



## wwPDB EM Validation Summary Report ⓘ

Nov 27, 2022 – 11:13 PM EST

PDB ID : 7KZM  
EMDB ID : EMD-23082  
Title : Outer dynein arm bound to doublet microtubules from *C. reinhardtii*  
Authors : Walton, T.; Wu, H.; Brown, A.B.  
Deposited on : 2020-12-10  
Resolution : 7.50 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](mailto: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

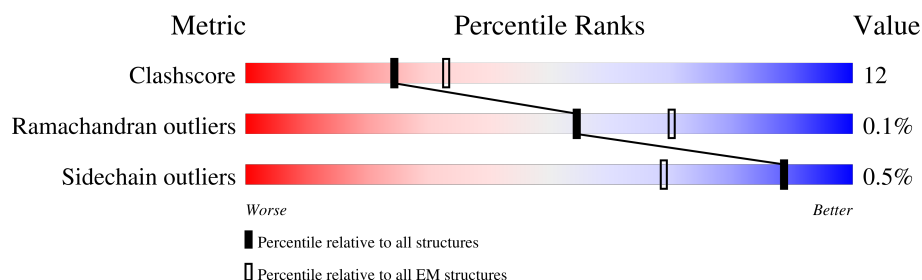
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.50 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A1	443	
1	A3	443	
1	A5	443	
1	A7	443	
1	B1	443	
1	B3	443	
1	B5	443	
1	B7	443	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	A2	451	
2	A4	451	
2	A6	451	
2	B2	451	
2	B4	451	
2	B6	451	
3	A	4503	
4	B	4568	
5	C	4485	
6	D	683	
7	E	567	
8	F	136	
9	G	159	
10	H	120	
11	I	105	
12	J	100	
13	K	91	
13	L	91	
13	M	91	
13	N	91	
14	O	117	
15	P	103	
16	X	749	
16	X1	749	
17	X0	162	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	Y	552	<div><div><div></div><div></div><div></div></div><div>8%5%87%</div></div>
18	Y1	552	<div><div><div></div><div></div><div></div></div><div>19%7%73%</div></div>
19	Y0	168	<div><div><div></div><div></div><div></div></div><div>11%99%</div></div>
20	Z	184	<div><div><div></div><div></div><div></div></div><div>20%60%31%8%</div></div>

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 124943 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 Tubulin beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A3	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A5	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A7	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	B1	419	Total	C	N	O	S	0	0
			3298	2077	563	628	30		
1	B3	410	Total	C	N	O	S	0	0
			3227	2030	553	614	30		
1	B5	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	B7	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		

- Molecule 2 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	430	Total	C	N	O	S	0	0
			3339	2114	568	636	21		
2	A4	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	A6	429	Total	C	N	O	S	0	0
			3335	2112	567	635	21		
2	B2	411	Total	C	N	O	S	0	0
			3204	2035	544	605	20		
2	B4	409	Total	C	N	O	S	0	0
			3193	2028	542	603	20		
2	B6	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

- Molecule 3 is a protein called Heavy chain alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	A	3275	Total	C	N	O	0	0
			16173	9623	3275	3275		

- Molecule 4 is a protein called Flagellar outer dynein arm heavy chain beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	3540	Total	C	N	O	S	0	0
			19163	11601	3735	3803	24		

- Molecule 5 is a protein called Dynein gamma chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	3890	Total	C	N	O	S	0	0
			21756	13184	4221	4314	37		

- Molecule 6 is a protein called Dynein, 78 kDa intermediate chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	456	Total	C	N	O	S	0	0
			3609	2297	610	678	24		

- Molecule 7 is a protein called Dynein, 70 kDa intermediate chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	474	Total	C	N	O	S	0	0
			3697	2332	623	725	17		

- Molecule 8 is a protein called Flagellar outer dynein arm light chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	F	100	Total	C	N	O	0	0
			495	295	100	100		

- Molecule 9 is a protein called Dynein 18 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	138	Total	C	N	O	S	0	0
			1089	677	183	220	9		

- Molecule 10 is a protein called Dynein 11 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	H	91	Total	C	N	O	0	0
			451	269	91	91		

- Molecule 11 is a protein called Dynein light chain roadblock LC7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	103	Total	C	N	O	S	0	0
			827	525	148	153	1		

- Molecule 12 is a protein called Dynein light chain roadblock LC7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	94	Total	C	N	O	S	0	0
			741	466	133	140	2		

- Molecule 13 is a protein called Dynein 8 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
13	L	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
13	M	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
13	N	82	Total	C	N	O		0	0
			407	243	82	82			

- Molecule 14 is a protein called Dynein light chain 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	97	Total	C	N	O	0	0
			481	286	97	98		

- Molecule 15 is a protein called Dynein light chain 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	98	Total	C	N	O	S	0	0
			805	523	128	146	8		

- Molecule 16 is a protein called Outer dynein arm-docking complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	56	Total	C	N	O	S	0	0
			481	292	97	89	3		
16	X1	142	Total	C	N	O	S	0	0
			1178	715	223	235	5		

- Molecule 17 is a protein called DC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X0	162	Total	C	N	O		0	0
			810	486	162	162			

- Molecule 18 is a protein called Outer dynein arm protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	73	Total	C	N	O	S	0	0
			595	360	112	120	3		
18	Y1	147	Total	C	N	O	S	0	0
			1185	729	223	224	9		

- Molecule 19 is a protein called DC2.

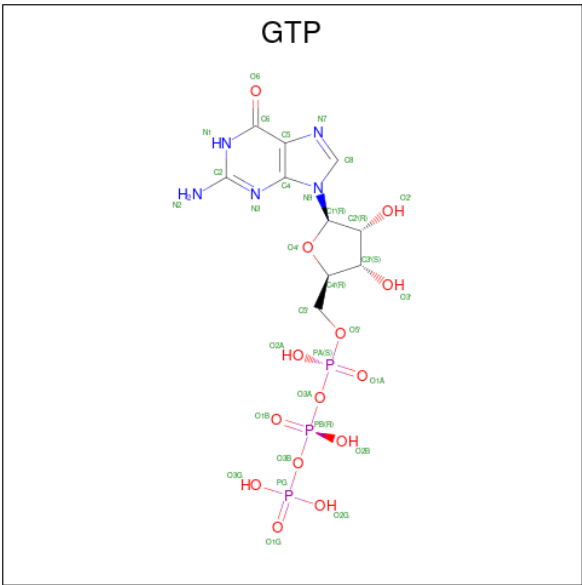
Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y0	168	Total	C	N	O		0	0
			840	504	168	168			

- Molecule 20 is a protein called Outer dynein arm-docking complex protein DC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	170	Total	C	N	O	S	0	0
			1384	863	242	270	9		

- Molecule 21 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).





Mol	Chain	Residues	Atoms					AltConf
21	A1	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	A3	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	A5	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	A7	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	B2	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	B5	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	B7	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

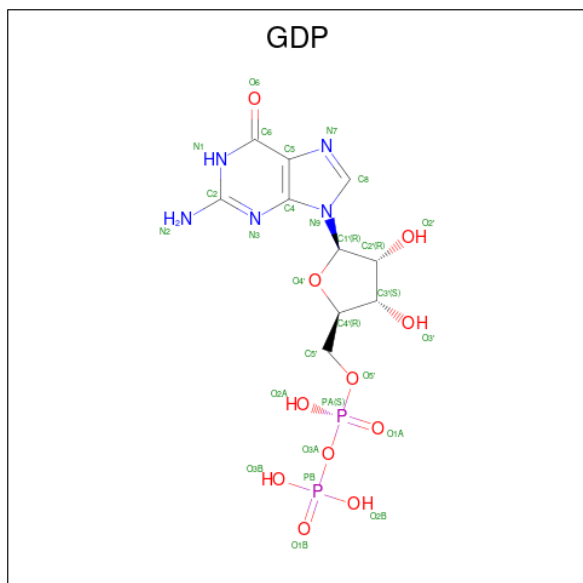
Mol	Chain	Residues	Atoms		AltConf
22	A1	1	Total	Mg	0
			1	1	
22	A2	1	Total	Mg	0
			1	1	
22	A4	1	Total	Mg	0
			1	1	
22	A6	1	Total	Mg	0
			1	1	
22	B3	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
22	B4	1	Total	Mg	0
			1	1	
22	B6	1	Total	Mg	0
			1	1	

- Molecule 23 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).

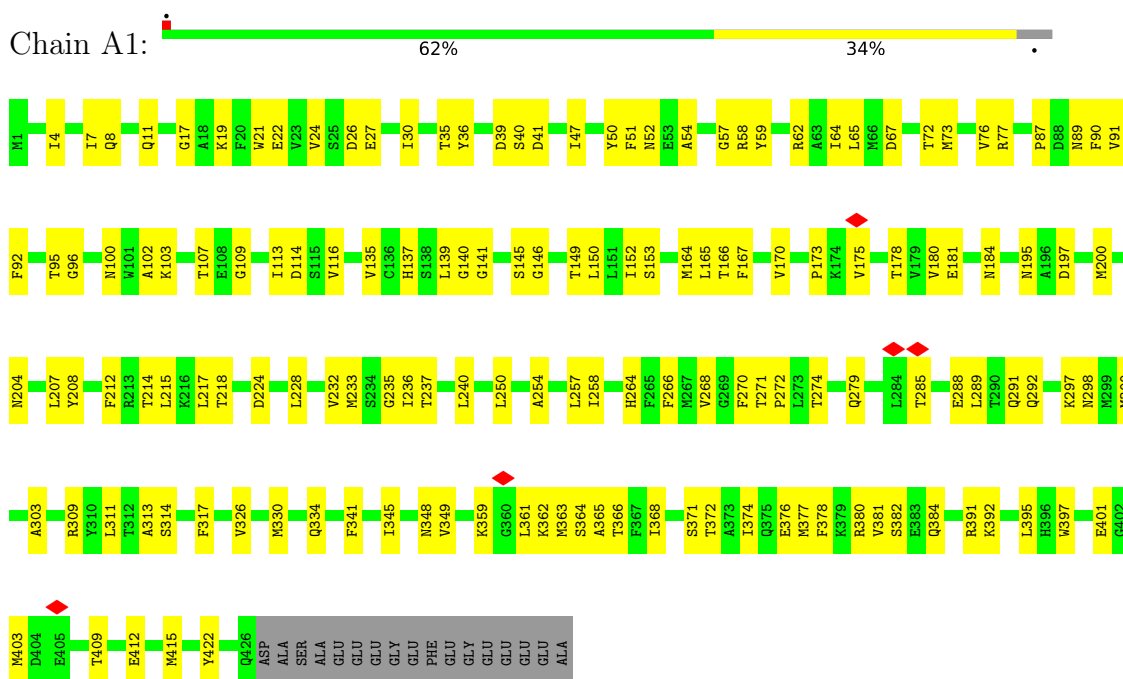


Mol	Chain	Residues	Atoms					AltConf
23	A1	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	A3	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	A5	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	A7	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	B1	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	B3	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	B5	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	B7	1	Total	C	N	O	P	0
			28	10	5	11	2	

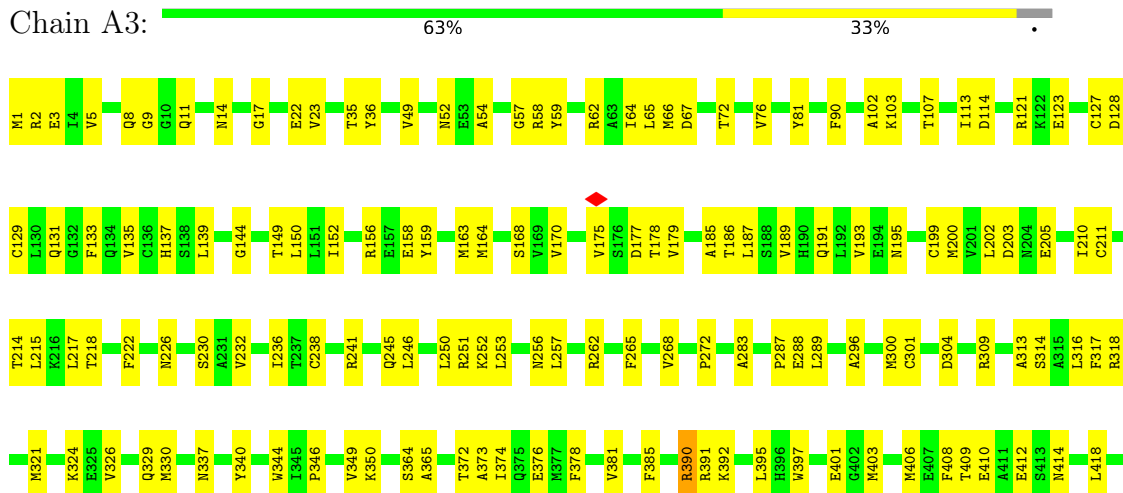
### 3 Residue-property plots

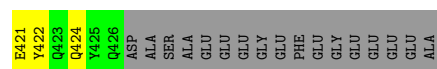
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Tubulin beta



