



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 10:52 PM UTC

PDB ID : 7MOQ / pdb_00007moq
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

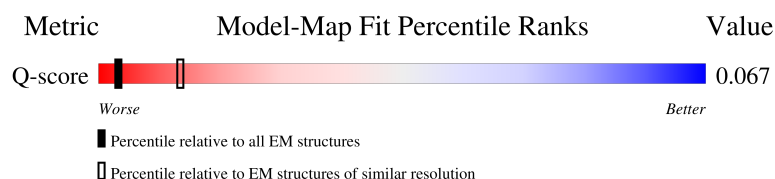
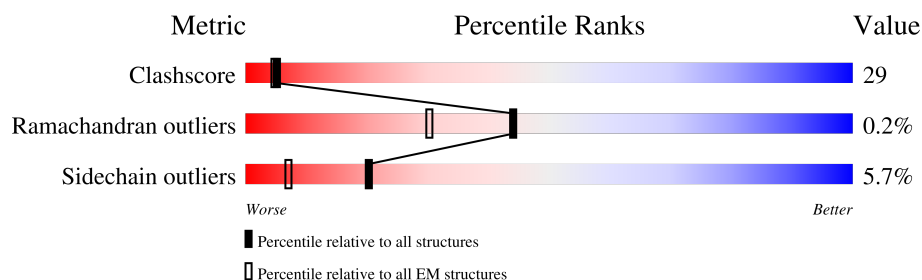
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



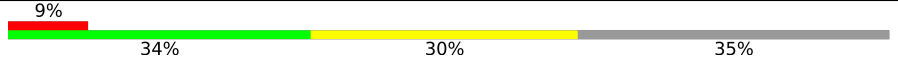
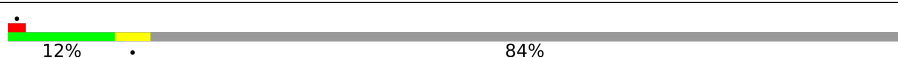
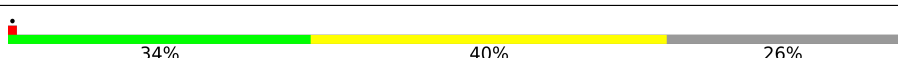
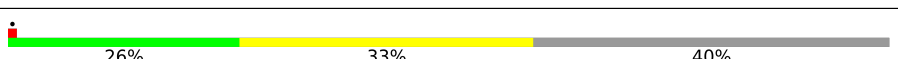
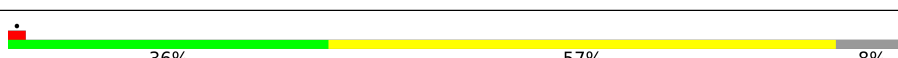
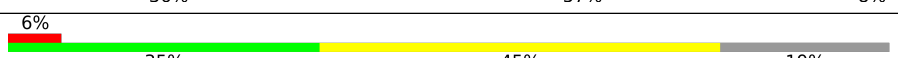
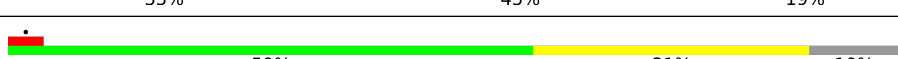
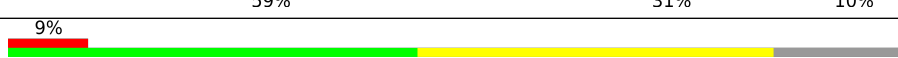
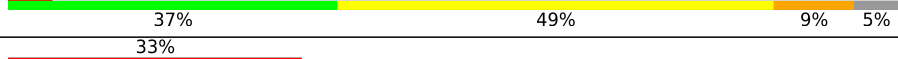
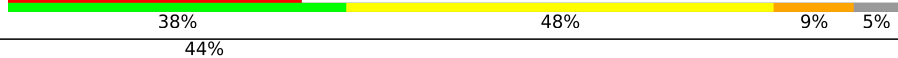
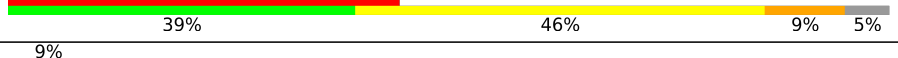
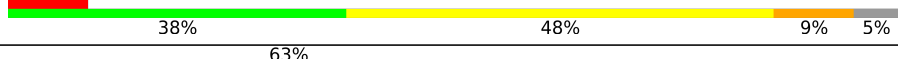
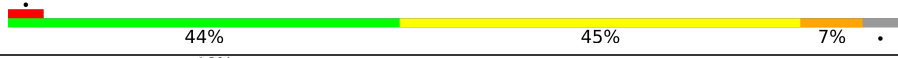
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	361 (7.50 - 8.50)

