)
17	y	0.32	0/3359	0.63	4/4546 (0.1%)
18	R	0.31	0/3413	0.56	0/4625
18	S	0.31	0/3413	0.56	0/4625
18	W	0.31	0/3413	0.56	0/4625
18	r	0.31	0/3413	0.56	0/4625
18	s	0.31	0/3413	0.56	0/4625
18	w	0.31	0/3413	0.56	0/4625
19	T	0.27	0/1070	0.43	0/1436
21	X	0.28	0/1164	0.51	3/1556 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	Z	0.28	0/998	0.50	0/1323
All	All	0.30	3/131010 (0.0%)	0.54	55/177049 (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	1
2	B	0	11
3	C	0	3
18	R	0	1
18	S	0	1
18	W	0	1
18	r	0	1
18	s	0	1
18	w	0	1
22	Z	0	1
All	All	0	22

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	77	GLN	N-CA	9.52	1.65	1.46
2	B	1330	TRP	CB-CG	7.05	1.62	1.50
2	B	2592	TYR	CD1-CE1	-5.02	1.31	1.39

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1330	TRP	CA-CB-CG	9.26	131.29	113.70
5	E	152	LEU	CB-CG-CD1	-9.24	95.29	111.00
2	B	956	LEU	CA-CB-CG	-9.19	94.17	115.30
2	B	4432	PRO	N-CA-CB	9.03	114.13	103.30
3	C	1878	LYS	CD-CE-NZ	-8.63	91.85	111.70

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	ARG	Peptide
2	B	1415	ILE	Peptide
2	B	2135	PRO	Peptide
2	B	2229	LYS	Peptide
2	B	966	LYS	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	336/4168 (8%)	292 (87%)	43 (13%)	1 (0%)	41	77
2	B	4037/4594 (88%)	3637 (90%)	384 (10%)	16 (0%)	34	72
3	C	4127/4620 (89%)	3813 (92%)	305 (7%)	9 (0%)	47	81
4	D	323/667 (48%)	286 (88%)	37 (12%)	0	100	100
4	d	122/667 (18%)	114 (93%)	8 (7%)	0	100	100
5	E	426/670 (64%)	370 (87%)	56 (13%)	0	100	100
5	e	103/670 (15%)	88 (85%)	14 (14%)	1 (1%)	15	55
6	F	96/133 (72%)	83 (86%)	13 (14%)	0	100	100
7	G	93/159 (58%)	80 (86%)	13 (14%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	97 (96%)	4 (4%)	0	100	100
17	Q	416/443 (94%)	389 (94%)	27 (6%)	0	100	100
17	U	416/443 (94%)	389 (94%)	27 (6%)	0	100	100
17	Y	416/443 (94%)	389 (94%)	27 (6%)	0	100	100
17	q	416/443 (94%)	389 (94%)	27 (6%)	0	100	100
17	u	416/443 (94%)	389 (94%)	27 (6%)	0	100	100
17	y	416/443 (94%)	389 (94%)	27 (6%)	0	100	100
18	R	425/449 (95%)	408 (96%)	17 (4%)	0	100	100
18	S	425/449 (95%)	408 (96%)	17 (4%)	0	100	100
18	W	425/449 (95%)	408 (96%)	17 (4%)	0	100	100
18	r	425/449 (95%)	408 (96%)	17 (4%)	0	100	100
18	s	425/449 (95%)	408 (96%)	17 (4%)	0	100	100
18	w	425/449 (95%)	408 (96%)	17 (4%)	0	100	100
19	T	127/309 (41%)	109 (86%)	16 (13%)	2 (2%)	9	44
21	X	138/555 (25%)	133 (96%)	5 (4%)	0	100	100
22	Z	113/538 (21%)	110 (97%)	1 (1%)	2 (2%)	8	40
All	All	15928/24065 (66%)	14686 (92%)	1211 (8%)	31 (0%)	50	81

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	THR
2	B	1651	ASN
2	B	1652	PRO
2	B	2030	PRO
2	B	2461	PHE

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	3646/4145 (88%)	3599 (99%)	47 (1%)	69	81
3	C	3699/4196 (88%)	3670 (99%)	29 (1%)	81	89
4	D	297/609 (49%)	297 (100%)	0	100	100
4	d	89/609 (15%)	88 (99%)	1 (1%)	73	84
5	E	322/597 (54%)	321 (100%)	1 (0%)	92	95
5	e	42/597 (7%)	42 (100%)	0	100	100
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	Q	356/376 (95%)	286 (80%)	70 (20%)	1	8
17	U	356/376 (95%)	286 (80%)	70 (20%)	1	8
17	Y	356/376 (95%)	286 (80%)	70 (20%)	1	8
17	q	356/376 (95%)	286 (80%)	70 (20%)	1	8
17	u	356/376 (95%)	286 (80%)	70 (20%)	1	8
17	y	356/376 (95%)	286 (80%)	70 (20%)	1	8
18	R	363/376 (96%)	308 (85%)	55 (15%)	3	14
18	S	363/376 (96%)	308 (85%)	55 (15%)	3	14
18	W	363/376 (96%)	308 (85%)	55 (15%)	3	14
18	r	363/376 (96%)	308 (85%)	55 (15%)	3	14
18	s	363/376 (96%)	308 (85%)	55 (15%)	3	14
18	w	363/376 (96%)	308 (85%)	55 (15%)	3	14
19	T	118/271 (44%)	118 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	X	122/502 (24%)	121 (99%)	1 (1%)	81	89
22	Z	108/491 (22%)	107 (99%)	1 (1%)	78	87
All	All	13982/21339 (66%)	13142 (94%)	840 (6%)	23	44

5 of 840 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	Z	180	LYS
17	u	322	SER
17	y	175	VAL
18	s	117	LEU
17	Y	417	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 257 such sidechains are listed below:

Mol	Chain	Res	Type
17	u	48	ASN
18	r	133	GLN
3	C	357	ASN
3	C	218	ASN
17	q	105	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 6 are monoatomic - leaving 15 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
25	GDP	u	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
24	ATP	C	4702	-	26,33,33	1.01	2 (7%)	31,52,52	1.56	4 (12%)
25	GDP	y	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
26	GTP	s	501	27	26,34,34	1.13	2 (7%)	32,54,54	1.56	7 (21%)
26	GTP	r	501	27	26,34,34	1.12	2 (7%)	32,54,54	1.56	7 (21%)
26	GTP	R	501	27	26,34,34	1.12	2 (7%)	32,54,54	1.56	7 (21%)
23	ADP	C	4701	-	24,29,29	0.95	1 (4%)	29,45,45	2.81	8 (27%)
26	GTP	W	501	27	26,34,34	1.12	2 (7%)	32,54,54	1.56	7 (21%)
25	GDP	U	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
25	GDP	q	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
26	GTP	w	501	27	26,34,34	1.12	2 (7%)	32,54,54	1.56	7 (21%)
25	GDP	Y	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
23	ADP	C	4703	-	24,29,29	1.59	4 (16%)	29,45,45	3.98	13 (44%)
25	GDP	Q	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
26	GTP	S	501	27	26,34,34	1.13	2 (7%)	32,54,54	1.56	7 (21%)

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
25	GDP	u	501	-	-	2/12/32/32	0/3/3/3
24	ATP	C	4702	-	-	1/18/38/38	0/3/3/3
25	GDP	y	501	-	-	2/12/32/32	0/3/3/3
26	GTP	s	501	27	-	3/18/38/38	0/3/3/3
26	GTP	r	501	27	-	3/18/38/38	0/3/3/3
26	GTP	R	501	27	-	3/18/38/38	0/3/3/3
23	ADP	C	4701	-	-	5/12/32/32	0/3/3/3
26	GTP	W	501	27	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	GDP	U	501	-	-	2/12/32/32	0/3/3/3
25	GDP	q	501	-	-	2/12/32/32	0/3/3/3
26	GTP	w	501	27	-	3/18/38/38	0/3/3/3
25	GDP	Y	501	-	-	2/12/32/32	0/3/3/3
23	ADP	C	4703	-	-	4/12/32/32	0/3/3/3
25	GDP	Q	501	-	-	2/12/32/32	0/3/3/3
26	GTP	S	501	27	-	3/18/38/38	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	s	501	GTP	C5-C6	-4.02	1.39	1.47
26	r	501	GTP	C5-C6	-4.00	1.39	1.47
26	S	501	GTP	C5-C6	-3.99	1.39	1.47
26	w	501	GTP	C5-C6	-3.99	1.39	1.47
26	W	501	GTP	C5-C6	-3.98	1.39	1.47