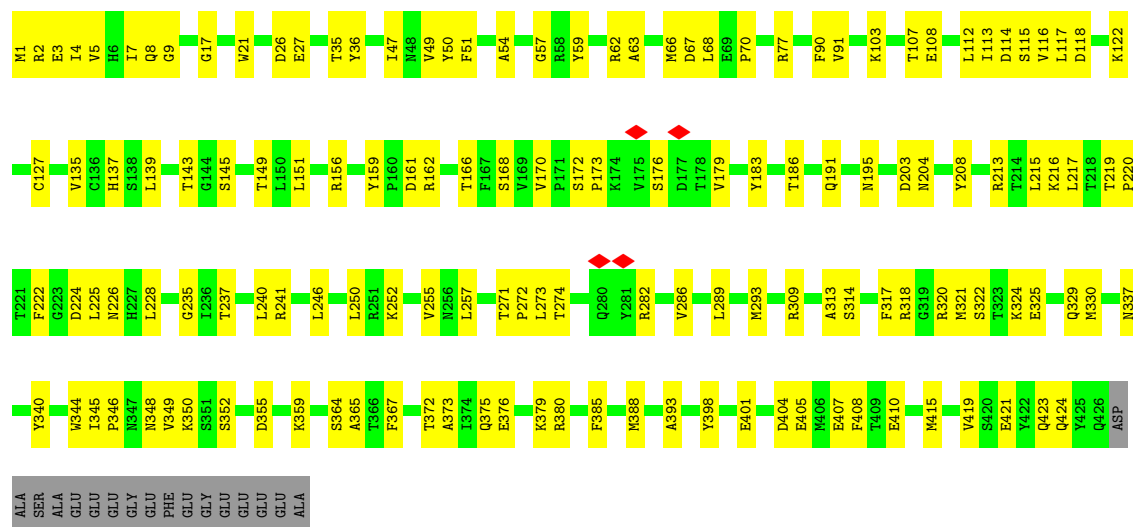
#### • Molecule 1: Tubulin beta





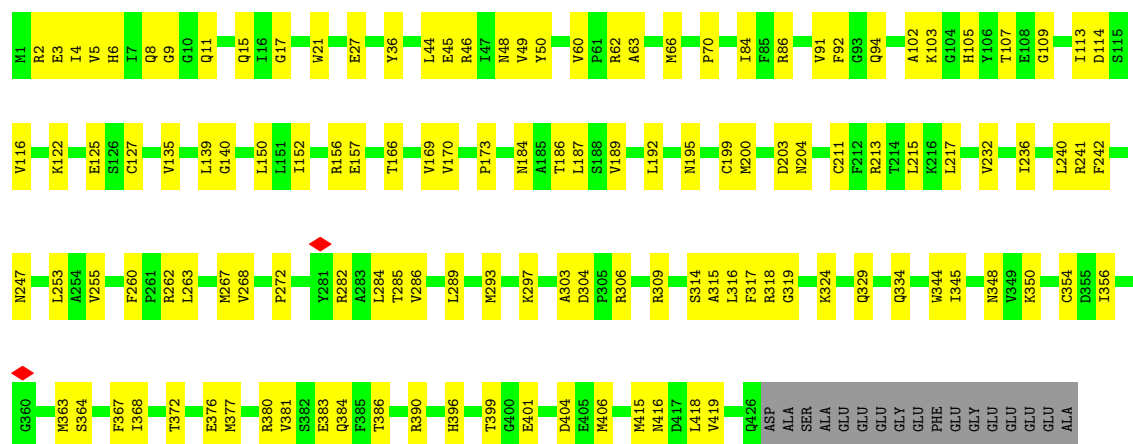
• Molecule 1: Tubulin beta

Chain A5: 64% 32%



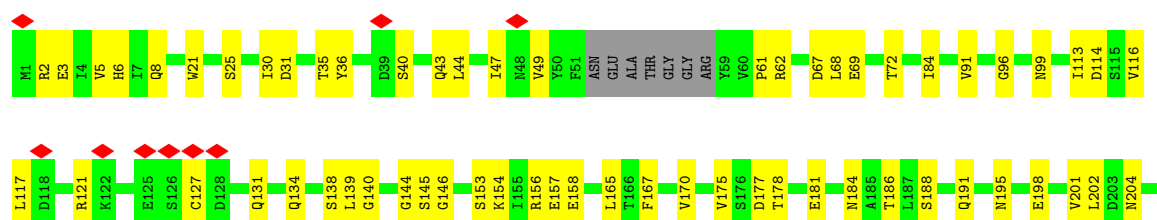
• Molecule 1: Tubulin beta

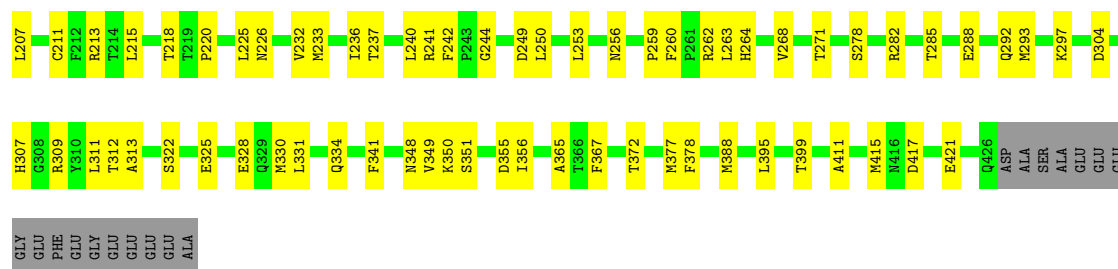
Chain A7: 67% 29%



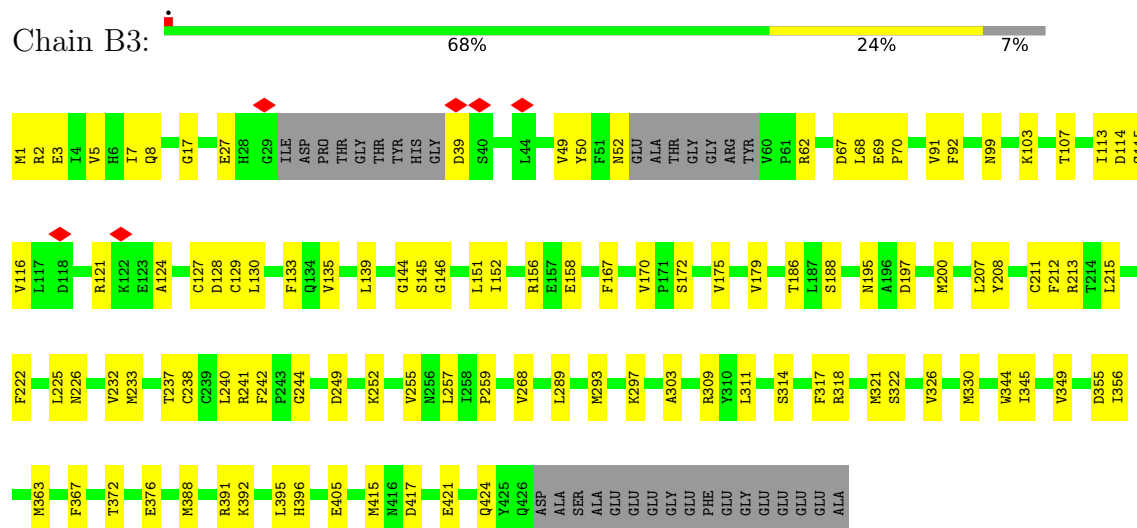
• Molecule 1: Tubulin beta

Chain B1: 66% 28% 5%

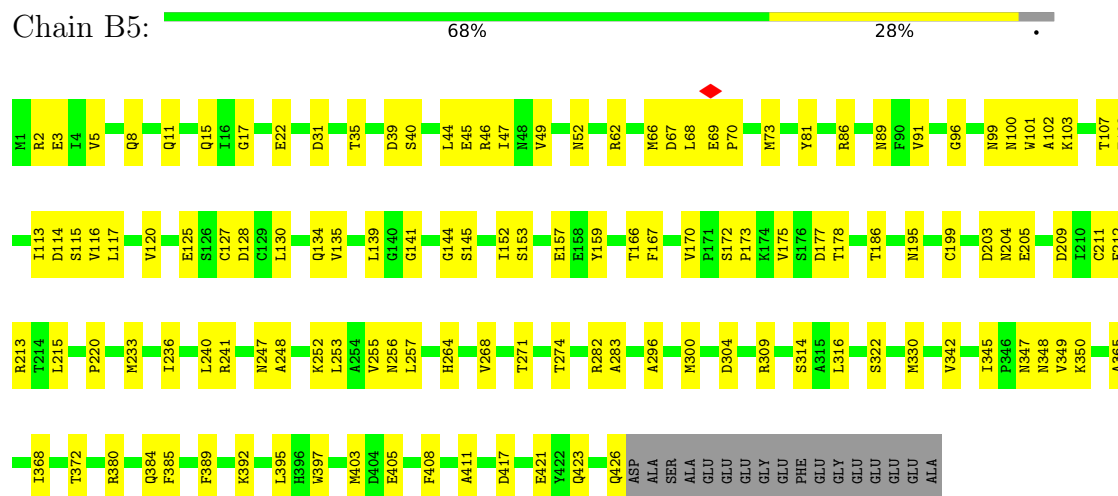




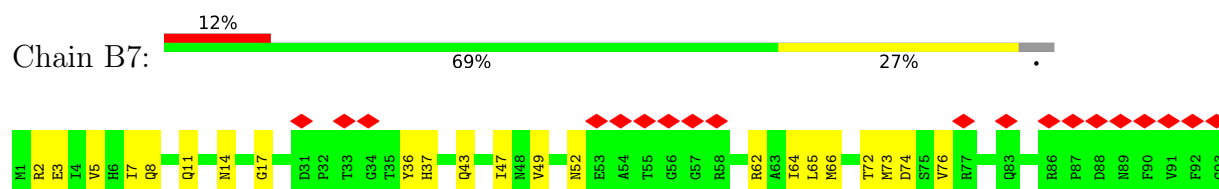
• Molecule 1: Tubulin beta

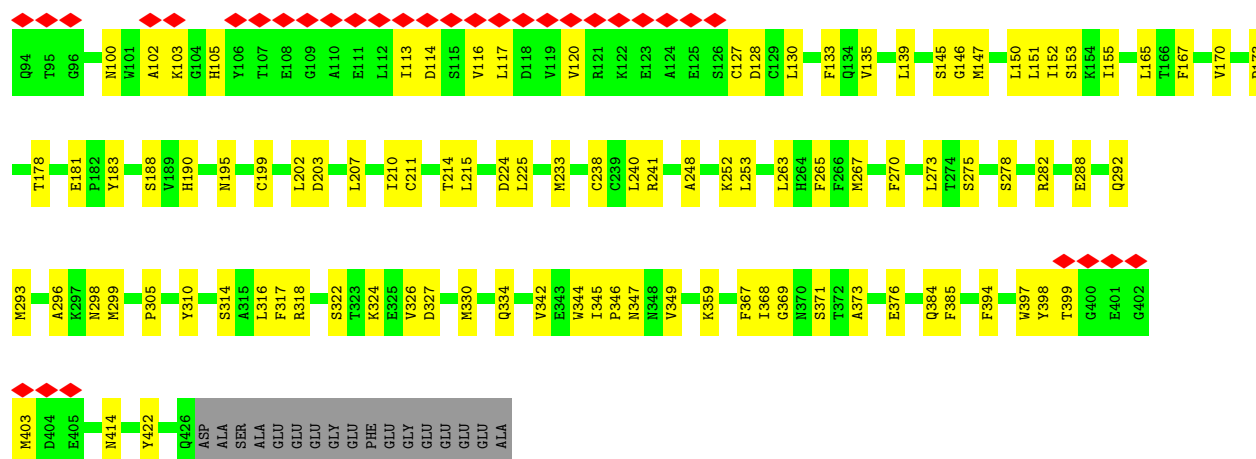


• Molecule 1: Tubulin beta



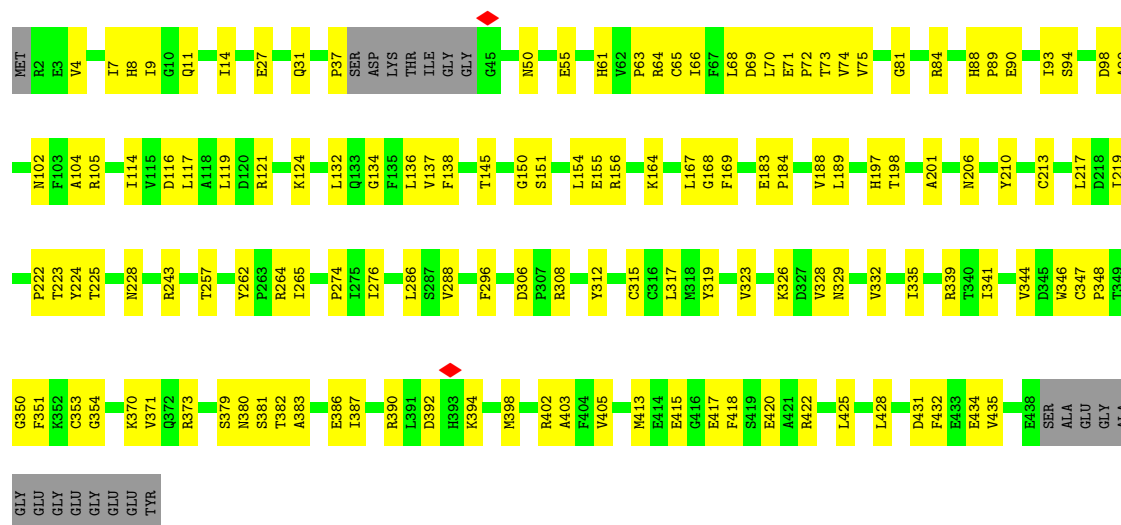
• Molecule 1: Tubulin beta





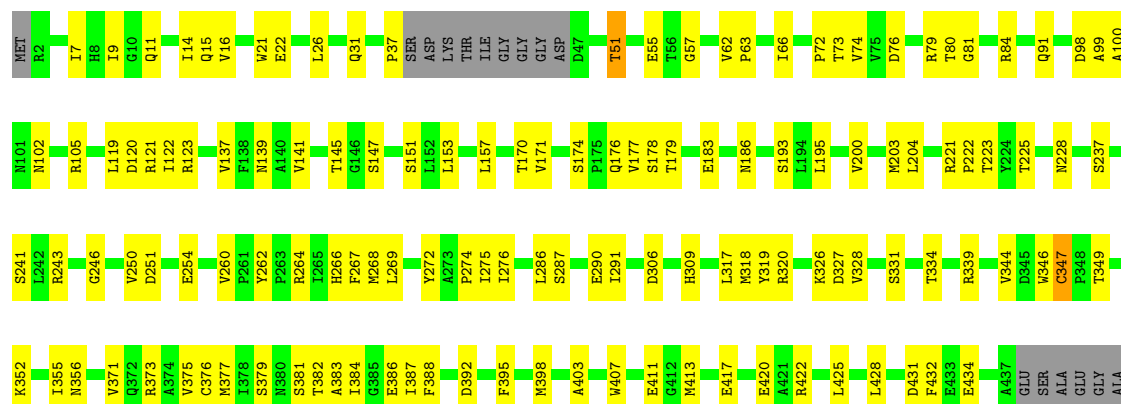
### • Molecule 2: Tubulin alpha

Chain A2:



### • Molecule 2: Tubulin alpha

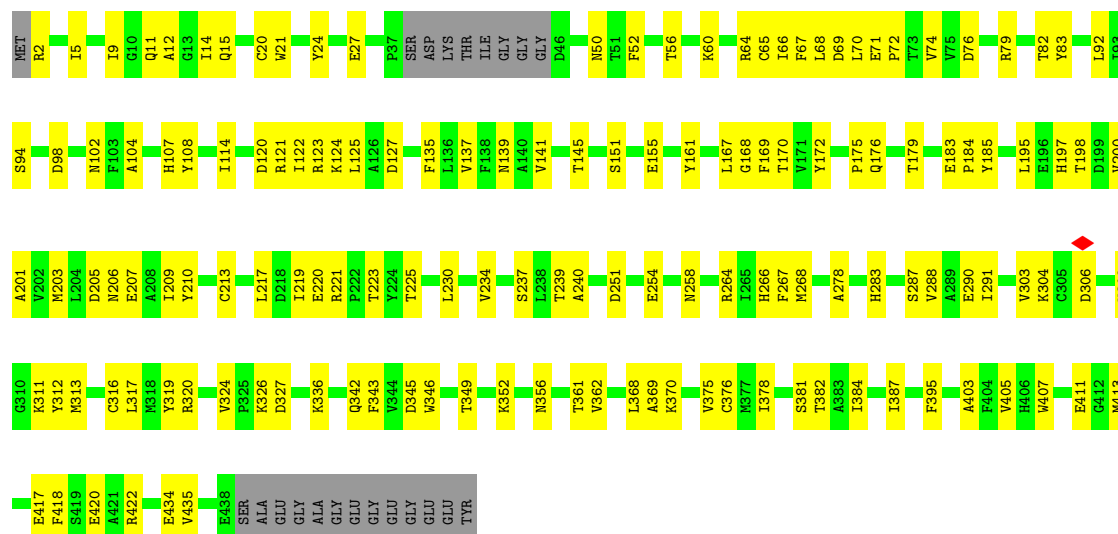
Chain A4:



GLY  
GLU  
GLY  
GLY  
GLY  
GLY  
GLY  
TYR

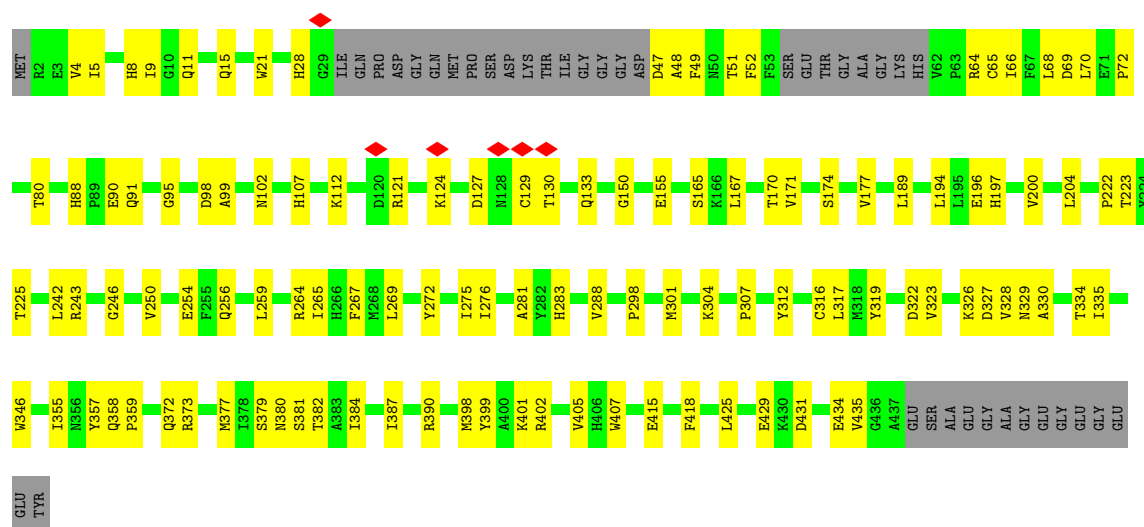
• Molecule 2: Tubulin alpha

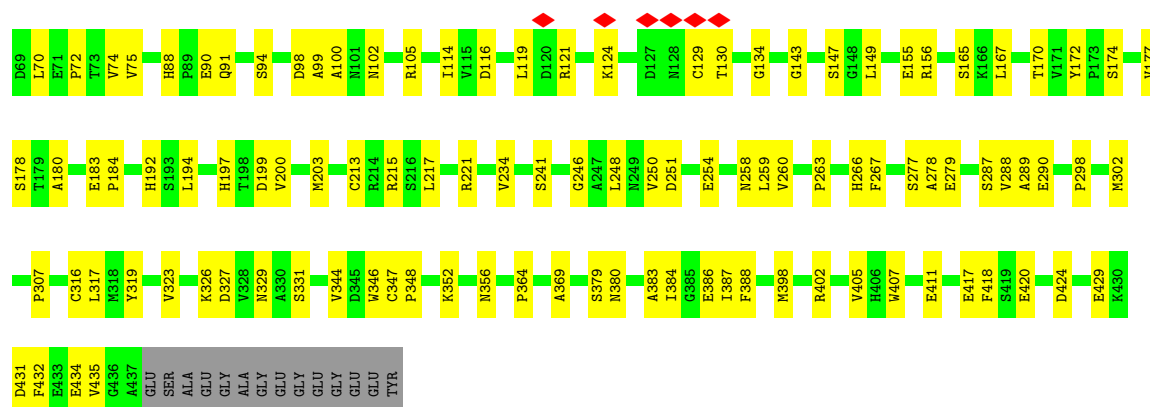
Chain A6: 63% 32% 5%



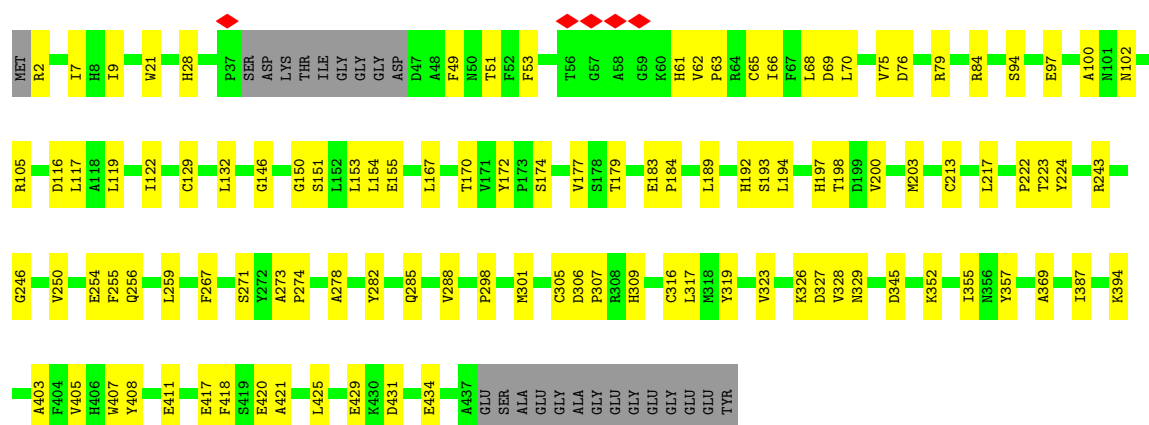
• Molecule 2: Tubulin alpha

Chain B2: 66% 25% 9%

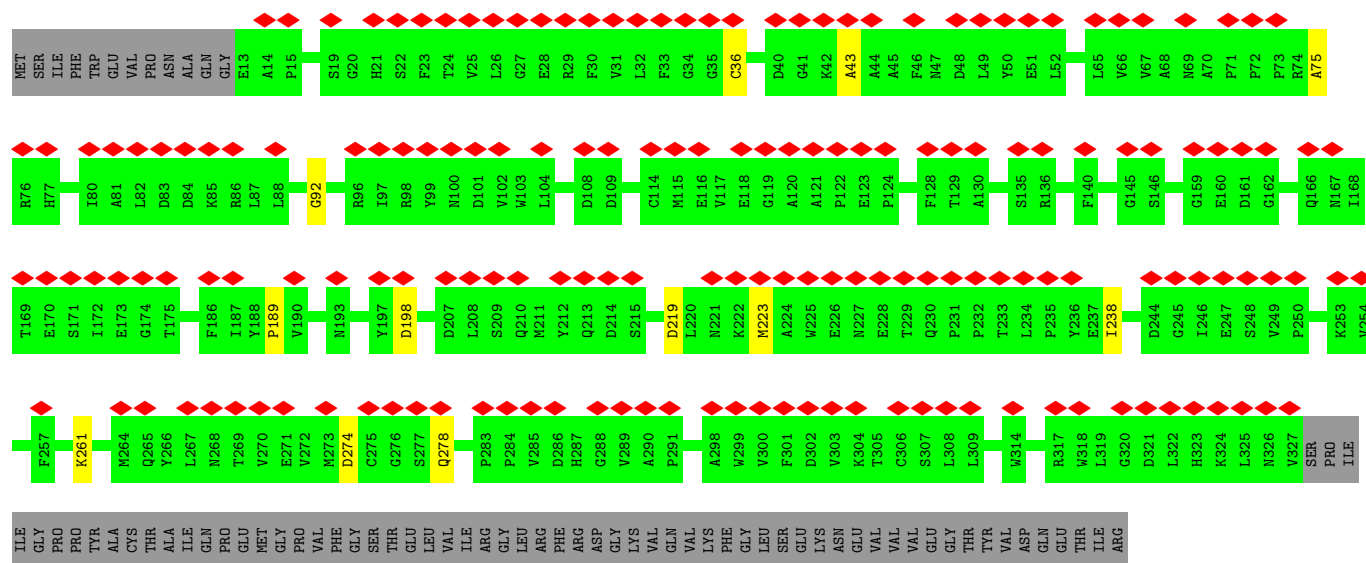




• Molecule 2: Tubulin alpha

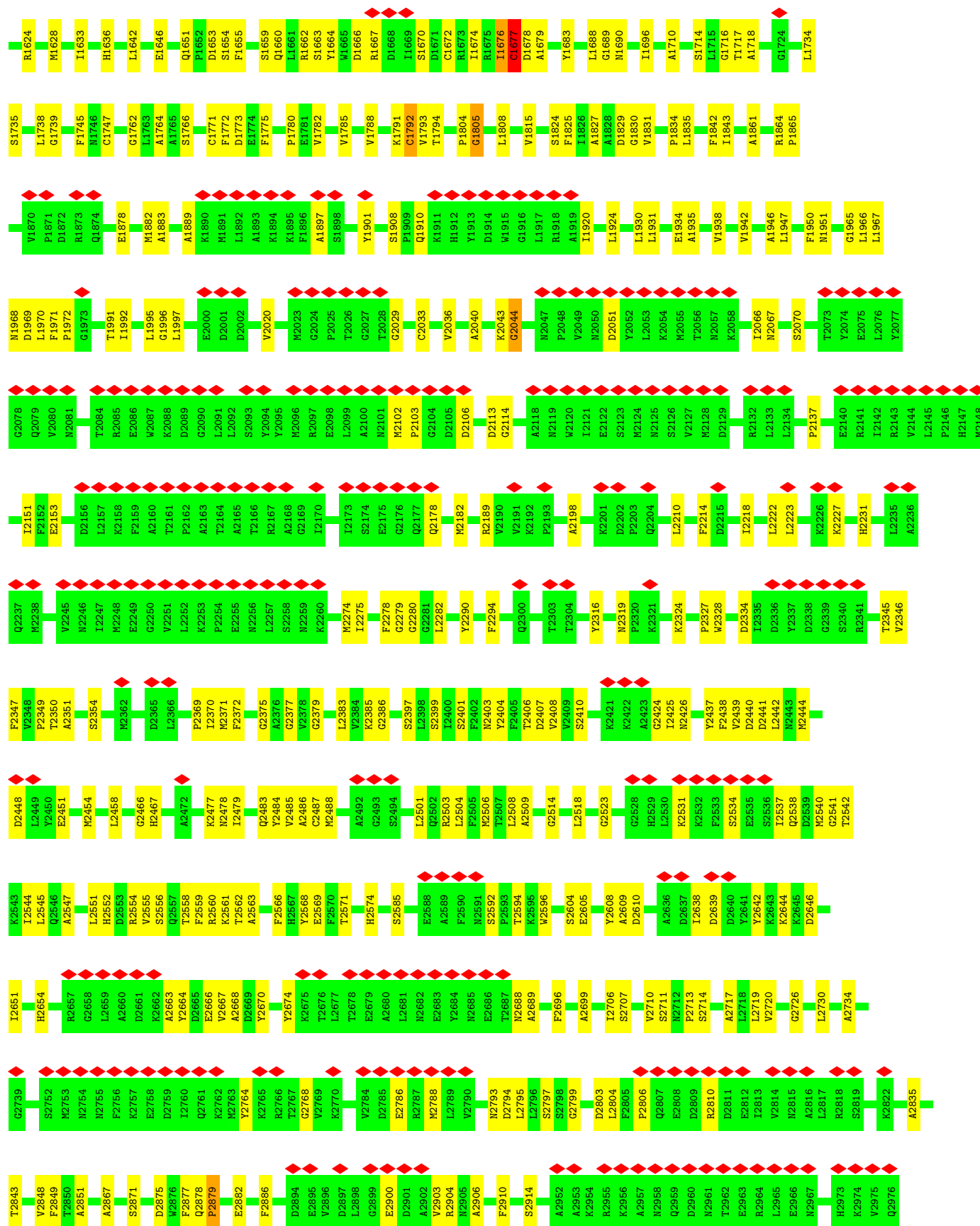


• Molecule 3: Heavy chain alpha

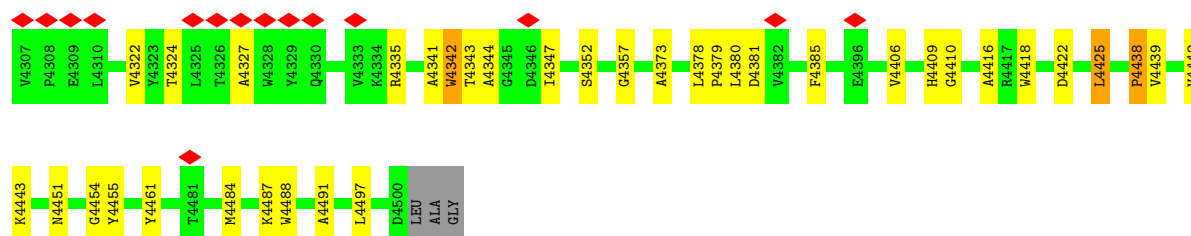




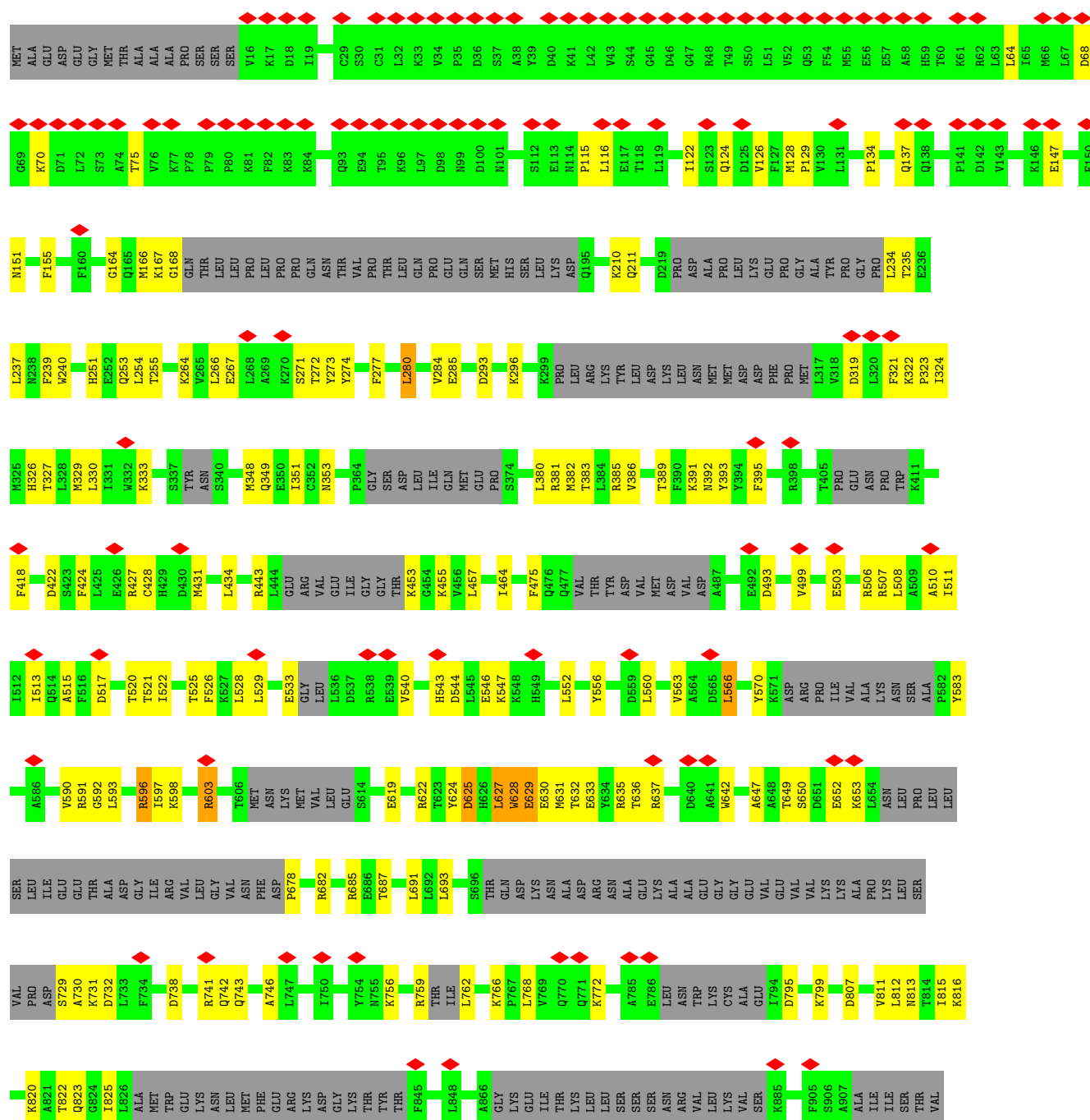






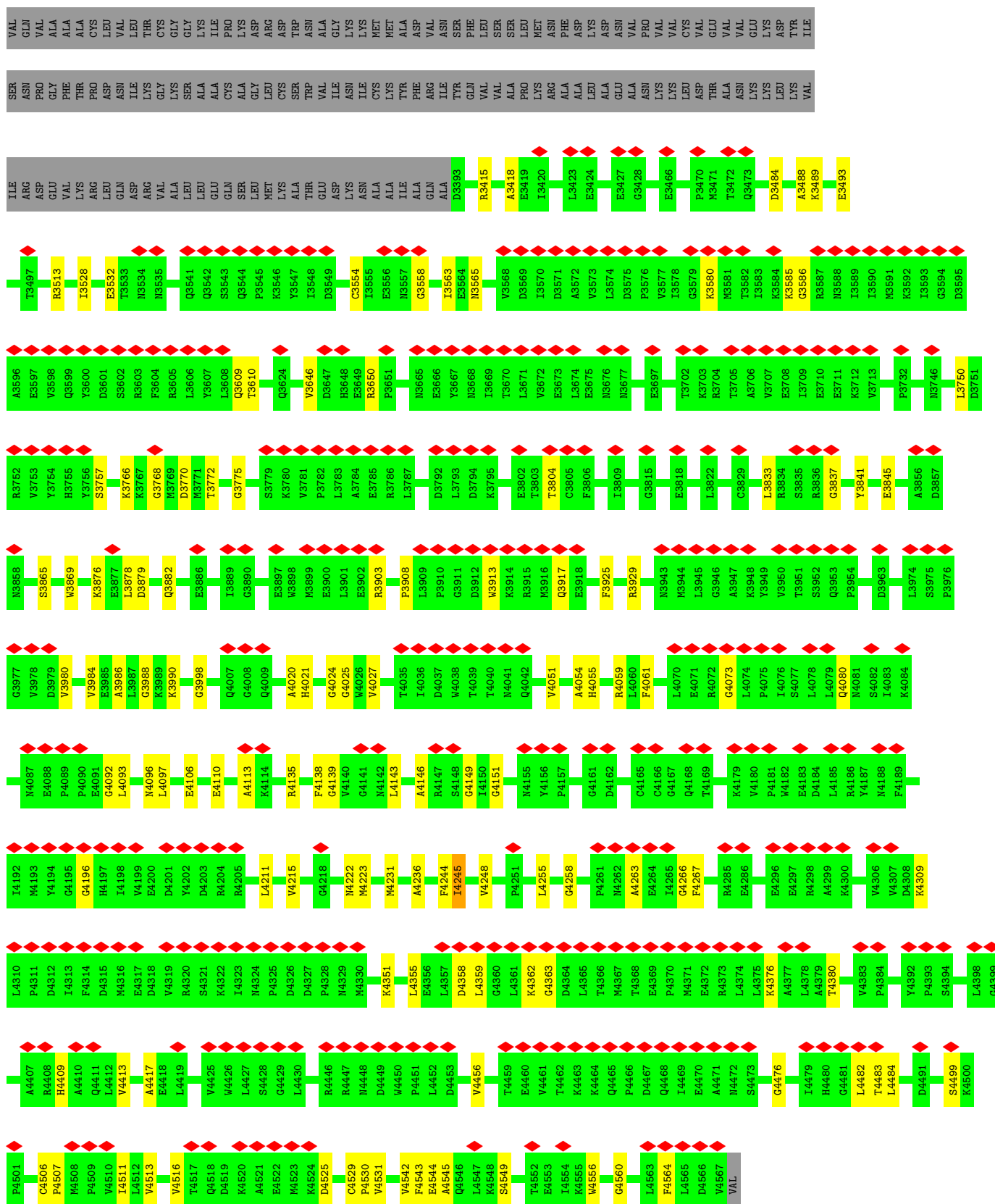


• Molecule 4: Flagellar outer dynein arm heavy chain beta









• Molecule 5: Dynein gamma chain, flagellar outer arm

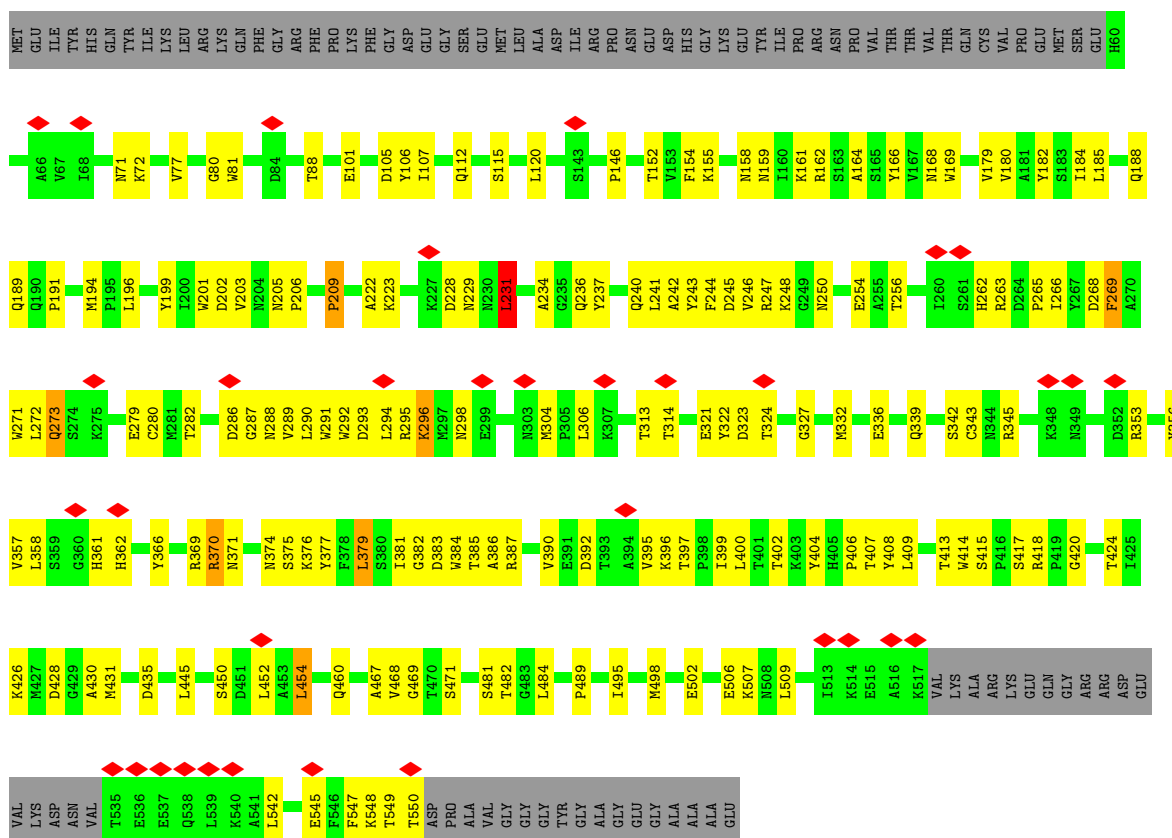




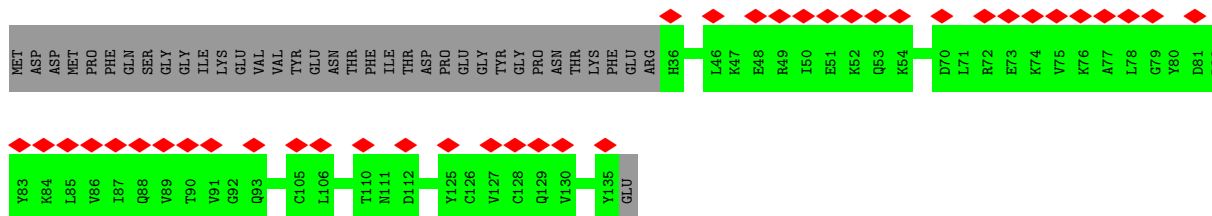
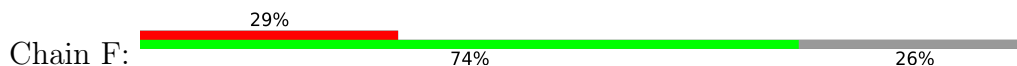
GLN	TYR	ALA	GLN	LEU	VAL	THR	L2402	G2408	A2409	L2410	L2411	N2412	L2413	S2414	Y2415	V2417	D2418	K2419	A2420	V2424	G2425	S2440	K2441	F2442	N2443	A2444	E2445	T2446	T2447	A2448	N2449	K2450	T2451	L2452	T2453	F2454	S2455	S2456	L2457	M2465	G2469	E2472	K2473	T2474	Q2475	K2476	L2477	T2478	F2479					
G2329	G2330	L2331	L2332	E2333	M2334	K2335	E2336	E2337	P2338	L2339	F2340	D2341	Q2342	R2345	T2346	F2347	A2348	H2349	N2350	M2351	P2352	P2353	K2354	E2355	E2356	D2357	S2358	D2359	T2360	L2361	F2362	V2366	N2367	T2368	T2369	D2370	A2371	E2372	H2375	TRP	ARG	HIS	CYS	VAL	PRO	TRP	THR	TYR	PRO	ASN	GLU	LYS	PRO	
S2227	R2228	A2229	G2230	I2231	D2236	V2237	W2248	L2249	Q2250	K2251	R2252	A2257	C2258	W2259	A2260	R2261	L2262	F2263	S2264	I2276	S2277	L2278	T2279	V2280	V2281	N2282	Y2283	L2284	E2285	S2288	T2289	V2290	K2305	E2306	A2307	G2308	T2309	A2310	N2311	D2312	L2313	A2314	K2315	V2319	F2320	L2321	Y2322	T2325	W2326					
D2053	A2054	T2055	R2056	P2057	D2058	V2059	N2060	K2061	K2065	E2069	V2074	L2090	V2091	P2100	G2104	A2107	E2118	L2119	G2120	H2123	V2124	L2125	V2126	R2127	P2130	K2131	A2132	I2133	T2134	A2135	Q2137	M2138	F2139	G2140	R2141	R2142	D2143	T2144	T2145	T2146	G2147	D2148	V2149	T2150	I2153	F2154	A2155							
W2158	R2159	E2160	A2161	A2162	K2163	T2164	K2165	N2166	Q2167	N2168	T2169	V2172	L2173	D2174	G2175	P2176	V2177	D2178	A2179	I2182	E2183	N2184	L2185	N2186	T2187	L2188	L2189	D2190	D2191	N2192	T2196	L2197	A2198	N2199	G2200	D2201	R2202	L2203	L2204	M2205	S2206	A2207	A2208	E2214	P2215	E2216	T2217	L2218	N2219	N2220	A2221	S2222	P2223	A2224
S2227	R2228	A2229	G2230	I2231	D2236	V2237	W2248	L2249	Q2250	K2251	R2252	A2257	C2258	W2259	A2260	R2261	L2262	F2263	S2264	I2276	S2277	L2278	T2279	V2280	V2281	N2282	Y2283	L2284	E2285	S2288	T2289	V2290	K2305	E2306	A2307	G2308	T2309	A2310	N2311	D2312	L2313	A2314	K2315	V2319	F2320	L2321	Y2322	T2325	W2326					
G2329	G2330	L2331	L2332	E2333	M2334	K2335	E2336	E2337	P2338	L2339	F2340	D2341	Q2342	R2345	T2346	F2347	A2348	H2349	N2350	M2351	P2352	P2353	K2354	E2355	E2356	D2357	S2358	D2359	T2360	L2361	F2362	V2366	N2367	T2368	T2369	D2370	A2371	E2372	H2375	TRP	ARG	HIS	CYS	VAL	PRO	TRP	THR	TYR	PRO	ASN	GLU	LYS	PRO	
GLN	TYR	ALA	GLN	LEU	VAL	ILE	PRO	THR	L2402	G2408	A2409	L2410	L2411	N2412	L2413	S2414	Y2415	V2417	D2418	K2419	A2420	V2424	G2425	S2440	K2441	F2442	N2443	A2444	E2445	T2446	T2447	A2448	N2449	K2450	T2451	L2452	T2453	F2454	S2455	S2456	L2457	M2465	G2469	E2472	K2473	T2474	Q2475	K2476	L2477	T2478	F2479			
L1251	D1252	R1253	L1254	Y1255	S1256	L1257	Y1258	V1259	A1260	V1261	I1262	T1263	T1264	W1273	V1276	V1277	E1278	K1279	I1280	H1353	F1354	Q1357	H1358	LEU	LEU	ASP	CYS	ASN	VAL	LEU	ARG	TYR	TYR	SER	GLY	GLY	GLU	LEU	PHE	GLY	LEU	PRO	VAL	THR	GLN	TYR	PRO	GLU	L1241	I1248	Q1249	M1250		



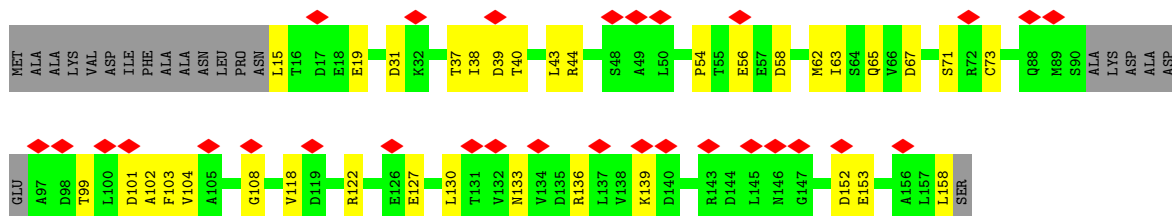




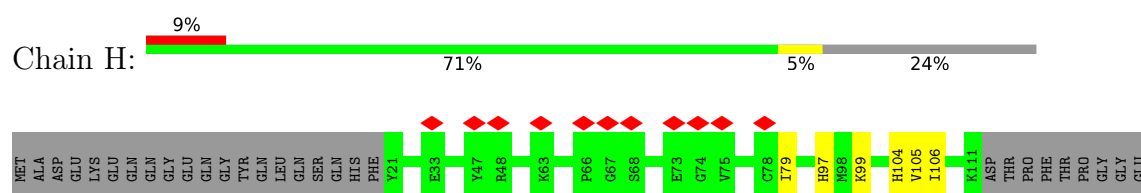
• Molecule 8: Flagellar outer dynein arm light chain 2