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	4703	ADP	O4'-C1'-C2'	-14.20	86.18	106.93
23	C	4701	ADP	O5'-PA-O1A	-8.60	75.47	109.07
23	C	4703	ADP	C2'-C3'-C4'	-8.40	86.32	102.64
23	C	4701	ADP	O2A-PA-O1A	7.06	147.16	112.24
23	C	4703	ADP	C1'-N9-C4	6.74	138.49	126.64

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

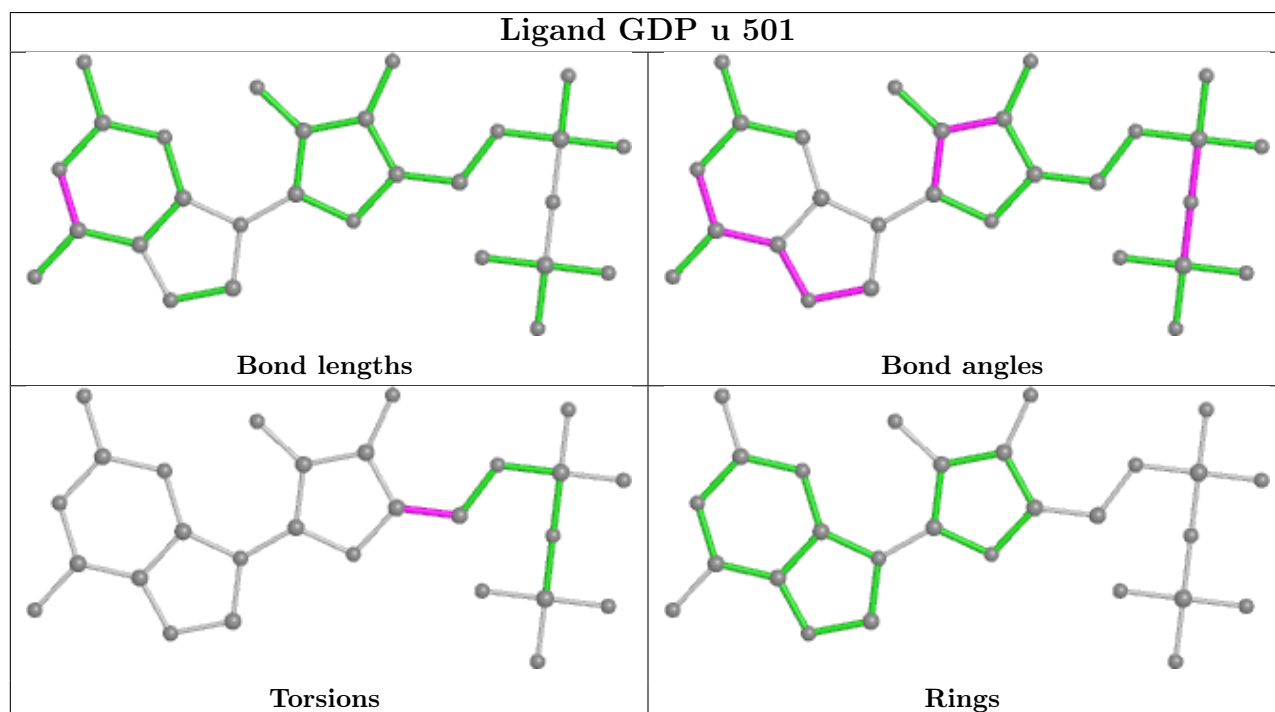
Mol	Chain	Res	Type	Atoms
23	C	4701	ADP	C5'-O5'-PA-O3A
23	C	4701	ADP	O4'-C4'-C5'-O5'
23	C	4701	ADP	C3'-C4'-C5'-O5'
26	R	501	GTP	C5'-O5'-PA-O3A
26	S	501	GTP	C5'-O5'-PA-O3A

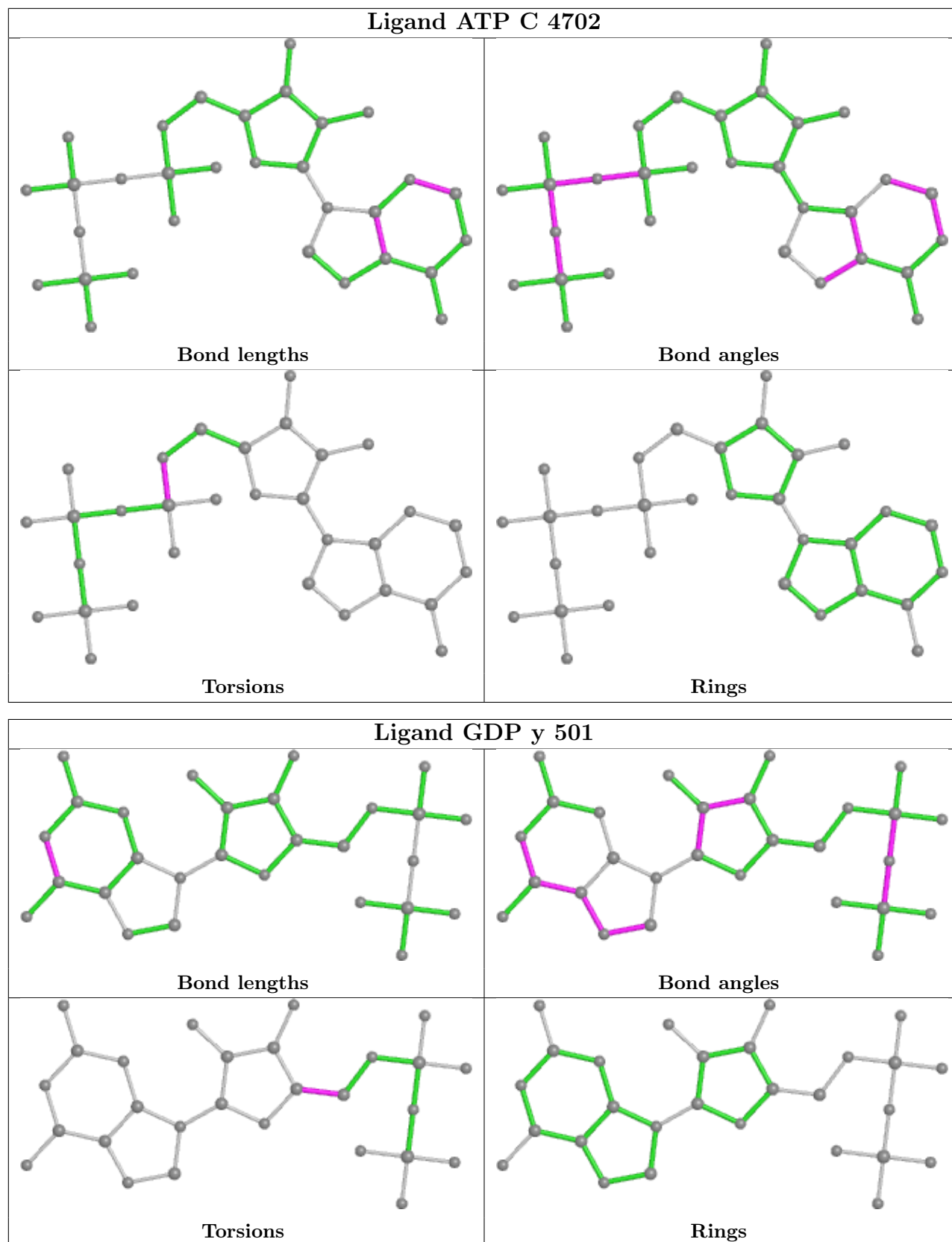
There are no ring outliers.