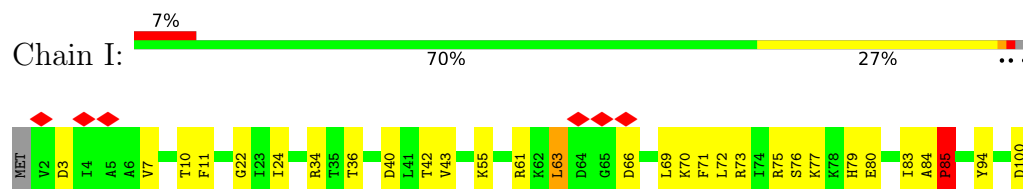
• Molecule 9: Dynein 18 kDa light chain, flagellar outer arm



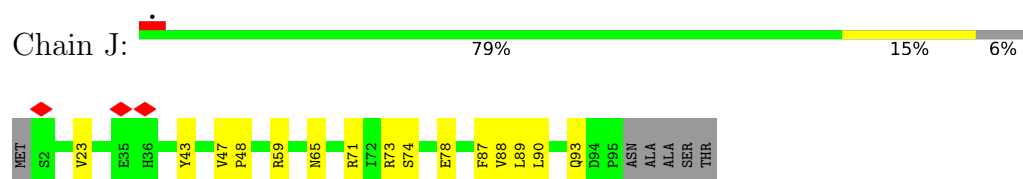
• Molecule 10: Dynein 11 kDa light chain, flagellar outer arm



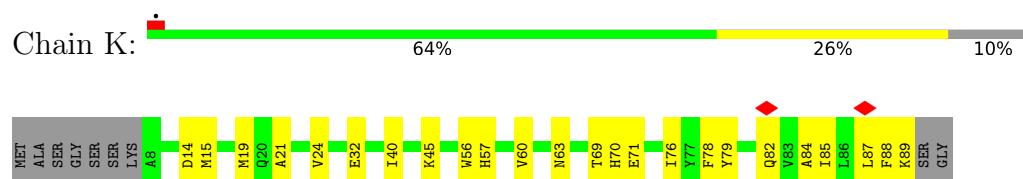
- Molecule 11: Dynein light chain roadblock LC7a



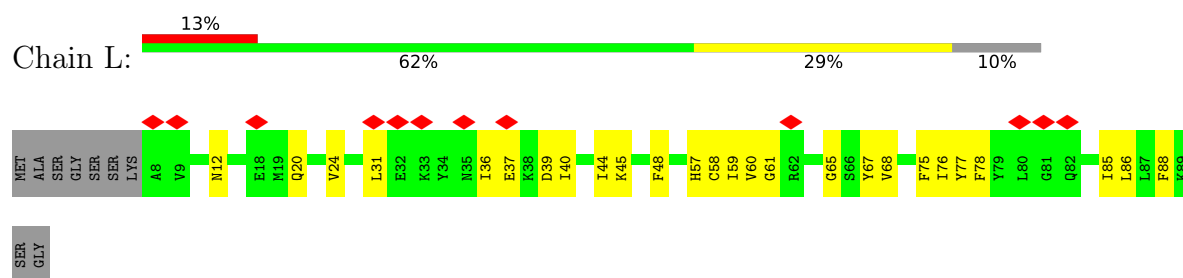
- Molecule 12: Dynein light chain roadblock LC7b



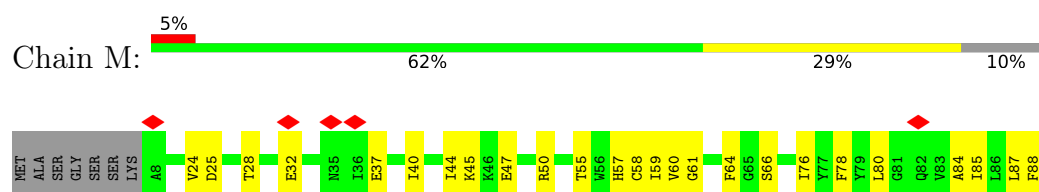
- Molecule 13: Dynein 8 kDa light chain, flagellar outer arm



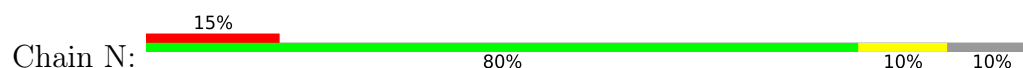
- Molecule 13: Dynein 8 kDa light chain, flagellar outer arm



- Molecule 13: Dynein 8 kDa light chain, flagellar outer arm



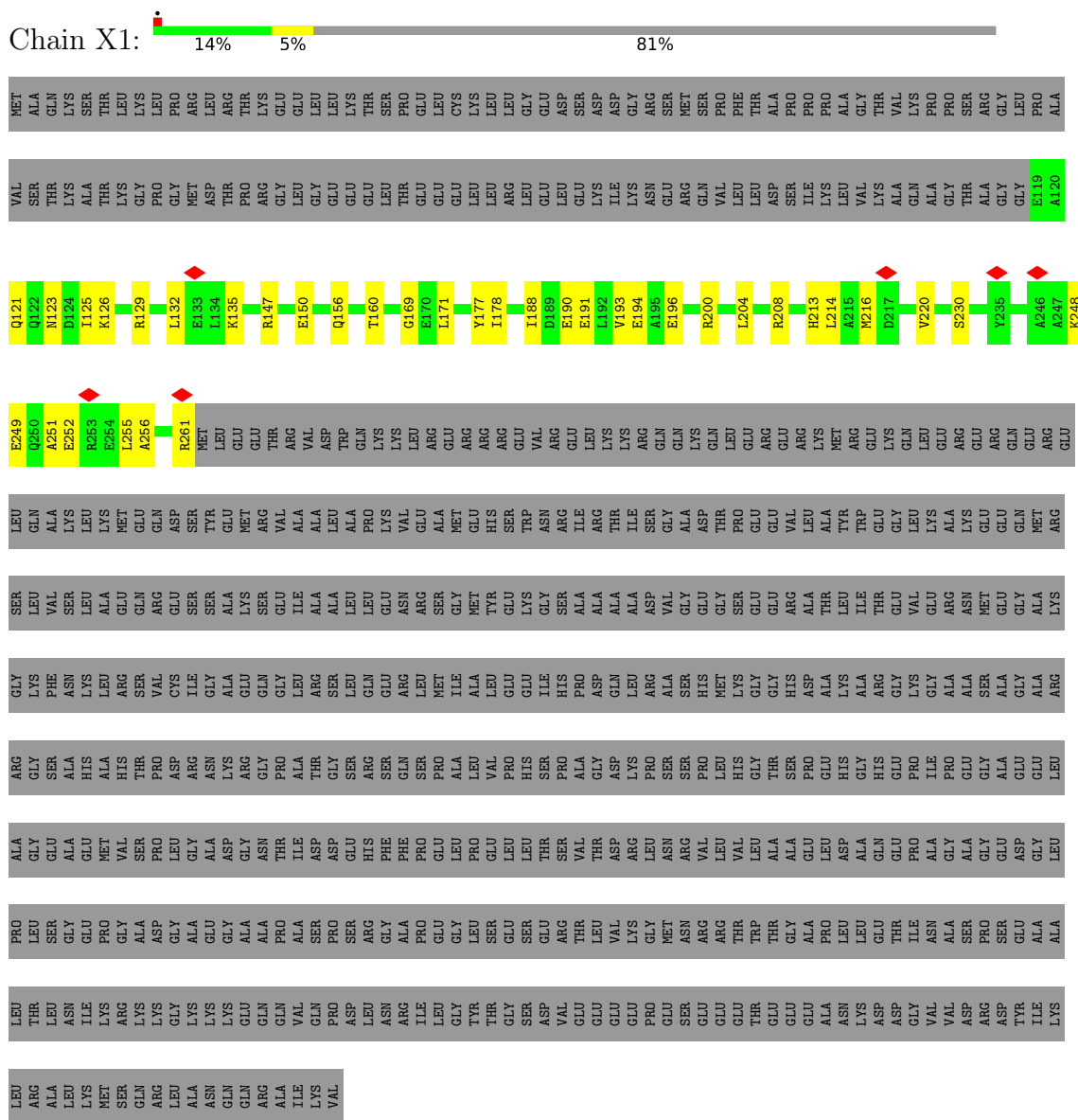
- Molecule 13: Dynein 8 kDa light chain, flagellar outer arm





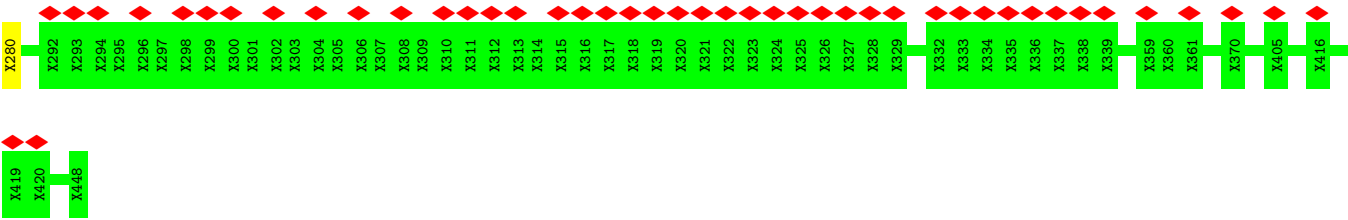
[illegible]

- Molecule 16: Outer dynein arm-docking complex subunit 1

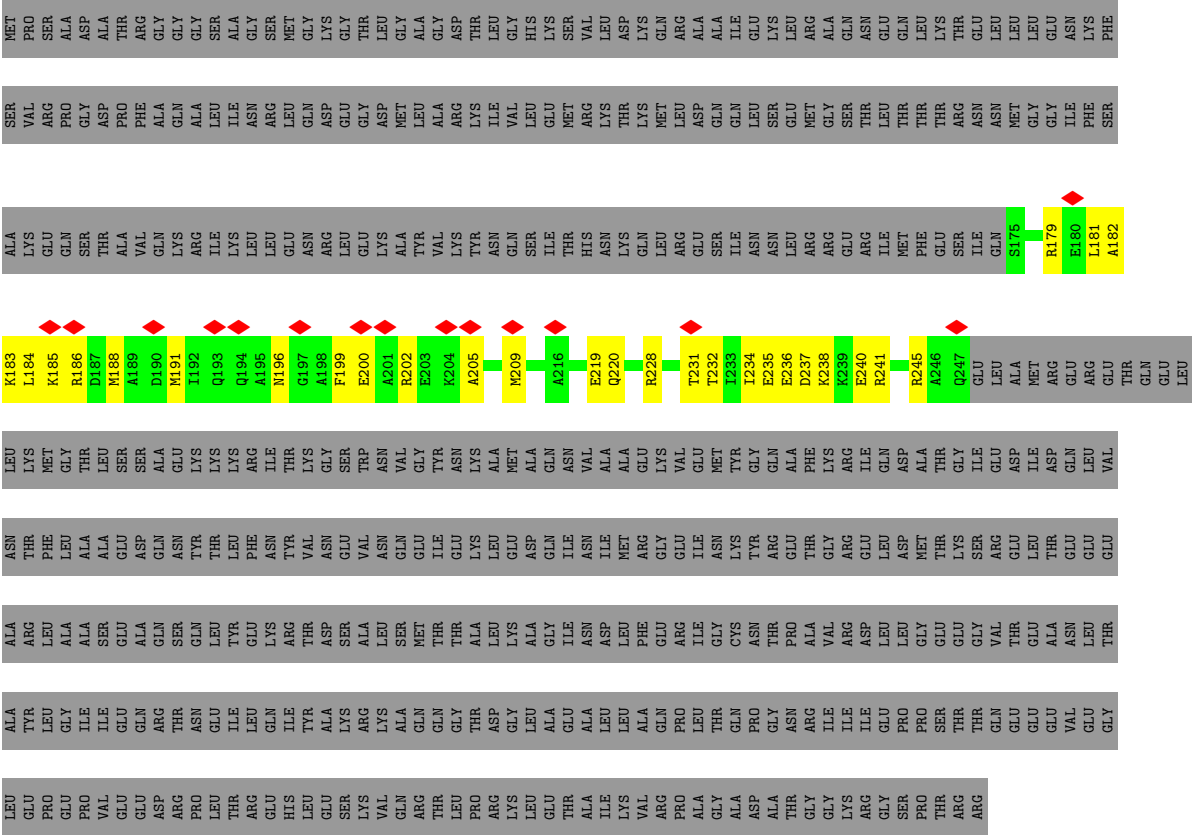


- Molecule 17: DC1

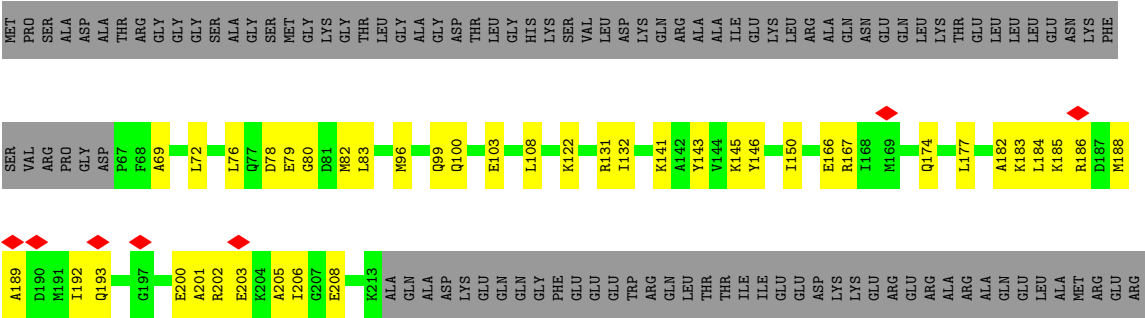




• Molecule 18: Outer dynein arm protein 1



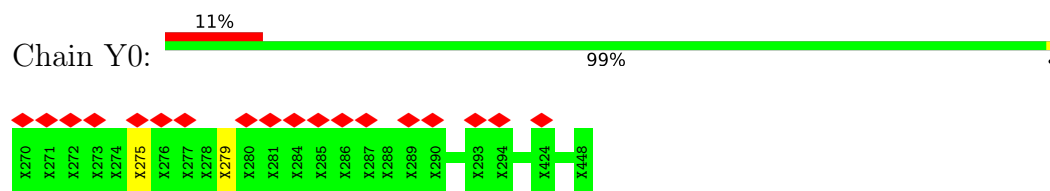
• Molecule 18: Outer dynein arm protein 1



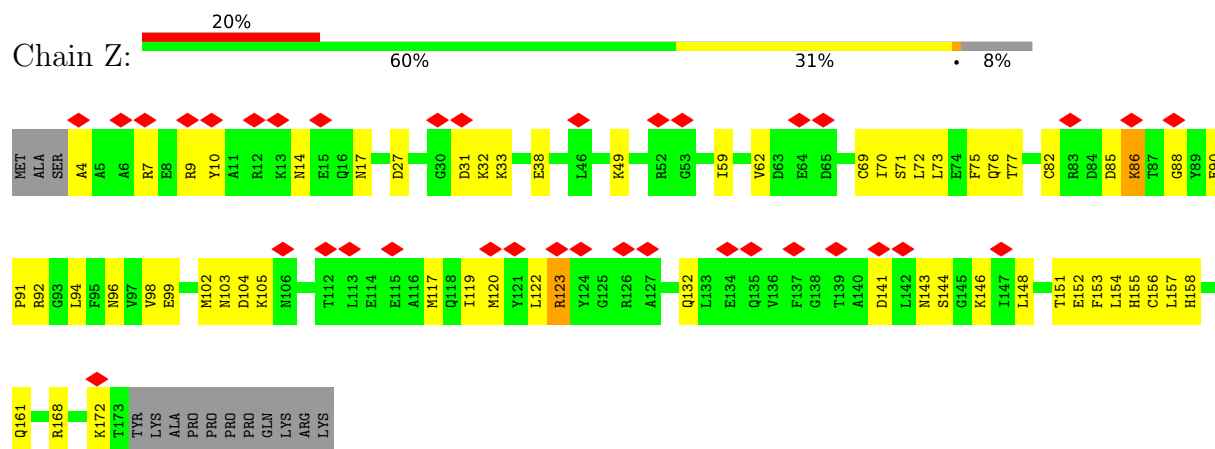




- Molecule 19: DC2



- Molecule 20: Outer dynein arm-docking complex protein DC3



## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=0°, rise=82 Å, axial sym=C1	Depositor
Number of segments used	485694	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The composite map was assembled on a box 700 reference map (7.5 Å) using the ODA-DC and ODA core composite maps (deposited separately), and maps targeting the aHC AAA+ domain (4.5 Å), bHC AAA+ domain (6.2 Å), aHC AAA+ domain (11.4 Å), and aHC tail domain (5.3 Å). A second conformation of bHC AAA+ domain (9.8 Å) is also provided.	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{Å}^2$ )	61.48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	952.0, 952.0, 952.0	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, GTP

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	A1	0.28	0/3420	0.53	0/4628
1	A3	0.31	0/3420	0.54	0/4628
1	A5	0.30	0/3420	0.52	0/4628
1	A7	0.28	0/3420	0.51	0/4628
1	B1	0.29	0/3371	0.49	0/4561
1	B3	0.32	0/3295	0.49	0/4454
1	B5	0.31	0/3420	0.51	0/4628
1	B7	0.29	0/3420	0.50	0/4628
2	A2	0.31	0/3410	0.53	0/4623
2	A4	0.34	0/3389	0.58	0/4595
2	A6	0.31	0/3406	0.54	0/4618
2	B2	0.31	0/3271	0.52	0/4434
2	B4	0.32	0/3260	0.52	0/4418
2	B6	0.29	0/3389	0.50	0/4595
3	A	0.32	0/16168	0.55	0/22506
4	B	0.34	1/19223 (0.0%)	0.61	7/26574 (0.0%)
5	C	0.34	0/21839	0.57	7/30089 (0.0%)
6	D	0.70	2/3699 (0.1%)	0.88	6/5023 (0.1%)
7	E	0.71	1/3784 (0.0%)	0.90	7/5152 (0.1%)
8	F	0.24	0/494	0.52	0/687
9	G	0.34	0/1098	0.63	0/1471
10	H	0.26	0/450	0.46	0/626
11	I	0.56	0/840	0.85	3/1133 (0.3%)
12	J	0.55	0/752	0.78	0/1019
13	K	0.53	0/687	0.70	0/926
13	L	0.56	0/687	0.74	0/926
13	M	0.43	0/687	0.73	0/926
13	N	0.25	0/406	0.49	0/565
14	O	0.26	0/480	0.56	0/666
15	P	0.58	0/823	0.87	1/1108 (0.1%)
16	X	0.29	0/485	0.57	0/642
16	X1	0.32	0/1186	0.51	0/1582

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
18	Y	0.30	0/598	0.52	0/793
18	Y1	0.29	0/1192	0.52	0/1585
20	Z	0.34	0/1403	0.67	0/1885
All	All	0.36	4/124292 (0.0%)	0.59	31/169950 (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
3	A	0	21
4	B	0	15
5	C	0	7
All	All	0	43

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	314	SER	CA-CB	-5.69	1.44	1.52
4	B	3908	PRO	C-N	-5.56	1.21	1.34
7	E	336	GLU	CA-C	-5.46	1.38	1.52
6	D	378	VAL	CB-CG2	-5.19	1.42	1.52

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	376	LEU	CB-CG-CD1	8.76	125.90	111.00
4	B	4073	GLY	C-N-CA	8.14	142.06	121.70
4	B	4499	SER	C-N-CA	7.97	141.63	121.70
5	C	129	PRO	CA-N-CD	-7.73	100.68	111.50
7	E	370	ARG	C-N-CA	-7.37	103.28	121.70

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1300	PHE	Peptide
3	A	1482	PHE	Peptide
3	A	1508	SER	Peptide
3	A	1633	ILE	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
3	A	1654	SER	Peptide

## 5.2 Too-close contacts ⓘ

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	A1	3346	0	3238	102	0
1	A3	3346	0	3238	110	0
1	A5	3346	0	3238	102	0
1	A7	3346	0	3238	88	0
1	B1	3298	0	3196	83	0
1	B3	3227	0	3134	80	0
1	B5	3346	0	3238	106	0
1	B7	3346	0	3238	91	0
2	A2	3339	0	3272	102	0
2	A4	3318	0	3259	94	0
2	A6	3335	0	3269	108	0
2	B2	3204	0	3152	84	0
2	B4	3193	0	3141	107	0
2	B6	3318	0	3259	80	0
3	A	16173	0	7306	417	0
4	B	19163	0	10961	281	0
5	C	21756	0	13263	244	0
6	D	3609	0	3534	90	0
7	E	3697	0	3534	133	0
8	F	495	0	221	0	0
9	G	1089	0	1072	24	0
10	H	451	0	204	3	0
11	I	827	0	841	24	0
12	J	741	0	750	12	0
13	K	671	0	654	20	0
13	L	671	0	654	20	0
13	M	671	0	654	23	0
13	N	407	0	192	5	0
14	O	481	0	230	1	0
15	P	805	0	801	19	0
16	X	481	0	488	19	0
16	X1	1178	0	1179	27	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	X0	810	0	170	1	0
18	Y	595	0	586	22	0
18	Y1	1185	0	1230	35	0
19	Y0	840	0	181	1	0
20	Z	1384	0	1359	46	0
21	A1	32	0	12	0	0
21	A3	32	0	12	1	0
21	A5	32	0	12	1	0
21	A7	32	0	12	4	0
21	B2	32	0	12	1	0
21	B5	32	0	12	1	0
21	B7	32	0	12	0	0
22	A1	1	0	0	0	0
22	A2	1	0	0	0	0
22	A4	1	0	0	0	0
22	A6	1	0	0	0	0
22	B3	1	0	0	0	0
22	B4	1	0	0	0	0
22	B6	1	0	0	0	0
23	A1	28	0	12	0	0
23	A3	28	0	12	2	0
23	A5	28	0	12	0	0
23	A7	28	0	12	2	0
23	B1	28	0	12	3	0
23	B3	28	0	12	2	0
23	B5	28	0	12	1	0
23	B7	28	0	12	1	0
All	All	124943	0	95354	2603	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 12.