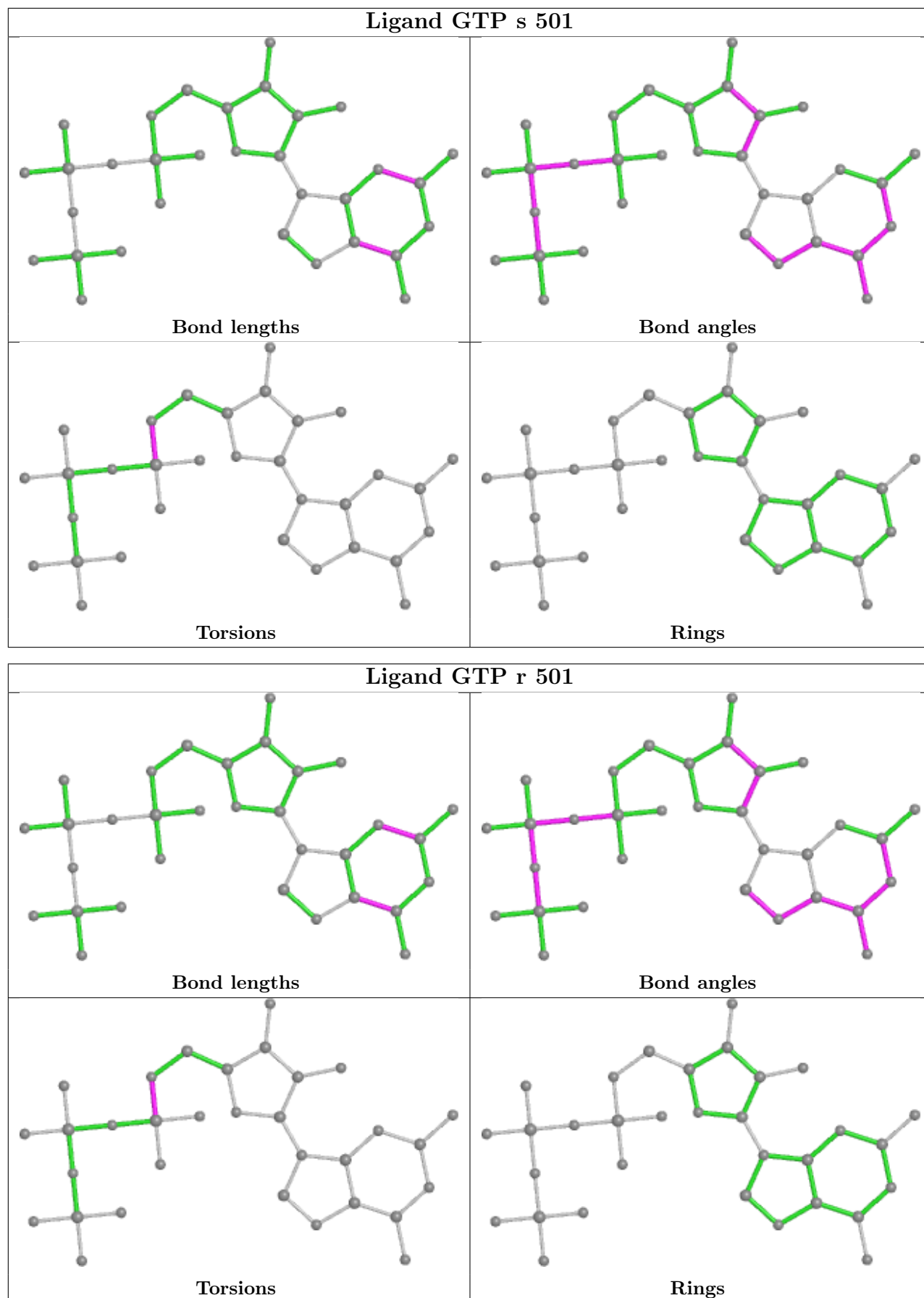
No monomer is involved in short contacts.

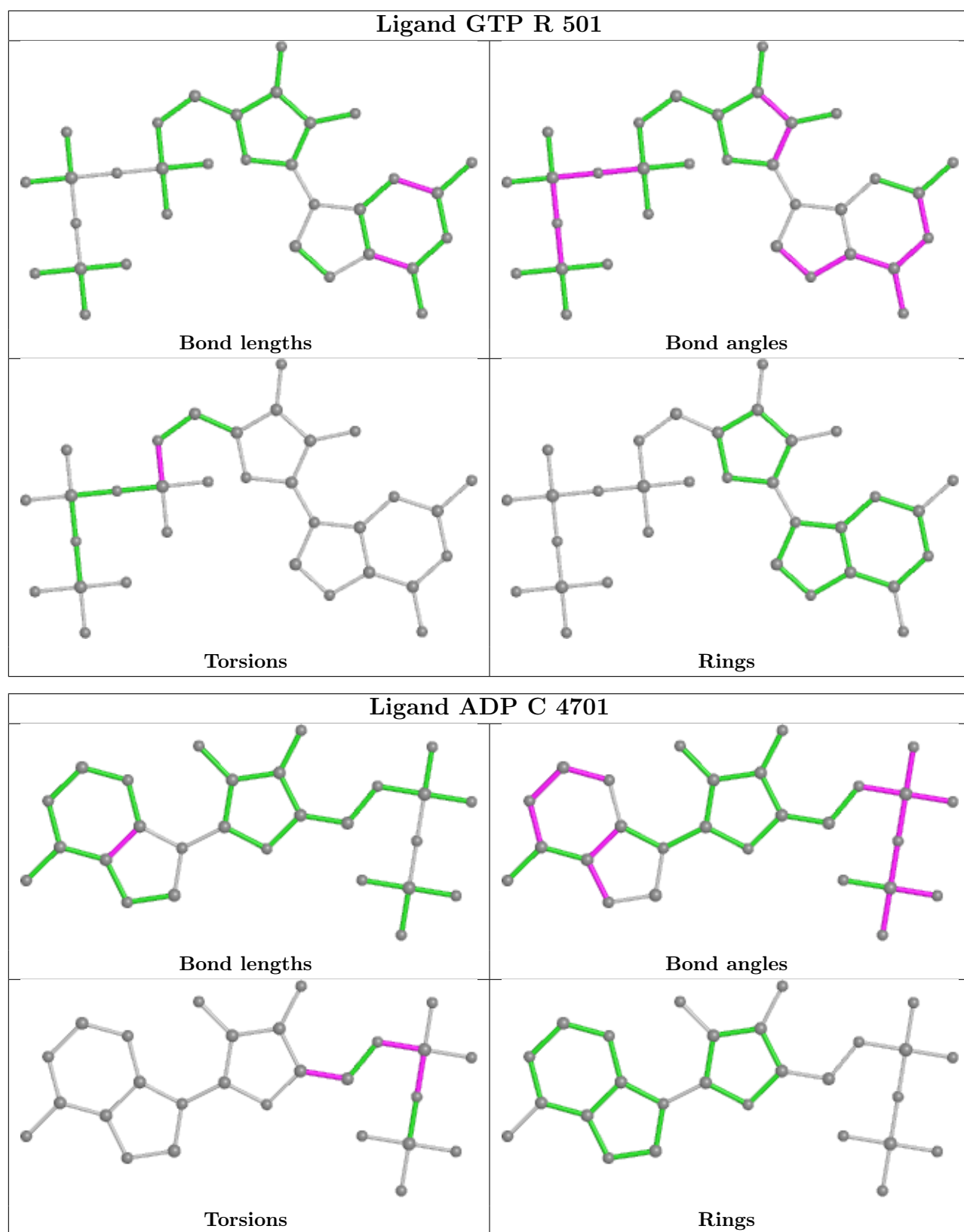
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

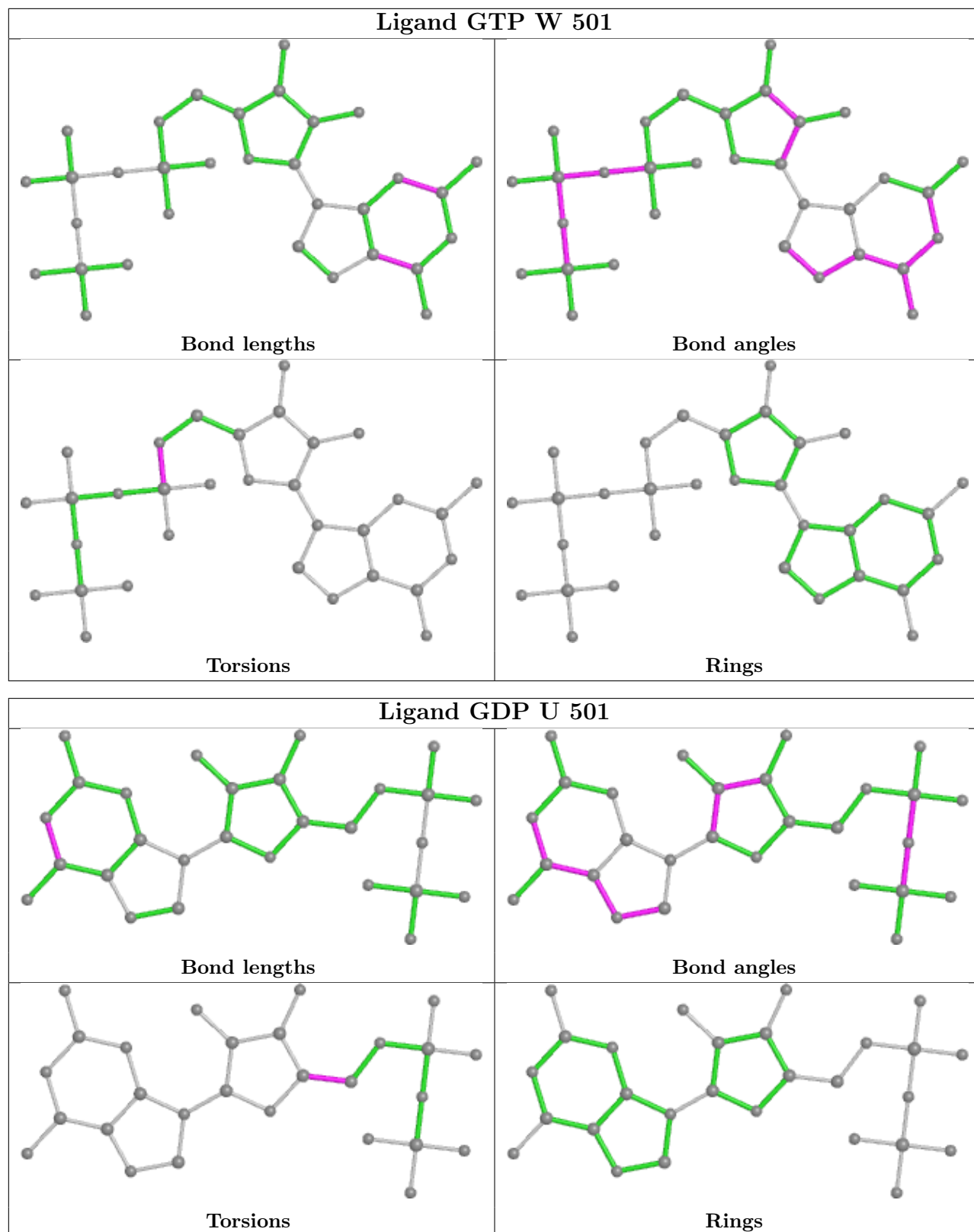
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