The worst 5 of 2603 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)
4:B:3879:ASP:HA	5:C:1534:GLU:CB	1.40	1.48
4:B:3879:ASP:CB	5:C:1530:PRO:O	1.86	1.23
4:B:3879:ASP:CA	5:C:1534:GLU:CB	2.17	1.23
3:A:1676:ILE:O	3:A:1679:ALA:HB3	1.56	1.05
3:A:2399:SER:HA	3:A:2438:PHE:O	1.57	1.03

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	A1	424/443 (96%)	399 (94%)	25 (6%)	0	100	100
1	A3	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
1	A5	424/443 (96%)	407 (96%)	17 (4%)	0	100	100
1	A7	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
1	B1	415/443 (94%)	396 (95%)	19 (5%)	0	100	100
1	B3	404/443 (91%)	392 (97%)	12 (3%)	0	100	100
1	B5	424/443 (96%)	403 (95%)	21 (5%)	0	100	100
1	B7	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
2	A2	426/451 (94%)	402 (94%)	24 (6%)	0	100	100
2	A4	423/451 (94%)	409 (97%)	14 (3%)	0	100	100
2	A6	425/451 (94%)	408 (96%)	17 (4%)	0	100	100
2	B2	405/451 (90%)	391 (96%)	14 (4%)	0	100	100
2	B4	403/451 (89%)	385 (96%)	18 (4%)	0	100	100
2	B6	423/451 (94%)	407 (96%)	16 (4%)	0	100	100
3	A	3266/4503 (72%)	2704 (83%)	550 (17%)	12 (0%)	34	72
4	B	3500/4568 (77%)	3121 (89%)	377 (11%)	2 (0%)	51	86
5	C	3840/4485 (86%)	3484 (91%)	353 (9%)	3 (0%)	51	86
6	D	450/683 (66%)	387 (86%)	63 (14%)	0	100	100
7	E	470/567 (83%)	371 (79%)	94 (20%)	5 (1%)	14	52
8	F	98/136 (72%)	94 (96%)	4 (4%)	0	100	100
9	G	134/159 (84%)	125 (93%)	9 (7%)	0	100	100
10	H	89/120 (74%)	77 (86%)	12 (14%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	I	101/105 (96%)	89 (88%)	11 (11%)	1 (1%)	15	54
12	J	92/100 (92%)	81 (88%)	11 (12%)	0	100	100
13	K	80/91 (88%)	73 (91%)	7 (9%)	0	100	100
13	L	80/91 (88%)	72 (90%)	8 (10%)	0	100	100
13	M	80/91 (88%)	73 (91%)	7 (9%)	0	100	100
13	N	80/91 (88%)	68 (85%)	12 (15%)	0	100	100
14	O	95/117 (81%)	92 (97%)	3 (3%)	0	100	100
15	P	96/103 (93%)	89 (93%)	7 (7%)	0	100	100
16	X	54/749 (7%)	54 (100%)	0	0	100	100
16	X1	140/749 (19%)	140 (100%)	0	0	100	100
18	Y	71/552 (13%)	71 (100%)	0	0	100	100
18	Y1	145/552 (26%)	145 (100%)	0	0	100	100
20	Z	168/184 (91%)	155 (92%)	11 (6%)	2 (1%)	13	50
All	All	18997/25046 (76%)	17179 (90%)	1793 (9%)	25 (0%)	54	86

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	1677	CYS
4	B	625	ASP
4	B	1876	ASP
5	C	4432	LEU
7	E	298	ASN

### 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	A1	367/379 (97%)	367 (100%)	0	100	100
1	A3	367/379 (97%)	366 (100%)	1 (0%)	92	95
1	A5	367/379 (97%)	367 (100%)	0	100	100

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A7	367/379 (97%)	367 (100%)	0	100	100
1	B1	363/379 (96%)	363 (100%)	0	100	100
1	B3	356/379 (94%)	356 (100%)	0	100	100
1	B5	367/379 (97%)	367 (100%)	0	100	100
1	B7	367/379 (97%)	366 (100%)	1 (0%)	92	95
2	A2	361/374 (96%)	360 (100%)	1 (0%)	92	95
2	A4	359/374 (96%)	354 (99%)	5 (1%)	67	80
2	A6	361/374 (96%)	361 (100%)	0	100	100
2	B2	347/374 (93%)	347 (100%)	0	100	100
2	B4	346/374 (92%)	346 (100%)	0	100	100
2	B6	359/374 (96%)	359 (100%)	0	100	100
4	B	463/3998 (12%)	455 (98%)	8 (2%)	60	78
5	C	702/3945 (18%)	696 (99%)	6 (1%)	78	87
6	D	401/584 (69%)	396 (99%)	5 (1%)	71	83
7	E	400/489 (82%)	396 (99%)	4 (1%)	76	86
9	G	121/136 (89%)	121 (100%)	0	100	100
11	I	90/91 (99%)	89 (99%)	1 (1%)	73	84
12	J	83/87 (95%)	83 (100%)	0	100	100
13	K	70/76 (92%)	70 (100%)	0	100	100
13	L	70/76 (92%)	69 (99%)	1 (1%)	67	80
13	M	70/76 (92%)	70 (100%)	0	100	100
15	P	86/90 (96%)	86 (100%)	0	100	100
16	X	50/618 (8%)	50 (100%)	0	100	100
16	X1	125/618 (20%)	121 (97%)	4 (3%)	39	61
18	Y	59/462 (13%)	59 (100%)	0	100	100
18	Y1	128/462 (28%)	127 (99%)	1 (1%)	81	89
20	Z	150/162 (93%)	146 (97%)	4 (3%)	44	65
All	All	8122/17246 (47%)	8080 (100%)	42 (0%)	89	93

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	E	279	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
16	X1	213	HIS
7	E	296	LYS
13	L	45	LYS
18	Y1	166	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	B5	348	ASN
5	C	500	GLN
1	B5	384	GLN
1	B7	100	ASN
5	C	515	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 22 ligands modelled in this entry, 7 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
23	GDP	A3	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	5 (16%)
21	GTP	A7	501	22	26,34,34	1.20	2 (7%)	32,54,54	1.67	7 (21%)
21	GTP	A1	501	22	26,34,34	1.13	2 (7%)	32,54,54	1.64	7 (21%)
23	GDP	A7	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.27	5 (16%)
23	GDP	A1	503	-	24,30,30	0.95	1 (4%)	30,47,47	1.28	4 (13%)
21	GTP	A3	501	22	26,34,34	1.18	2 (7%)	32,54,54	1.72	7 (21%)
23	GDP	A5	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	5 (16%)
21	GTP	A5	501	22	26,34,34	1.22	2 (7%)	32,54,54	1.66	7 (21%)
21	GTP	B7	501	22	26,34,34	1.20	2 (7%)	32,54,54	1.58	7 (21%)
23	GDP	B7	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.41	5 (16%)
21	GTP	B2	501	22	26,34,34	1.19	2 (7%)	32,54,54	1.73	7 (21%)
21	GTP	B5	501	22	26,34,34	1.21	2 (7%)	32,54,54	1.62	7 (21%)
23	GDP	B5	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
23	GDP	B3	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.35	4 (13%)
23	GDP	B1	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.34	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	A3	502	-	-	1/12/32/32	0/3/3/3
21	GTP	A7	501	22	-	7/18/38/38	0/3/3/3
21	GTP	A1	501	22	-	5/18/38/38	0/3/3/3
23	GDP	A7	502	-	-	4/12/32/32	0/3/3/3
23	GDP	A1	503	-	-	3/12/32/32	0/3/3/3
21	GTP	A3	501	22	-	7/18/38/38	0/3/3/3
23	GDP	A5	502	-	-	1/12/32/32	0/3/3/3
21	GTP	A5	501	22	-	6/18/38/38	0/3/3/3
21	GTP	B7	501	22	-	6/18/38/38	0/3/3/3
23	GDP	B7	502	-	-	6/12/32/32	0/3/3/3
21	GTP	B2	501	22	-	4/18/38/38	0/3/3/3
21	GTP	B5	501	22	-	7/18/38/38	0/3/3/3
23	GDP	B5	502	-	-	4/12/32/32	0/3/3/3
23	GDP	B3	502	-	-	3/12/32/32	0/3/3/3

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	B1	501	-	-	2/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A7	501	GTP	C5-C6	-4.28	1.38	1.47
21	B7	501	GTP	C5-C6	-4.26	1.38	1.47
21	A5	501	GTP	C5-C6	-4.26	1.38	1.47
21	B5	501	GTP	C5-C6	-4.24	1.38	1.47
21	B2	501	GTP	C5-C6	-4.16	1.39	1.47

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B2	501	GTP	PB-O3B-PG	-5.00	115.69	132.83
21	A5	501	GTP	PA-O3A-PB	-4.67	116.82	132.83
21	A3	501	GTP	PB-O3B-PG	-4.46	117.52	132.83
21	A3	501	GTP	PA-O3A-PB	-4.46	117.53	132.83
21	A7	501	GTP	PA-O3A-PB	-4.46	117.53	132.83

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A1	501	GTP	C5'-O5'-PA-O1A
21	A3	501	GTP	C5'-O5'-PA-O1A
21	A3	501	GTP	C5'-O5'-PA-O2A
21	A5	501	GTP	C5'-O5'-PA-O1A
21	A7	501	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

11 monomers are involved in 19 short contacts:

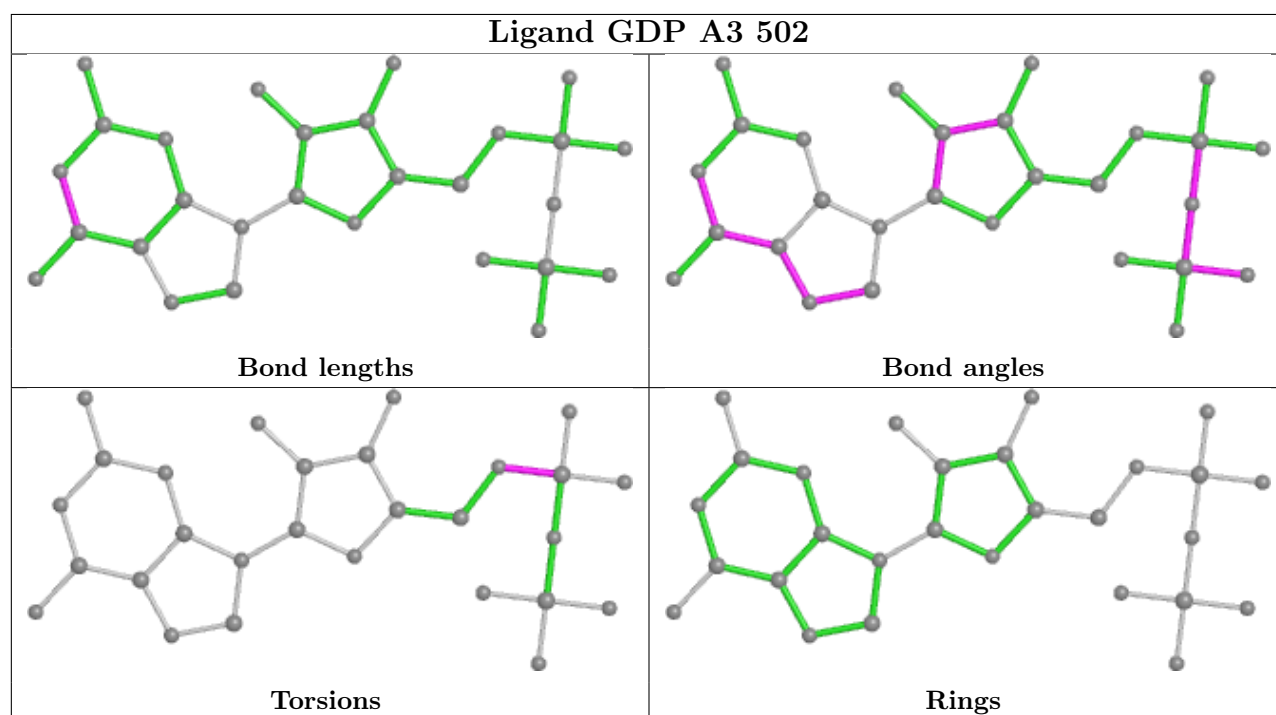
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A3	502	GDP	2	0
21	A7	501	GTP	4	0
23	A7	502	GDP	2	0
21	A3	501	GTP	1	0
21	A5	501	GTP	1	0
23	B7	502	GDP	1	0
21	B2	501	GTP	1	0

*Continued on next page...*

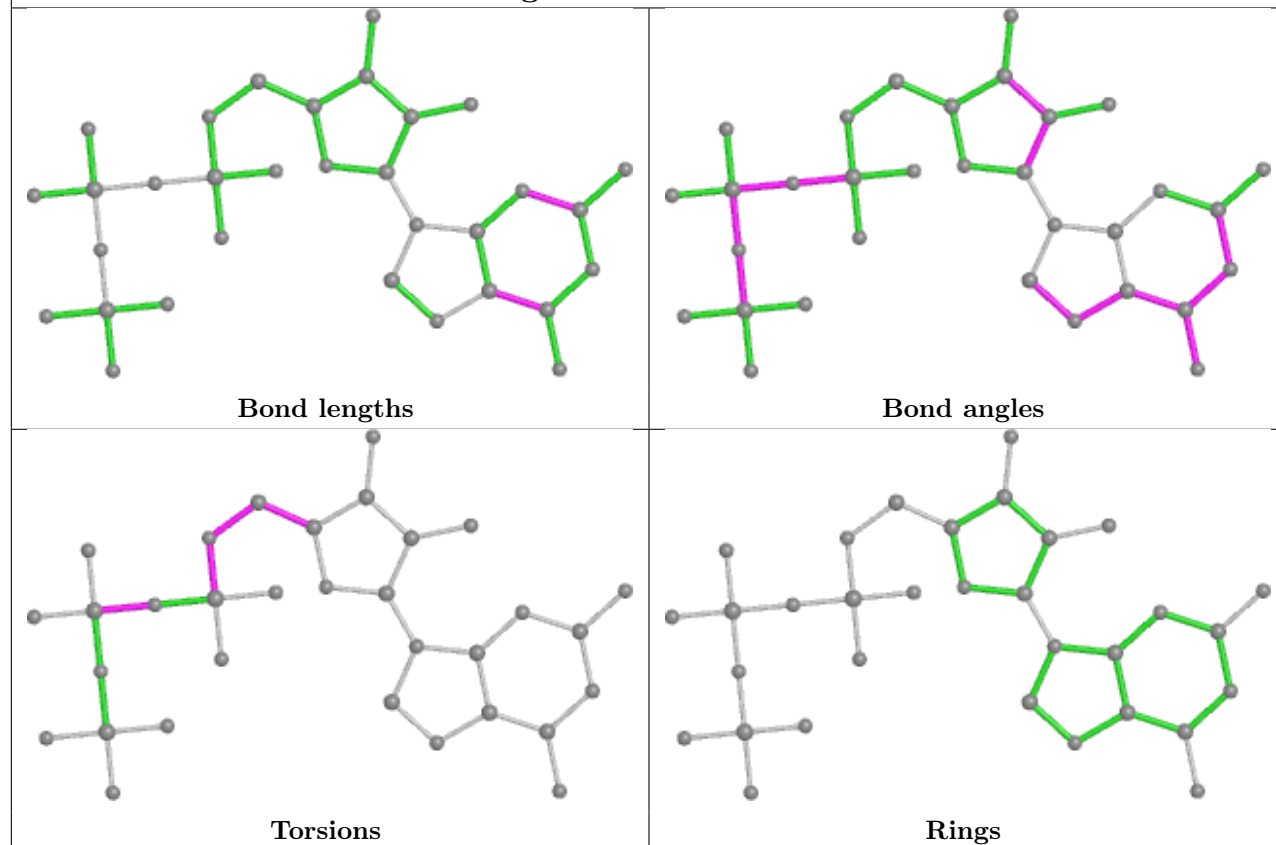
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B5	501	GTP	1	0
23	B5	502	GDP	1	0
23	B3	502	GDP	2	0
23	B1	501	GDP	3	0

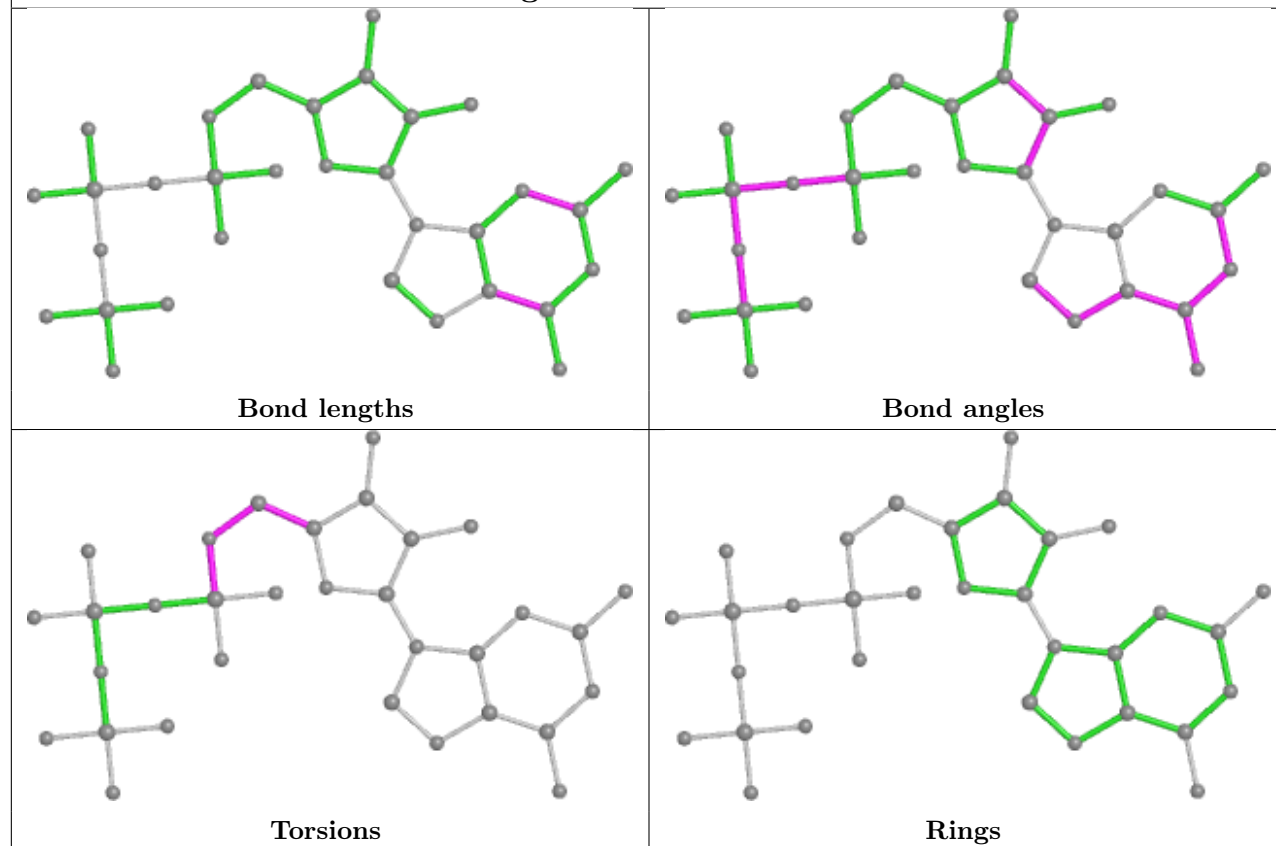
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

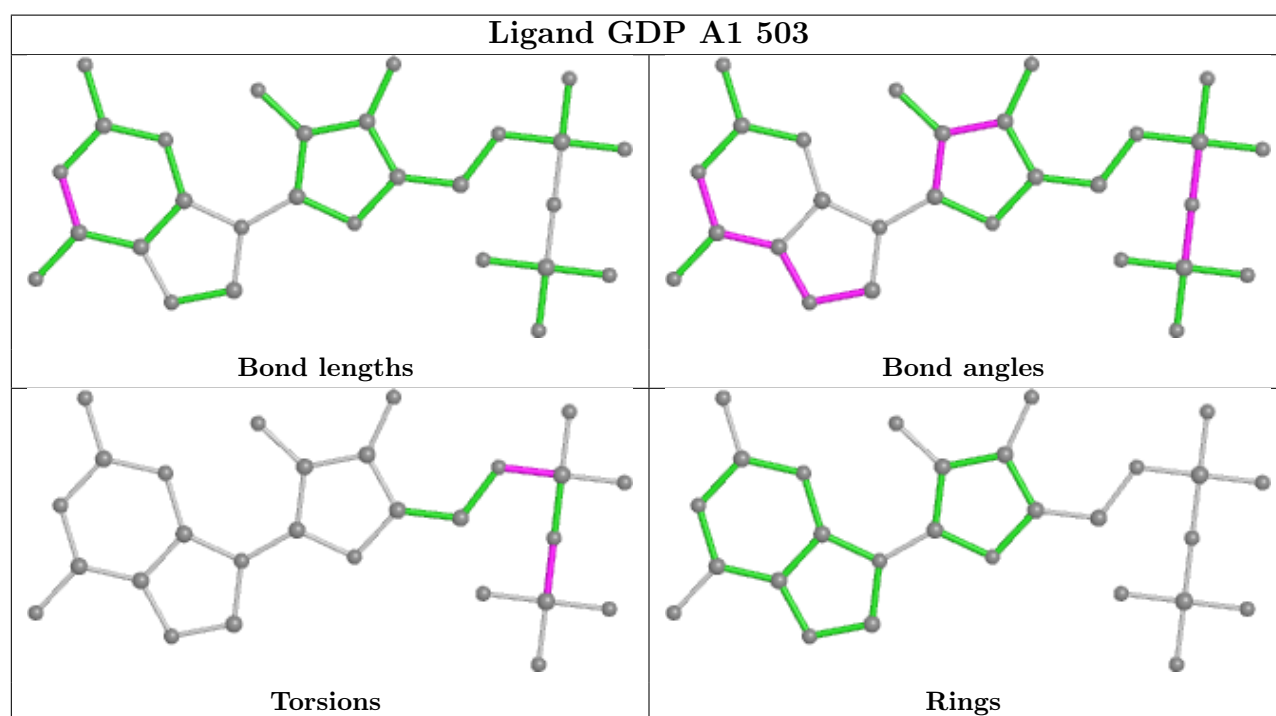
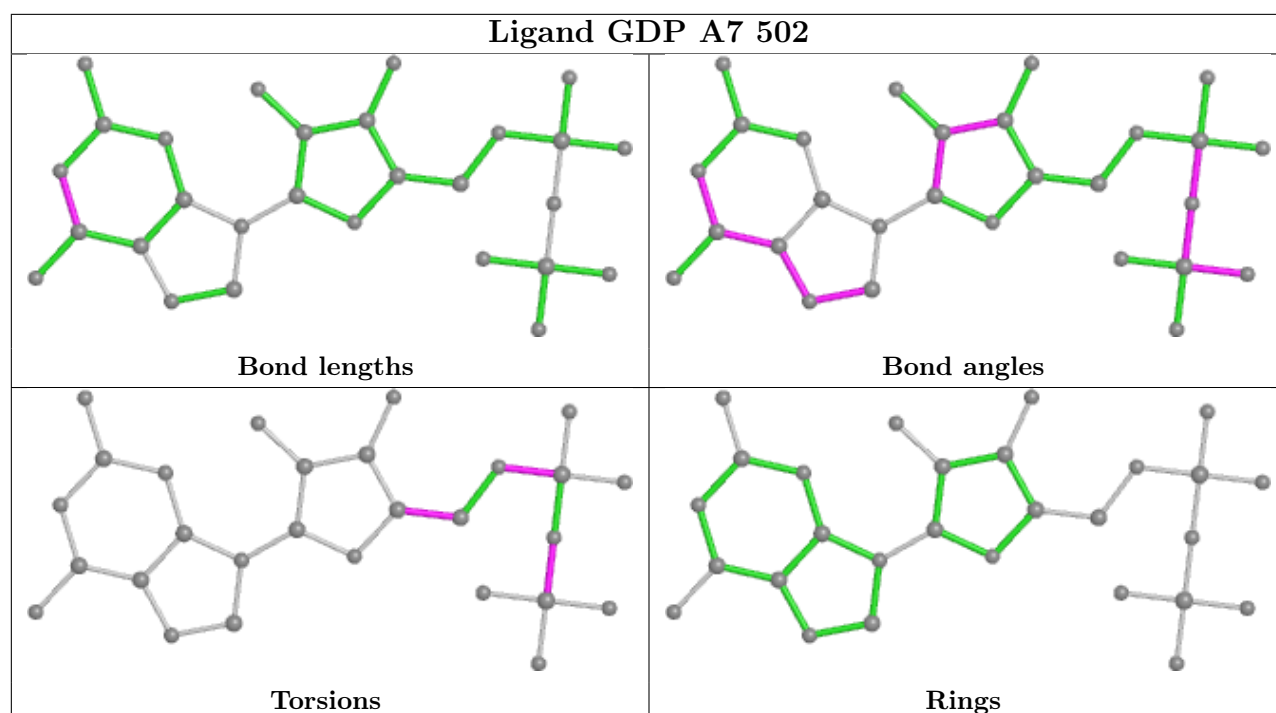


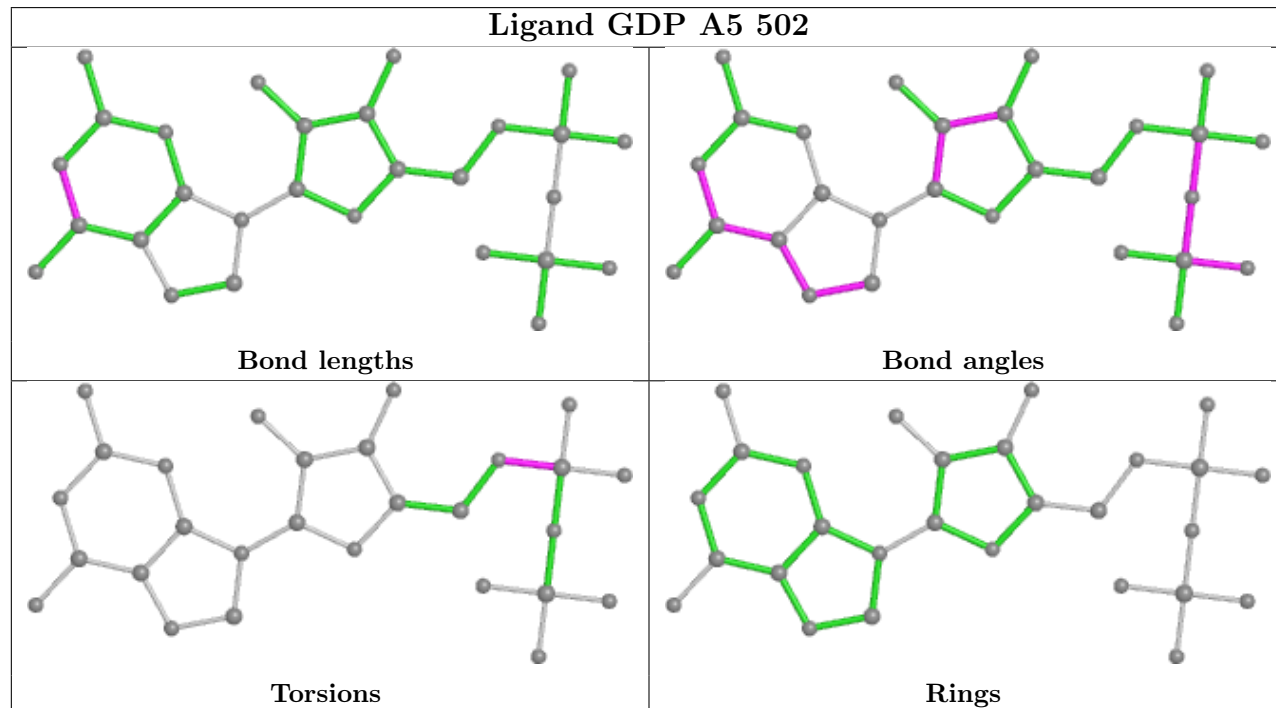
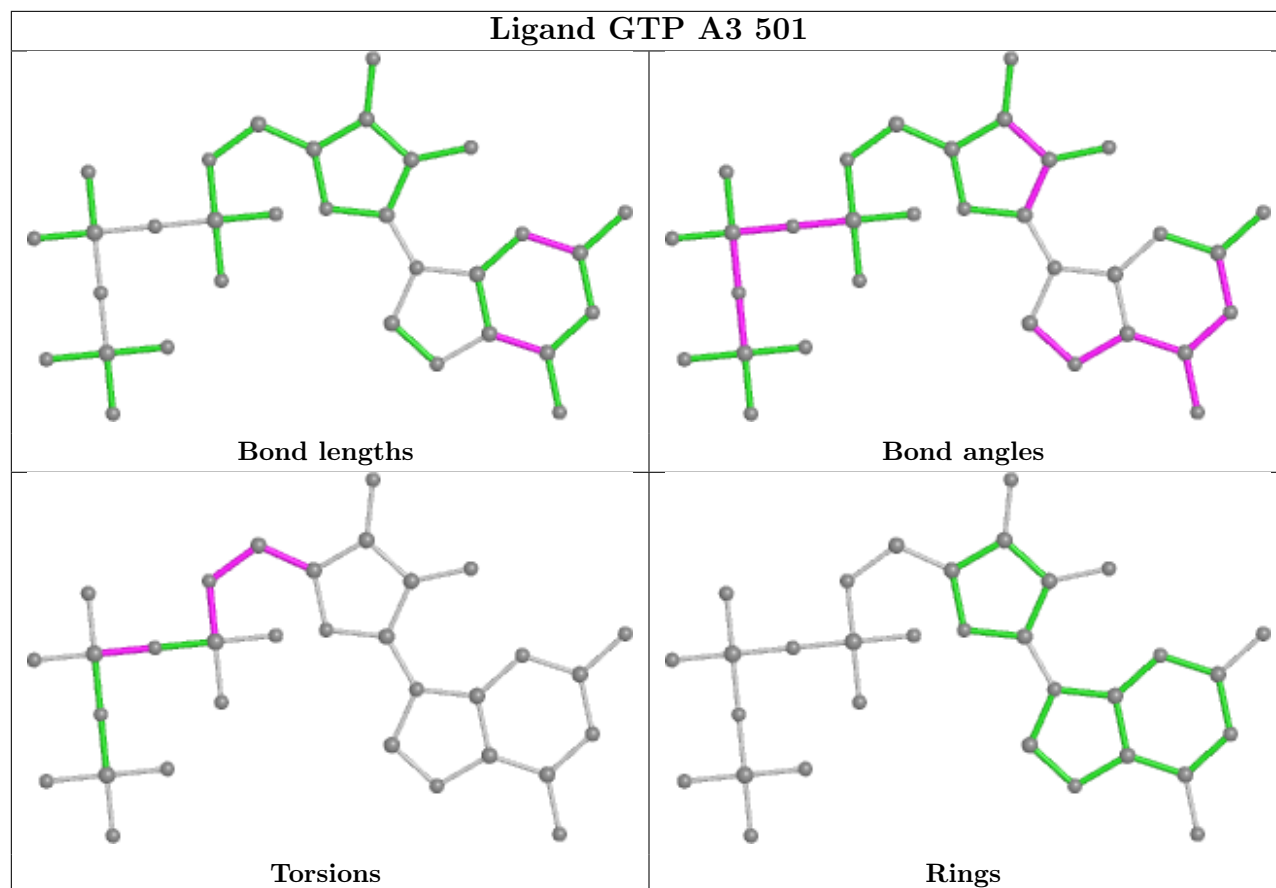
## Ligand GTP A7 501