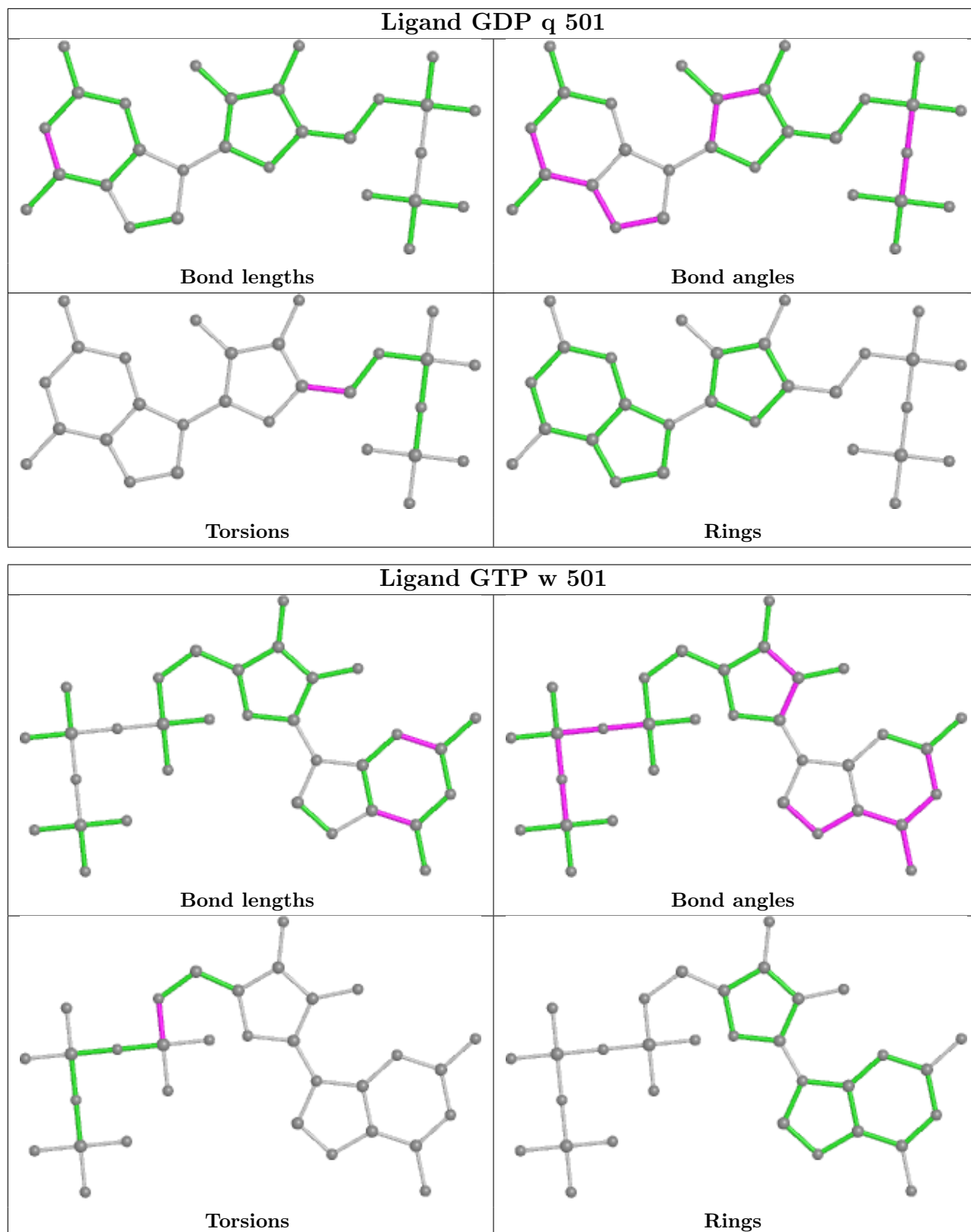


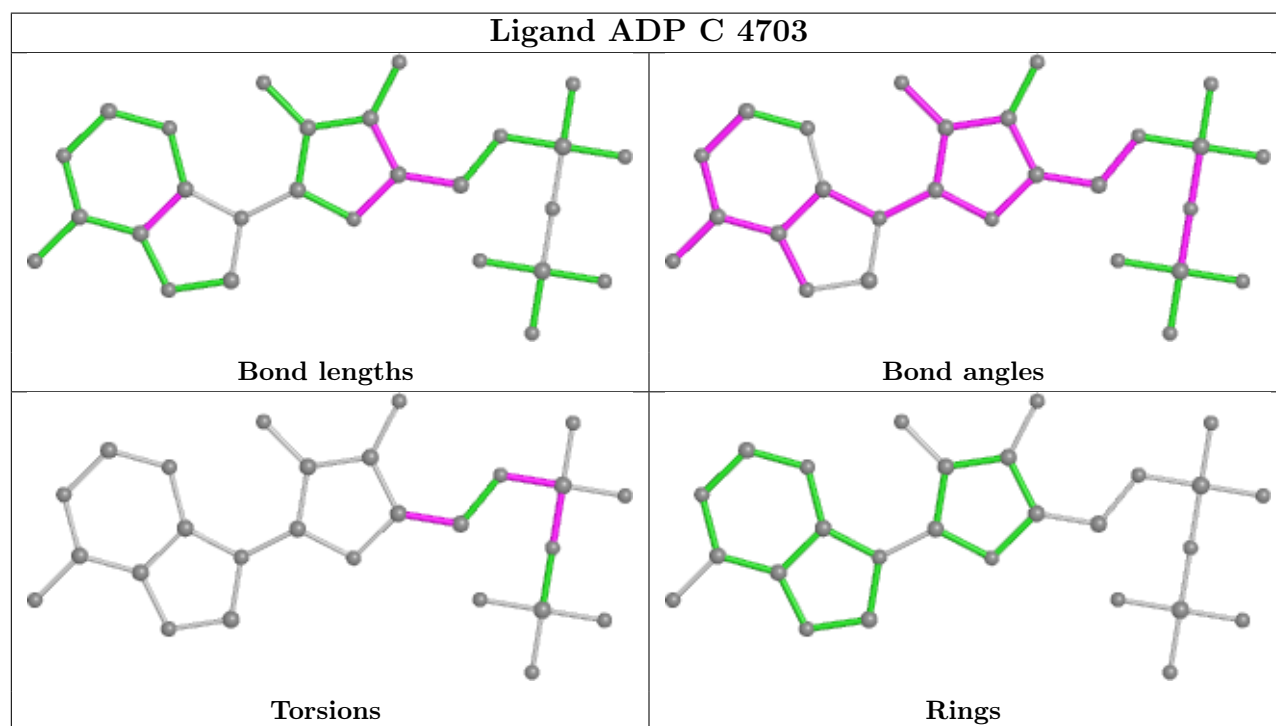
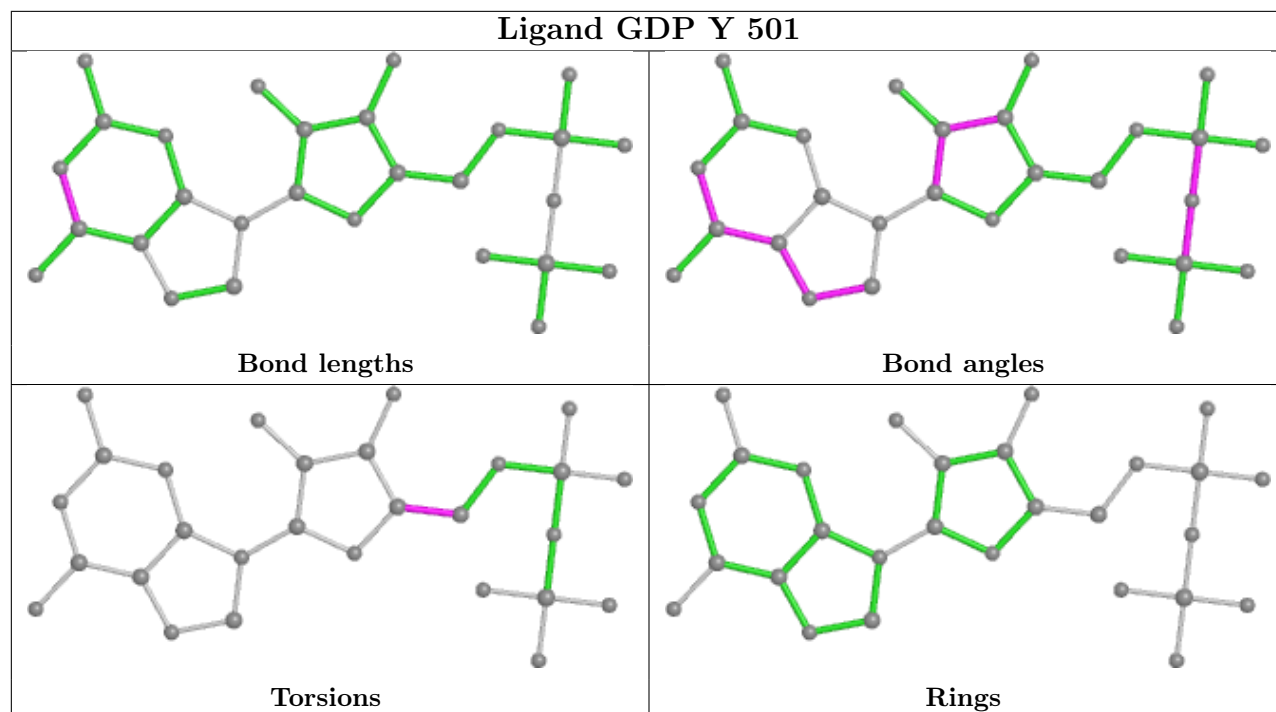