## Ligand GTP A1 501

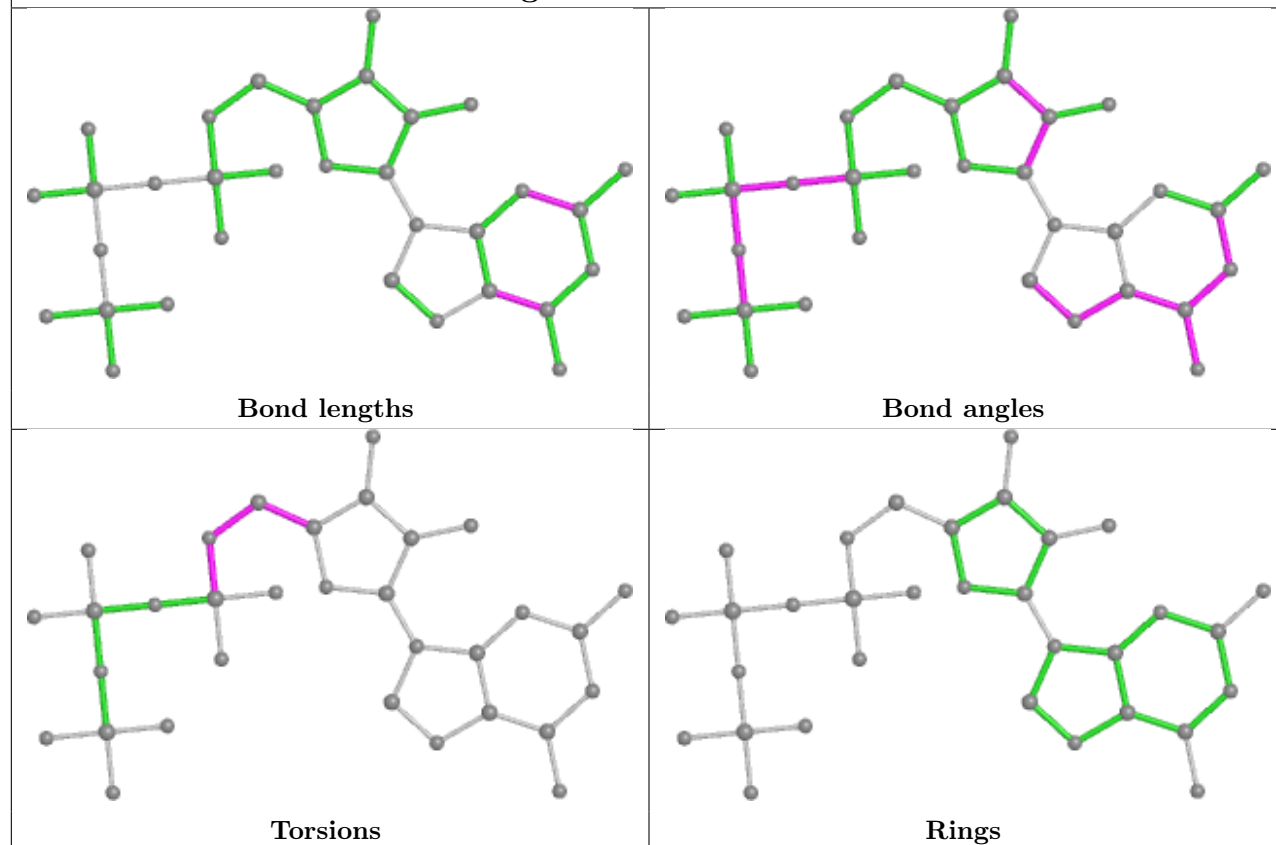




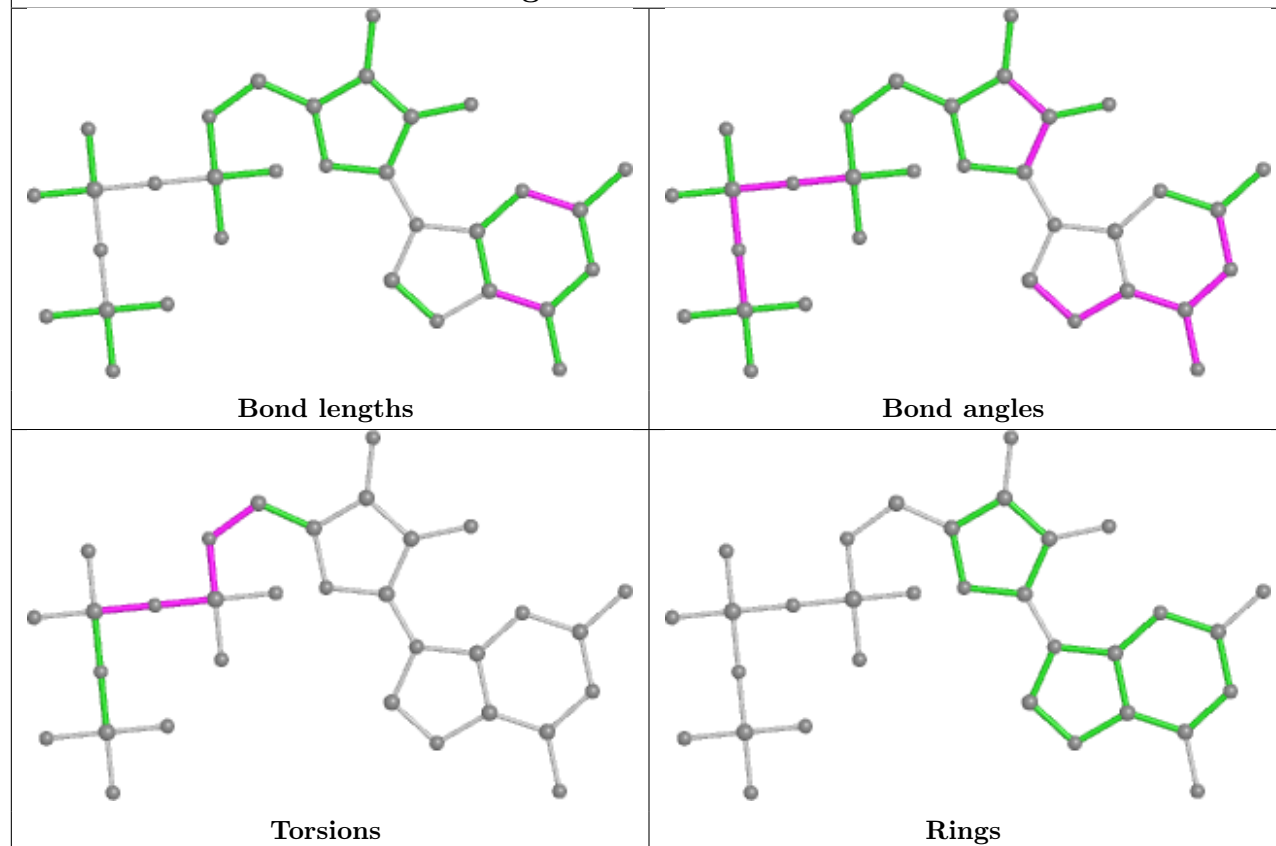


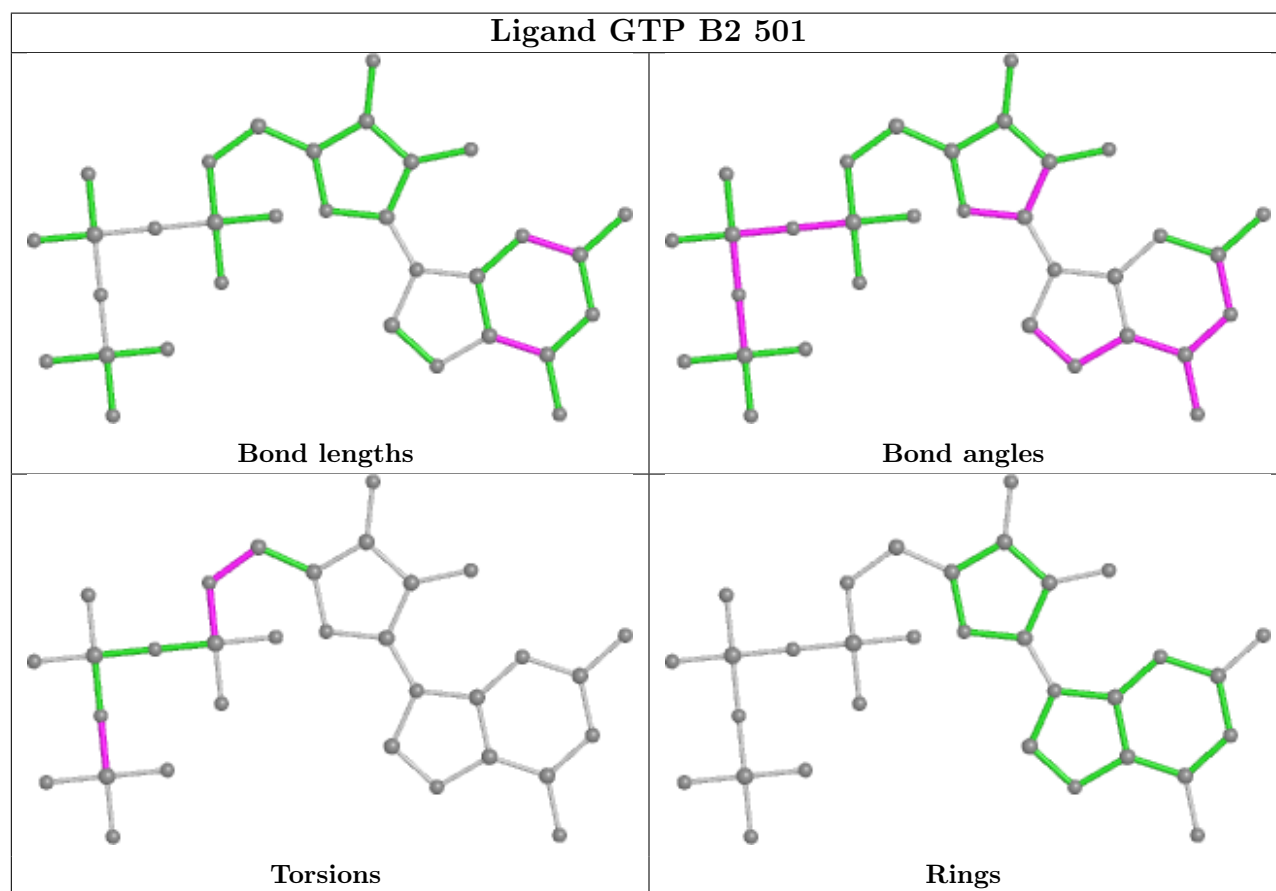
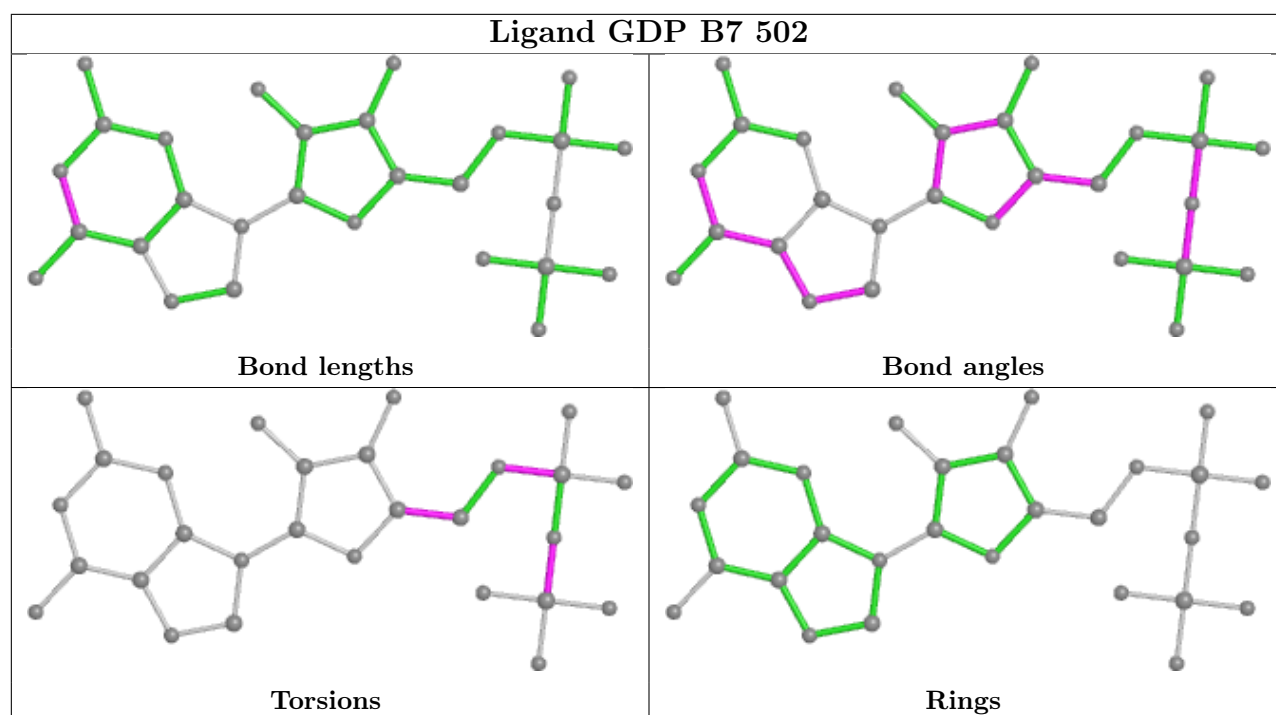


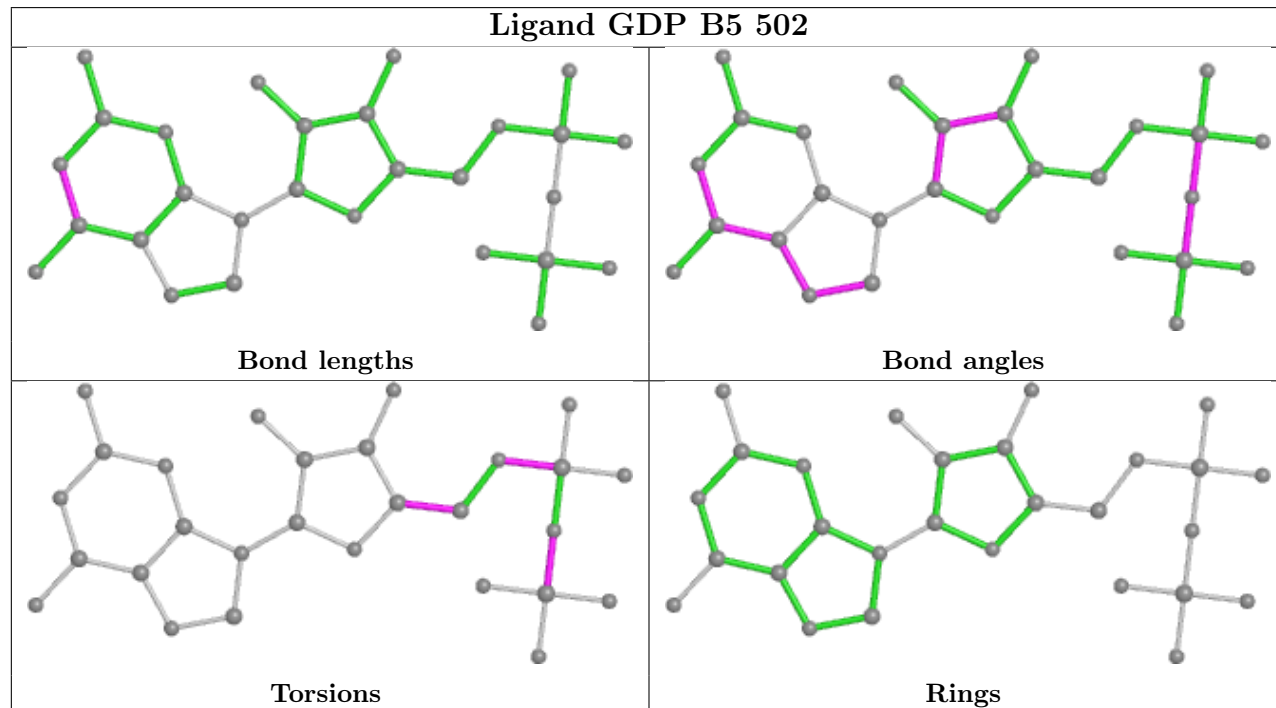
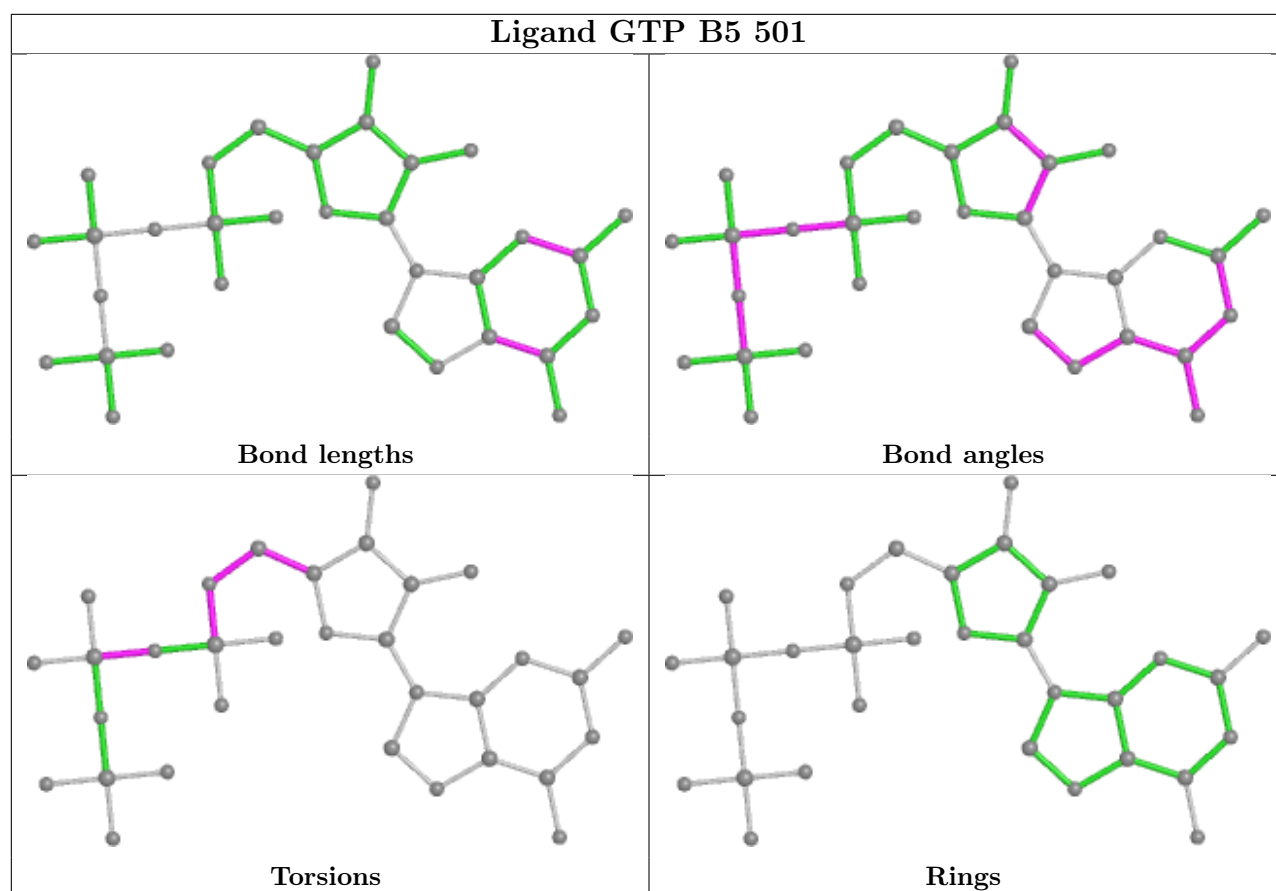
## Ligand GTP A5 501

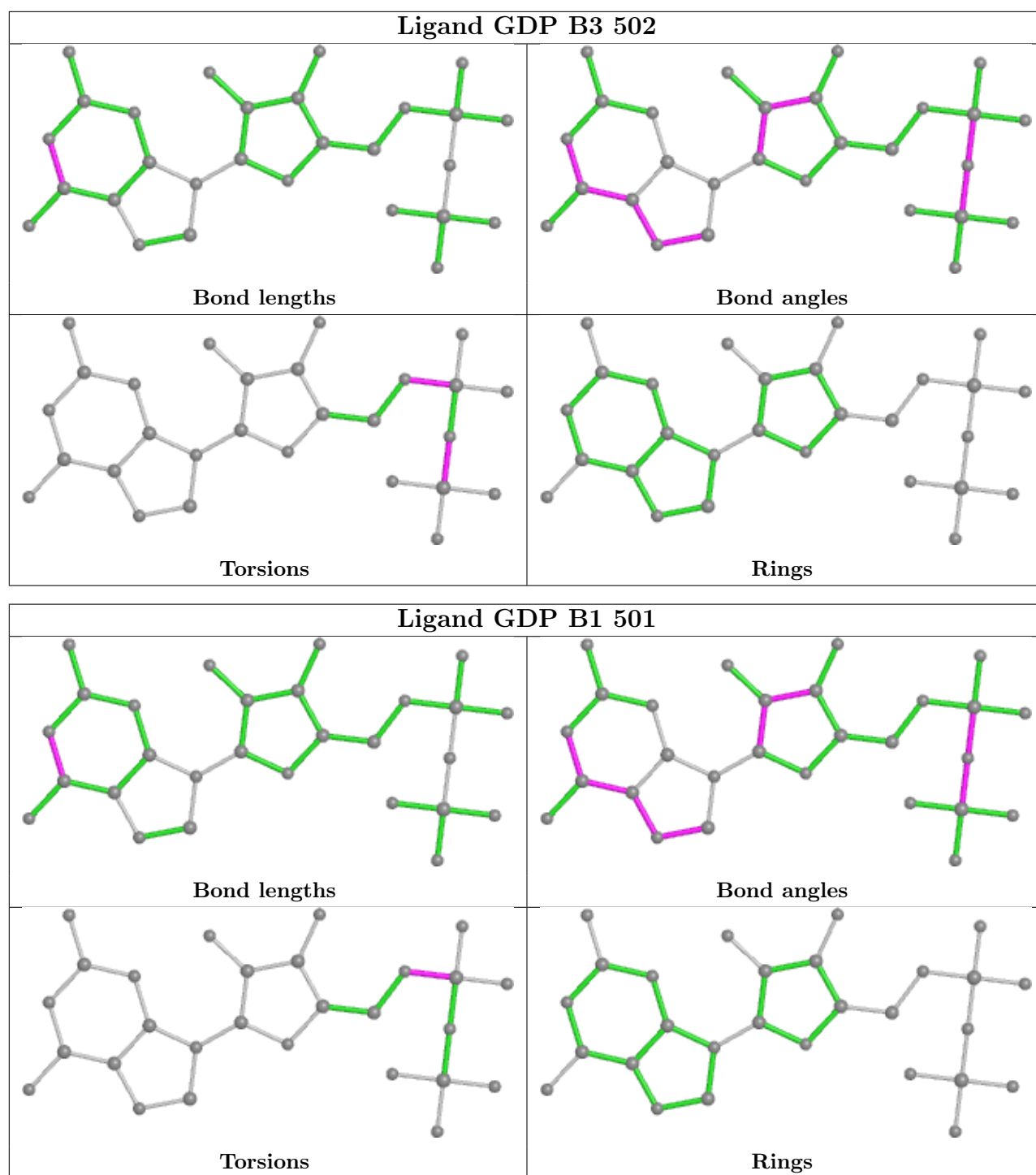


## Ligand GTP B7 501









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
19	Y0	3
17	X0	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X0	396:UNK	C	403:UNK	N	28.65
1	Y0	387:UNK	C	394:UNK	N	22.26
1	Y0	420:UNK	C	424:UNK	N	12.82
1	X0	346:UNK	C	348:UNK	N	9.65
1	Y0	281:UNK	C	284:UNK	N	6.72

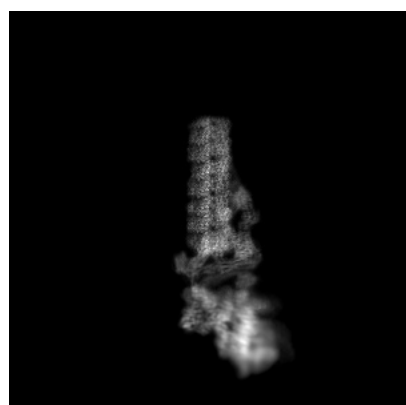
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23082. These allow visual inspection of the internal detail of the map and identification of artifacts.

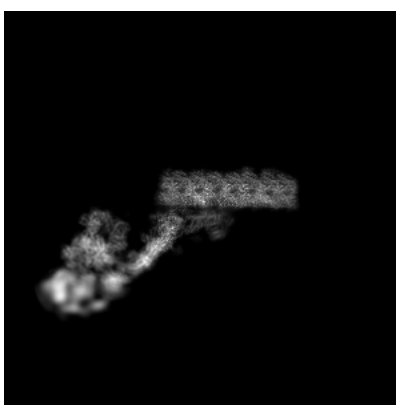
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

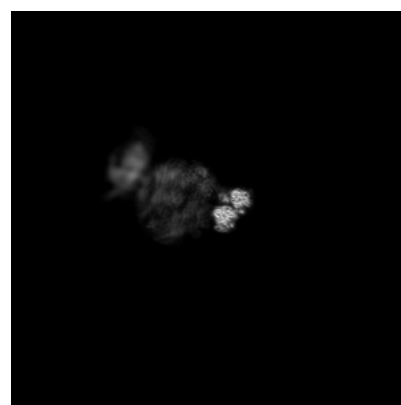
#### 6.1.1 Primary map



X



Y

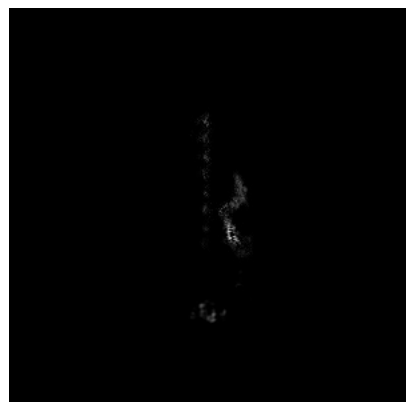


Z

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

### 6.2 Central slices [i](#)

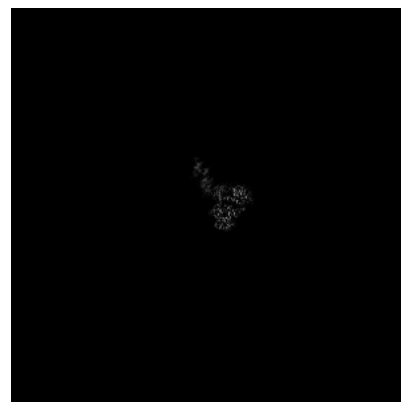
#### 6.2.1 Primary map



X Index: 350



Y Index: 350

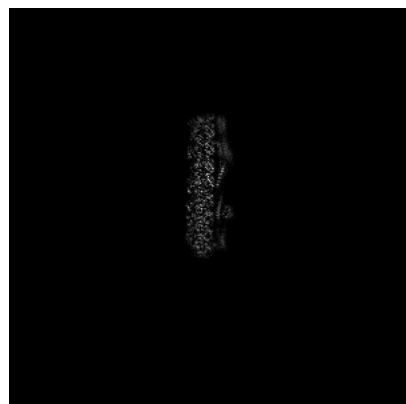


Z Index: 350

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

## 6.3 Largest variance slices [i](#)

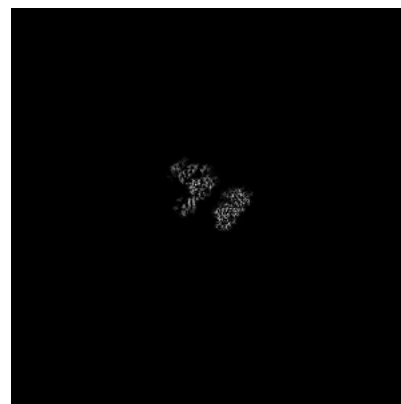
### 6.3.1 Primary map



X Index: 372



Y Index: 347



Z Index: 294

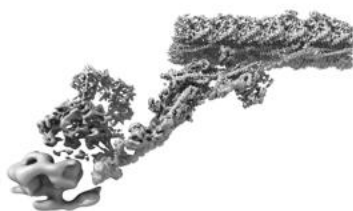
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

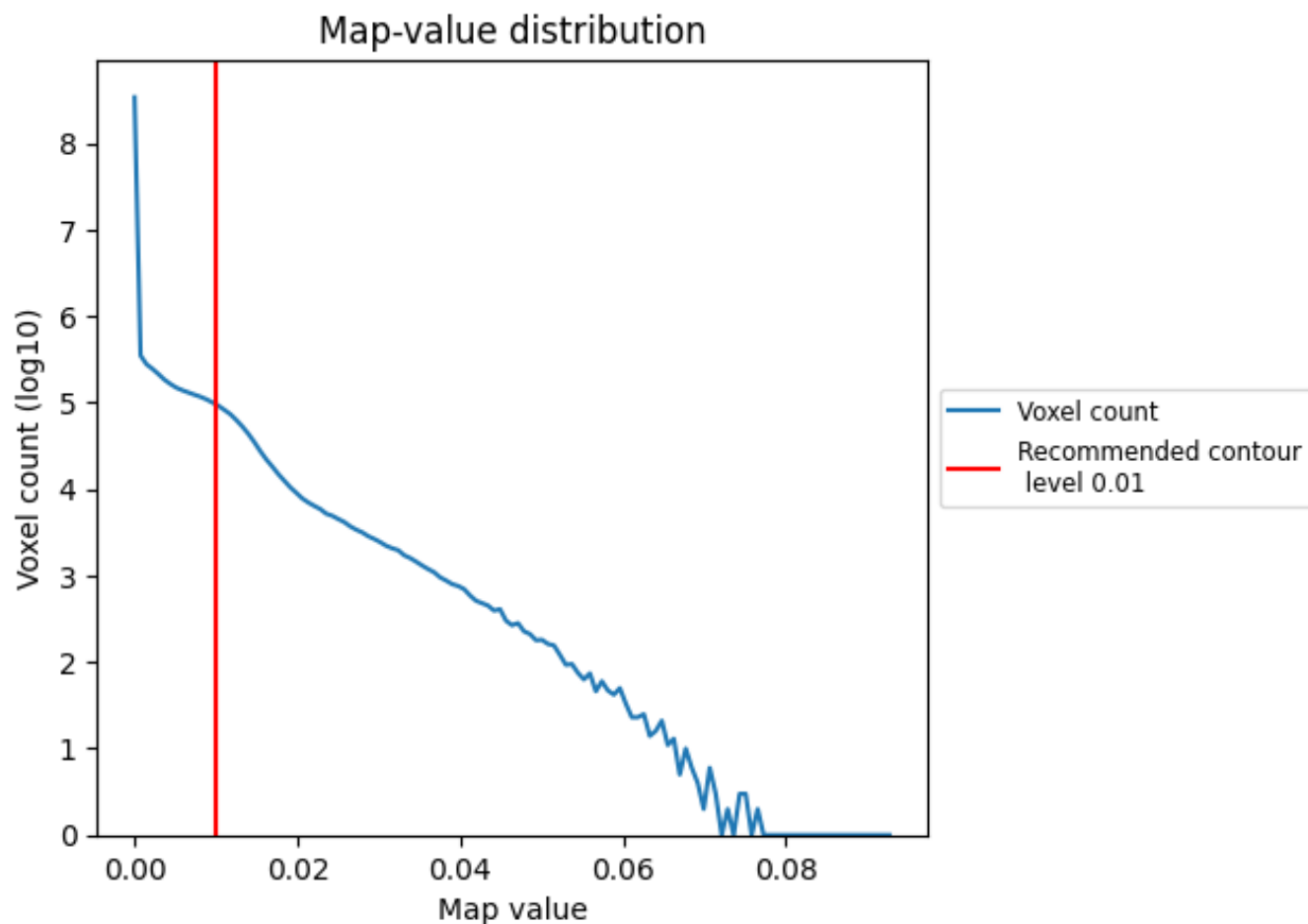
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

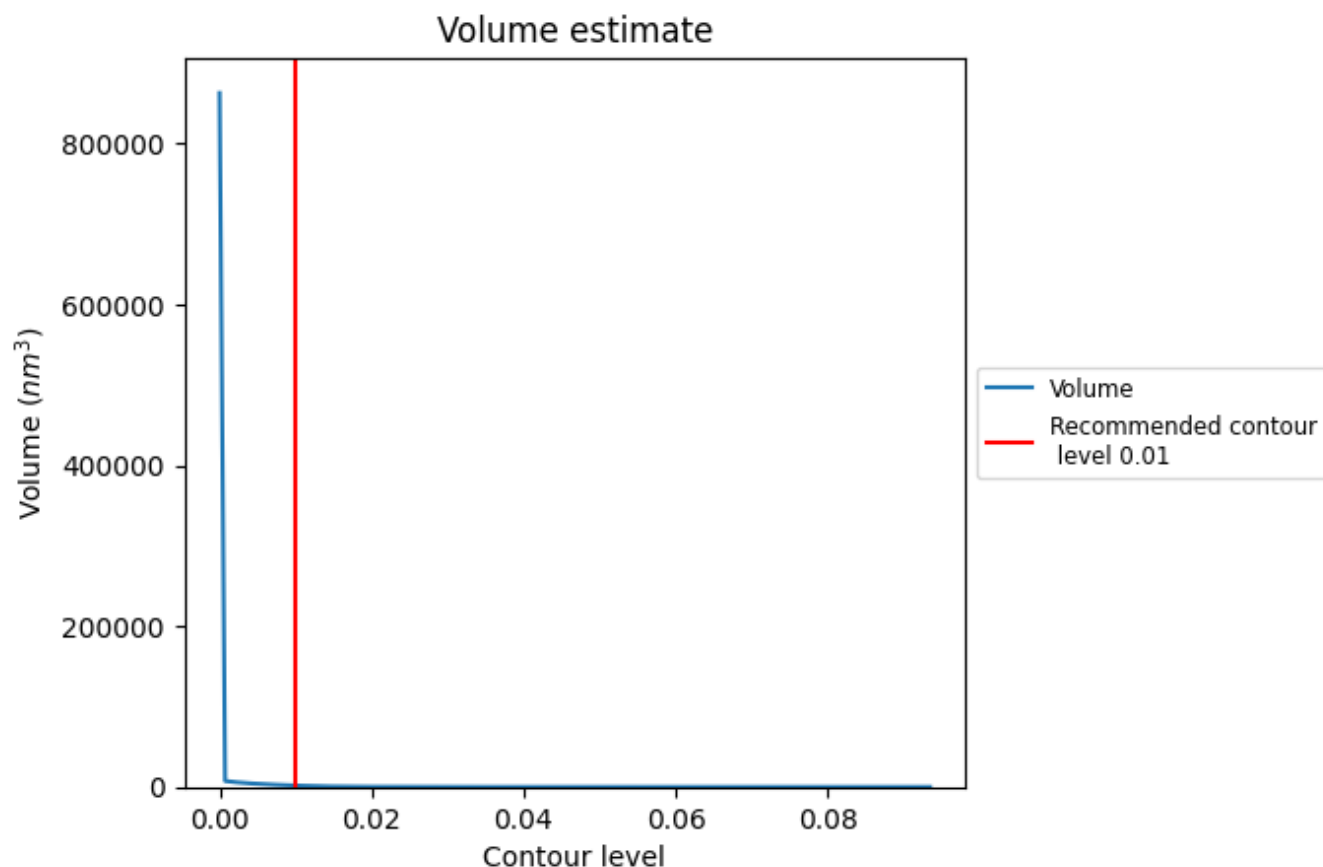
This section contains the results of statistical analysis of the map.

### 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.

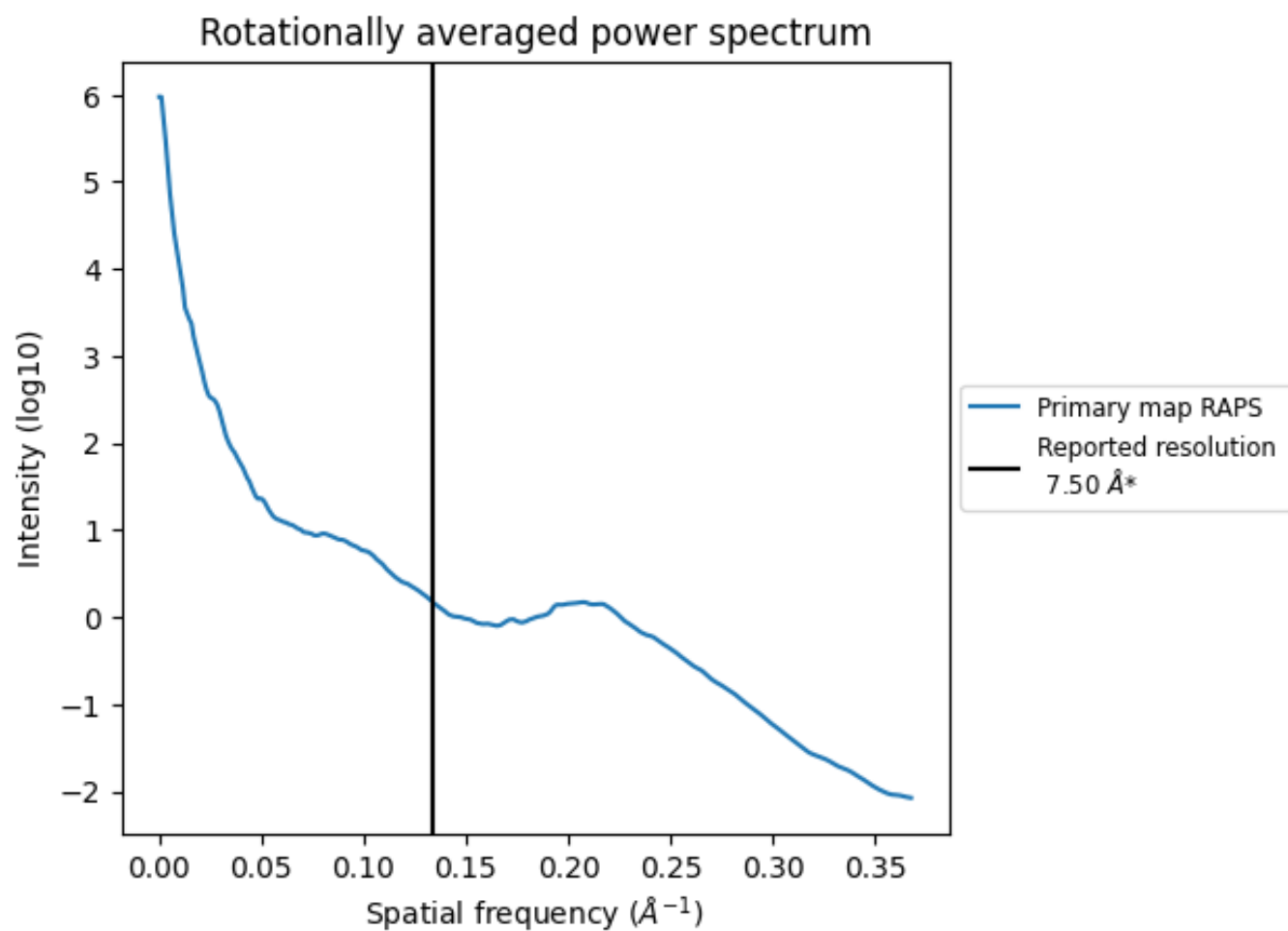
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1728 nm<sup>3</sup>; this corresponds to an approximate mass of 1561 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 0.133 Å<sup>-1</sup>

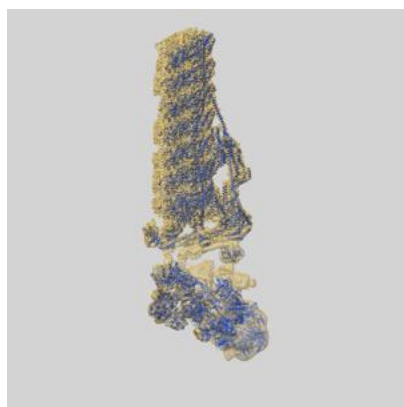
## 8 Fourier-Shell correlation

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

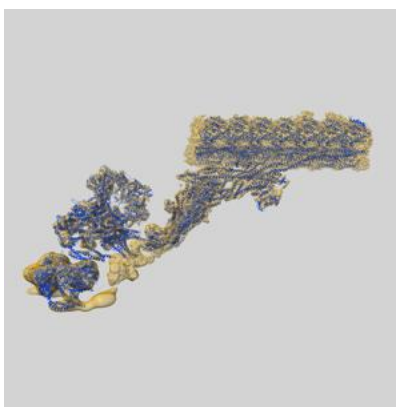
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23082 and PDB model 7KZM. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

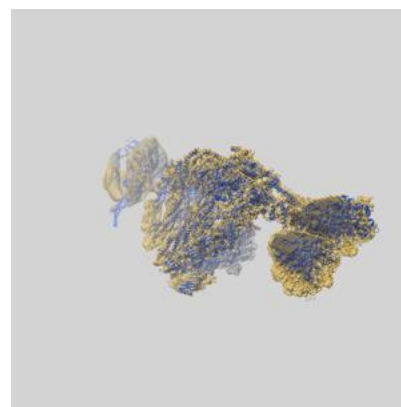
### 9.1 Map-model overlay [i](#)



X



Y



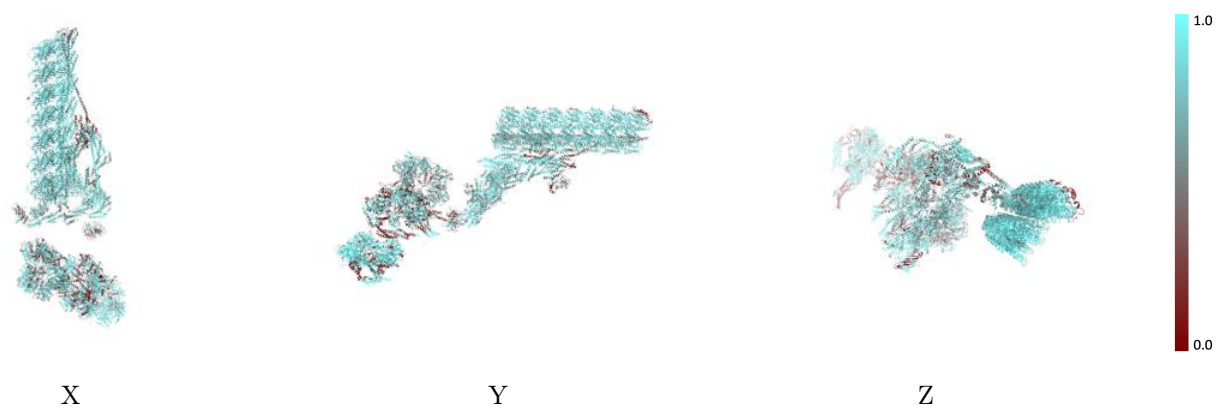
Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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](#)

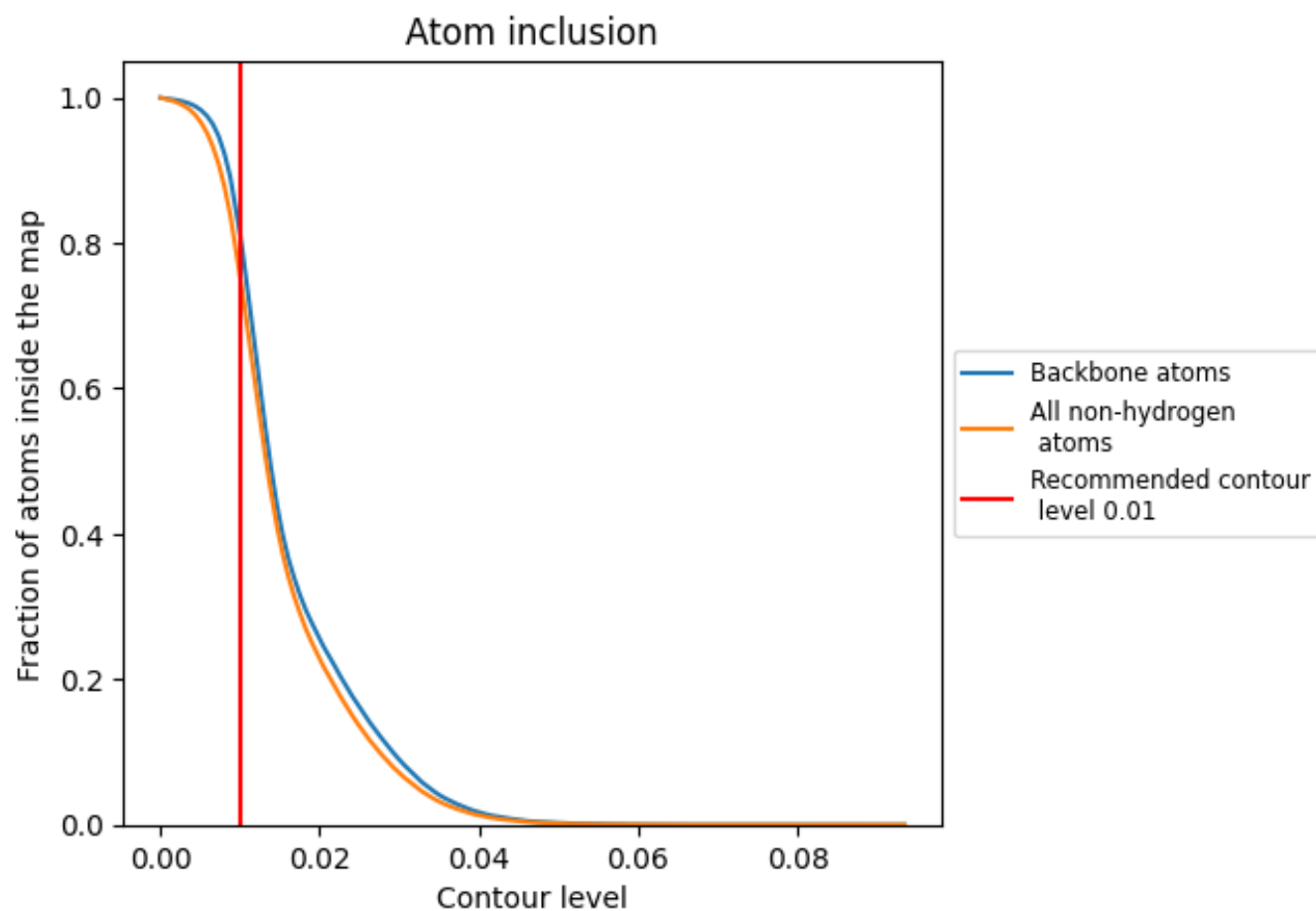
This section was not generated.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).




































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 75% 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 (0.01) and Q-score for the entire model and for each chain.




Chain	Atom inclusion
All	 0.7538
A	 0.7811
A1	 0.8454
A2	 0.8872
A3	 0.8974
A4	 0.9156
A5	 0.8980
A6	 0.8773
A7	 0.8657
B	 0.6073
B1	 0.8395
B2	 0.8844
B3	 0.8993
B4	 0.8975
B5	 0.9162
B6	 0.8637
B7	 0.7598
C	 0.6326
D	 0.7966
E	 0.7605
F	 0.5859
G	 0.6019
H	 0.8027
I	 0.7092
J	 0.7692
K	 0.7761
L	 0.6551
M	 0.7186
N	 0.7936
O	 0.5343
P	 0.7181
X	 0.5987
X0	 0.6877
X1	 0.7474
Y	 0.6534



*Continued on next page...*



*Continued from previous page...*

Chain	Atom inclusion
Y0	 0.8321
Y1	 0.7727
Z	 0.6064