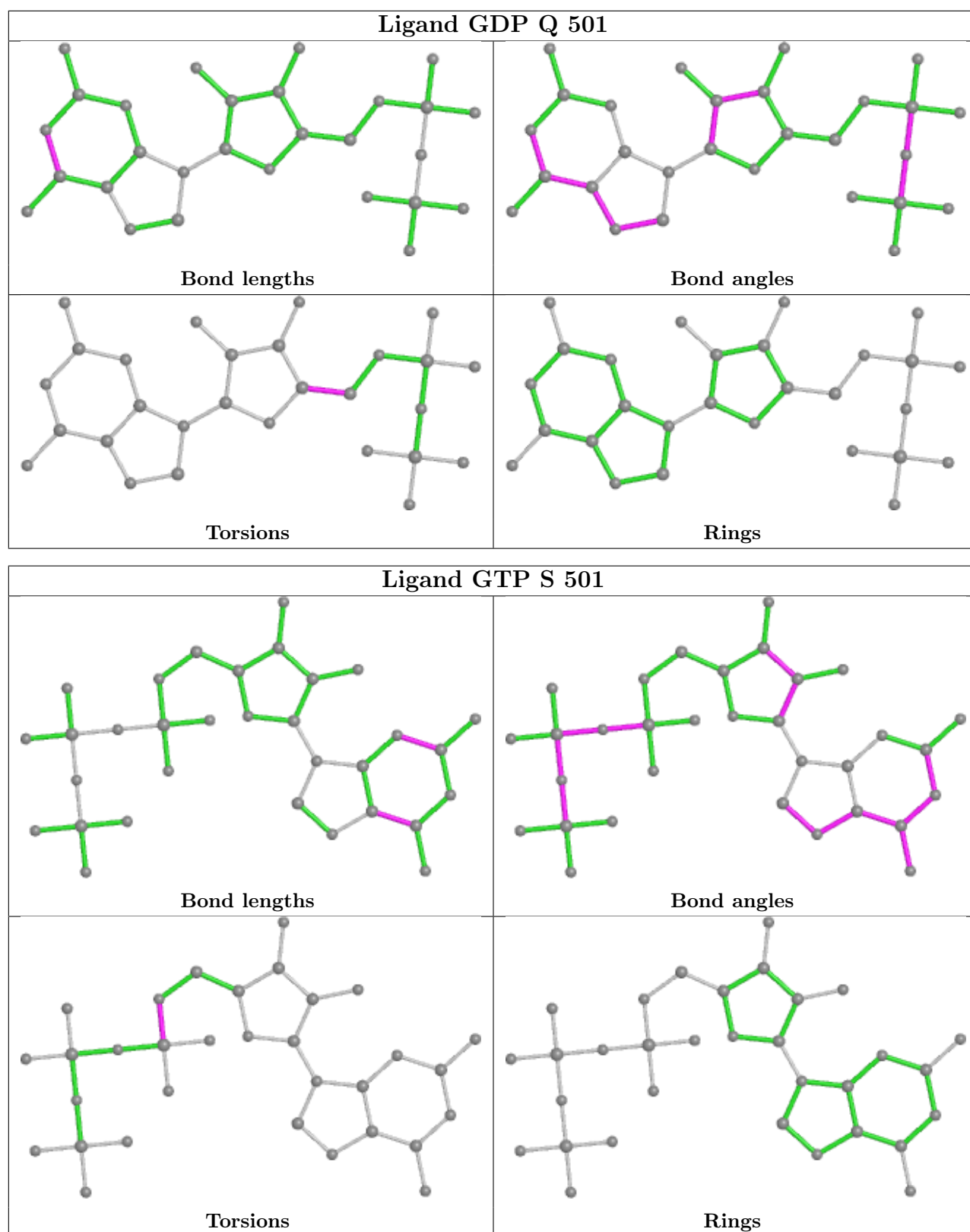












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	E	3
20	V	1
20	x	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	161:UNK	C	202:UNK	N	59.24
1	x	161:UNK	C	202:UNK	N	58.84
1	E	566:LEU	C	577:ALA	N	29.14
1	E	531:ARG	C	535:GLN	N	19.87
1	E	594:GLU	C	605:LYS	N	15.83

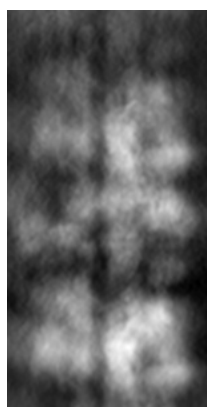
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23926. These allow visual inspection of the internal detail of the map and identification of artifacts.

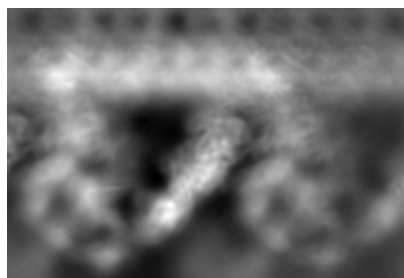
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

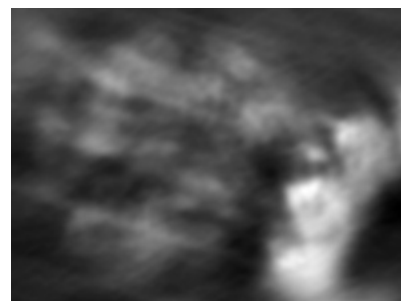
6.1.1 Primary map



X



Y

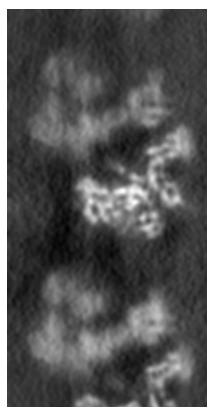


Z

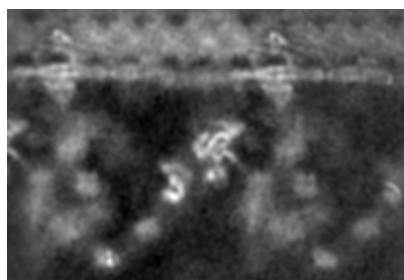
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

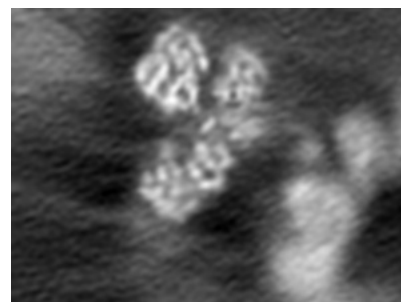
6.2.1 Primary map



X Index: 57



Y Index: 42



Z Index: 84

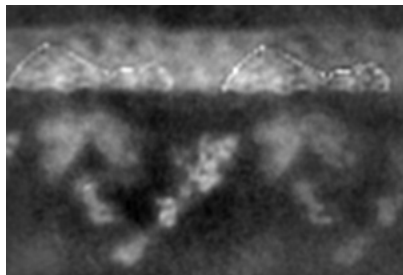
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

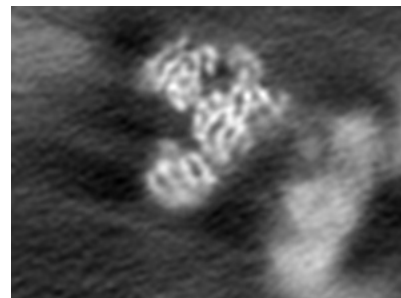
6.3.1 Primary map



X Index: 86



Y Index: 32



Z Index: 88

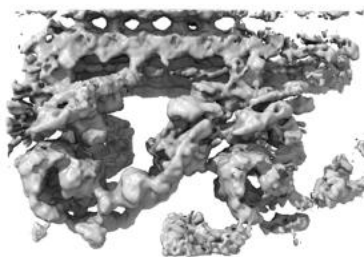
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

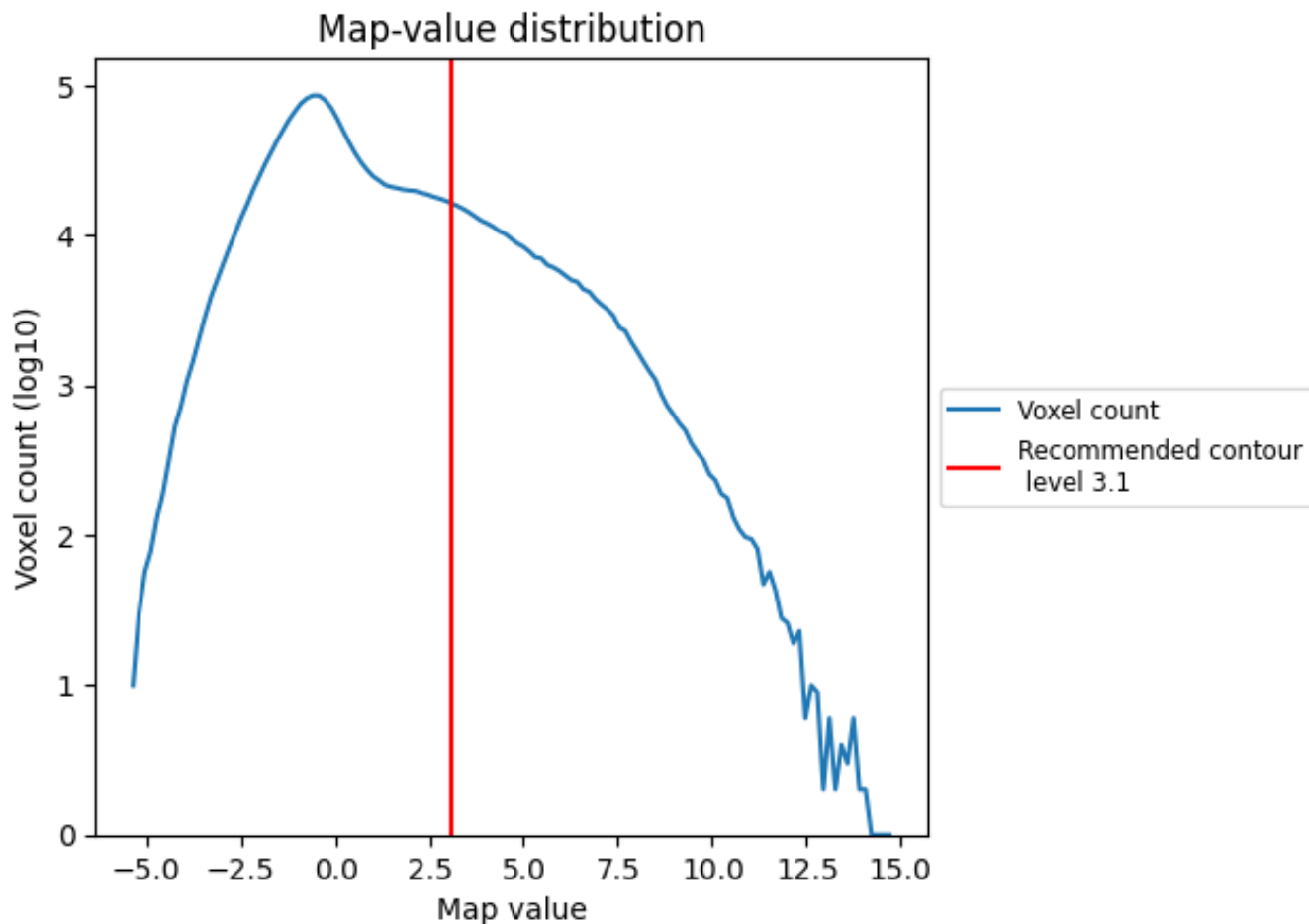
6.5 Mask visualisation

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

7 Map analysis [i](#)

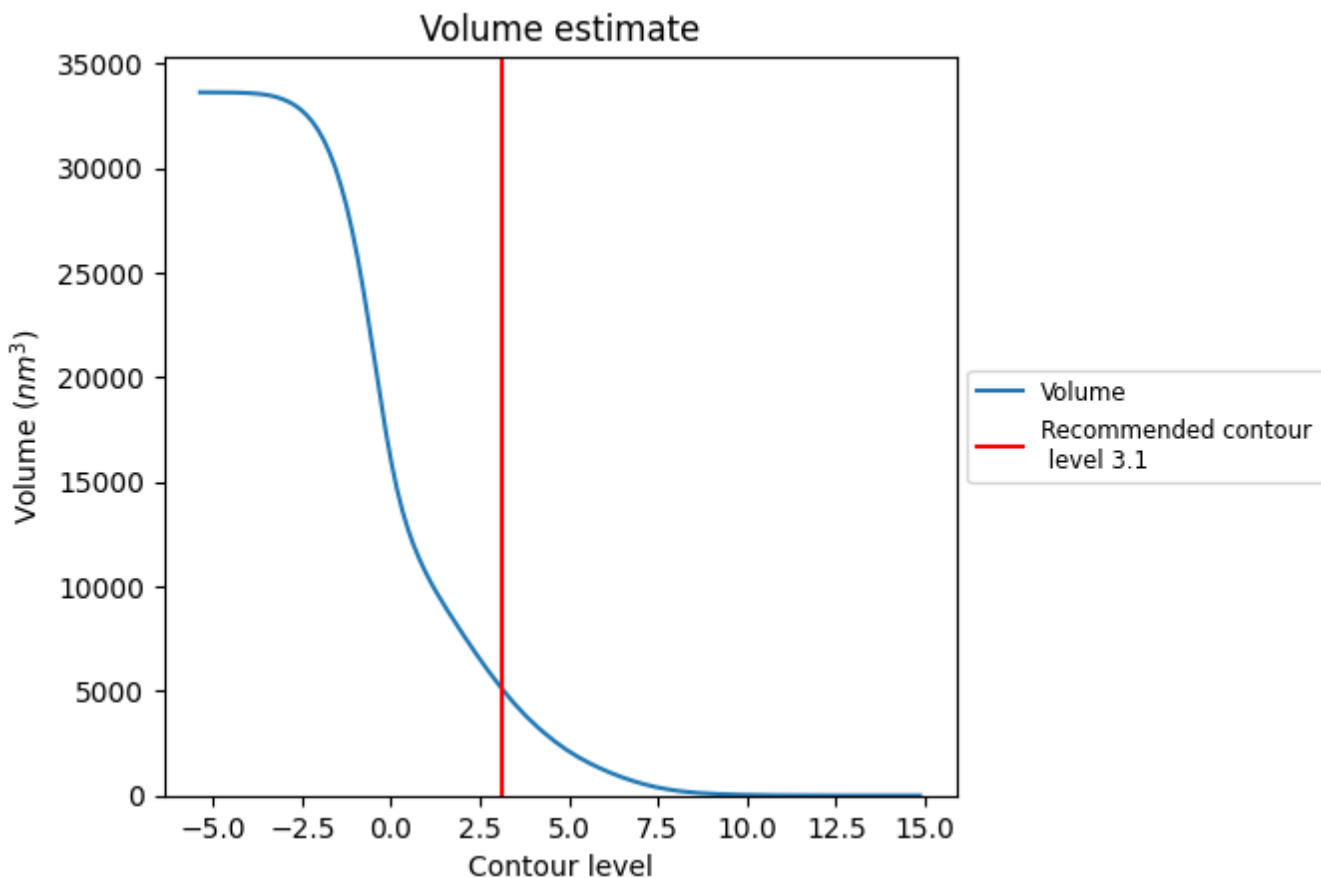
This section contains the results of statistical analysis of the map.

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 5148 nm³; this corresponds to an approximate mass of 4650 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

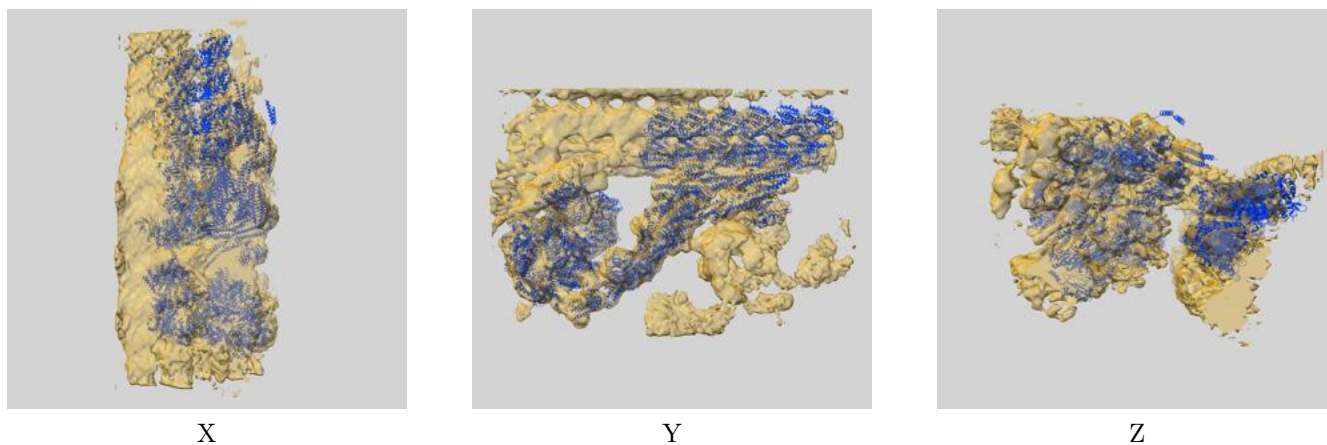
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

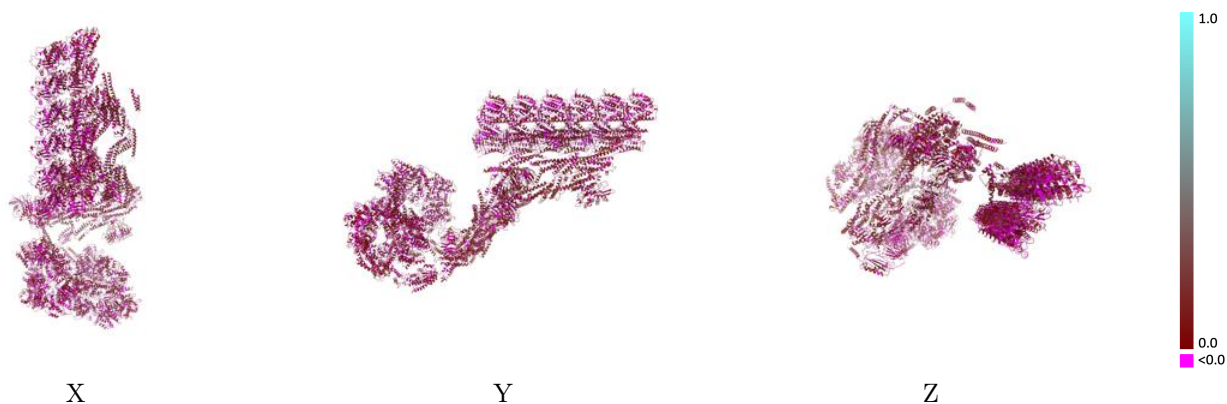
This section contains information regarding the fit between EMDB map EMD-23926 and PDB model 7MOQ. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



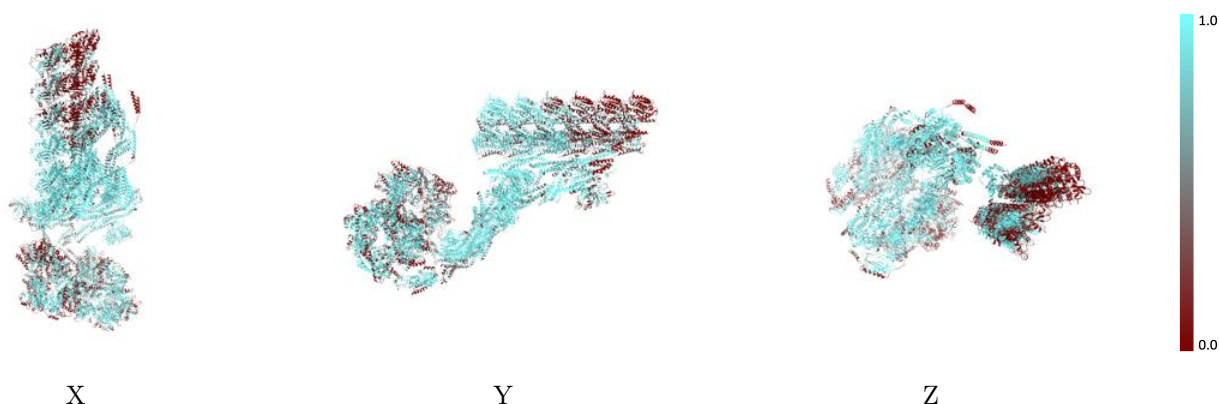
The images above show the 3D surface view of the map at the recommended contour level 3.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



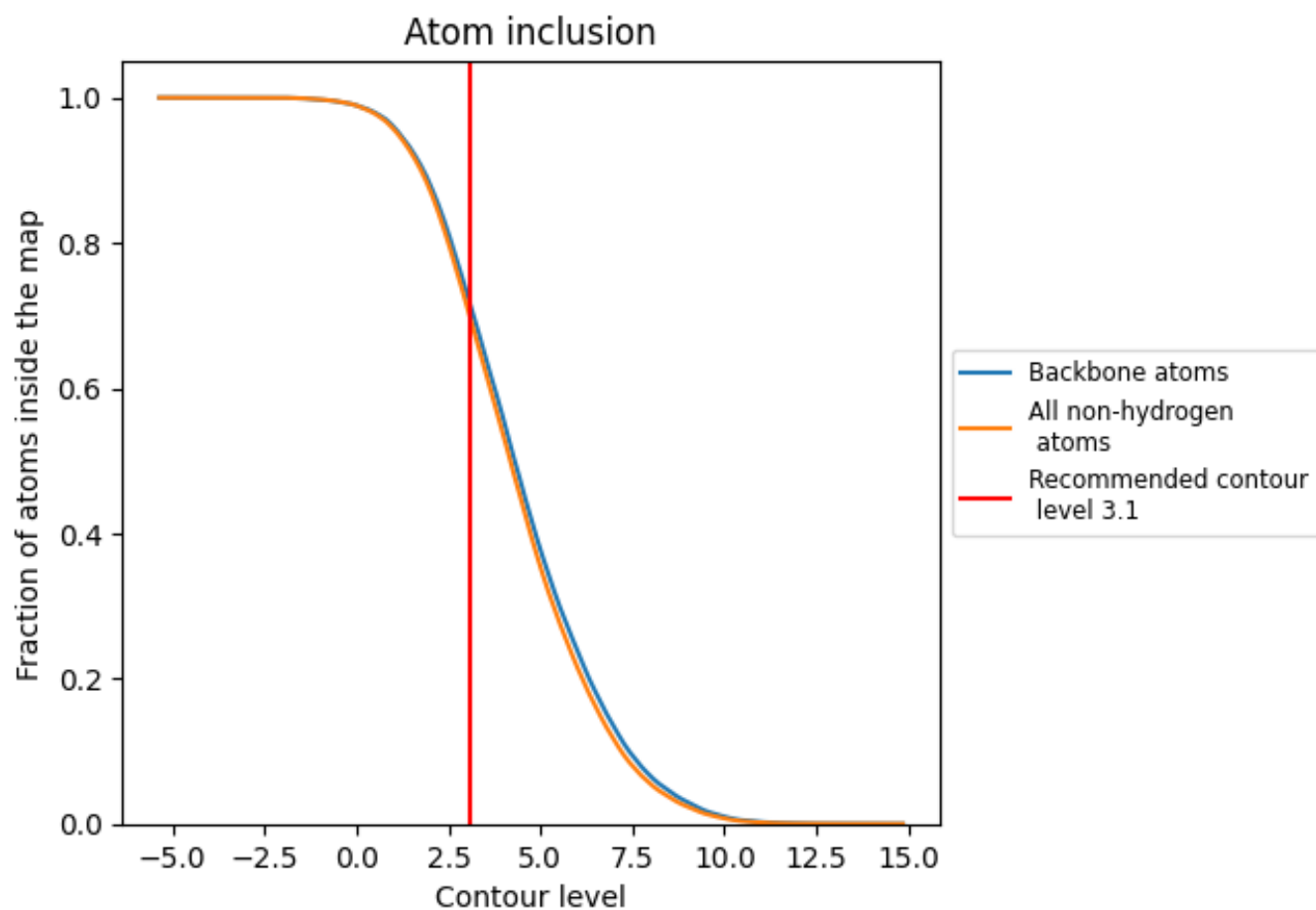
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.1).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 70% 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 (3.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6957	 0.0670
A	 0.9339	 0.0870
B	 0.7122	 0.0750
C	 0.6662	 0.0700
D	 0.9627	 0.1060
E	 0.8603	 0.0950
F	 0.9779	 0.1290
G	 0.9441	 0.1420
H	 0.9360	 0.1260
I	 0.9013	 0.1210
J	 0.8903	 0.0960
K	 0.8679	 0.0410
L	 0.7715	 0.0560
M	 0.9287	 0.0870
N	 0.8144	 0.0540
O	 0.6935	 0.0750
P	 0.8551	 0.0730
Q	 0.9428	 0.0300
R	 0.9134	 0.0270
S	 0.9415	 0.0250
T	 0.8722	 0.0870
U	 0.6192	 0.0270
V	 0.8163	 0.1200
W	 0.4647	 0.0350
X	 0.4591	 0.1170
Y	 0.4905	 0.0460
Z	 0.4943	 0.1210
d	 0.8625	 0.0940
e	 0.8417	 0.1200
q	 0.8906	 0.0480
r	 0.8684	 0.0360
s	 0.6107	 0.0400
u	 0.3230	 0.0620
w	 0.2133	 0.0700
x	 0.8178	 0.1580
y	 0.1663	 0.0460