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	92%
2	B	4594	23% 44% 45% 11%
3	C	4620	27% 52% 38% 10%
4	D	667	21% 28% 50%

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Mol	Chain	Length	Quality of chain
4	d	667	
5	E	670	
5	e	670	
6	F	133	
7	G	159	
8	H	92	
9	I	110	
10	J	93	
11	K	111	
12	L	111	
13	M	87	
14	N	132	
15	O	117	
16	P	110	
17	Q	443	
17	U	443	
17	Y	443	
17	q	443	
17	u	443	
17	y	443	
18	R	449	
18	S	449	
18	W	449	
18	r	449	
18	s	449	

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Mol	Chain	Length	Quality of chain
18	w	449	
19	T	309	
20	V	130	
20	x	130	
21	X	555	
22	Z	538	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	ADP	C	4703	-	-	X	-

2 Entry composition

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
1	A	340	Total	C	N	O	S	0	0
			2698	1720	458	508	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4091	Total	C	N	O	S	0	0
			33080	21201	5547	6175	157		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	4159	Total	C	N	O	S	0	0
			33529	21421	5645	6289	174		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	331	Total	C	N	O	S	0	0
			2669	1719	439	493	18		
4	d	128	Total	C	N	O	S	0	0
			957	597	170	187	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	436	Total	C	N	O	S	0	0
			3264	2059	565	621	19		
5	e	109	Total	C	N	O		0	0
			684	414	132	138			

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

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

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

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

- Molecule 8 is a protein called Dynein light chain.

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

- Molecule 9 is a protein called Dynein light chain.

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

- Molecule 10 is a protein called Dynein light chain.

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

- Molecule 11 is a protein called Dynein light chain.

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

- Molecule 12 is a protein called Dynein light chain.

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

- Molecule 13 is a protein called Dynein light chain.

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

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

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

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

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

- Molecule 16 is a protein called Thioredoxin.

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

- Molecule 17 is a protein called Tubulin beta chain.

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

- Molecule 18 is a protein called Tubulin alpha chain.

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

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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		

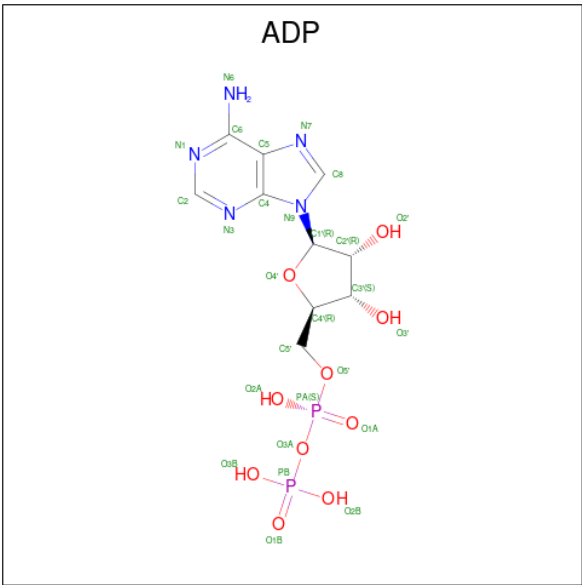
- Molecule 21 is a protein called Docking complex 1 protein.

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.

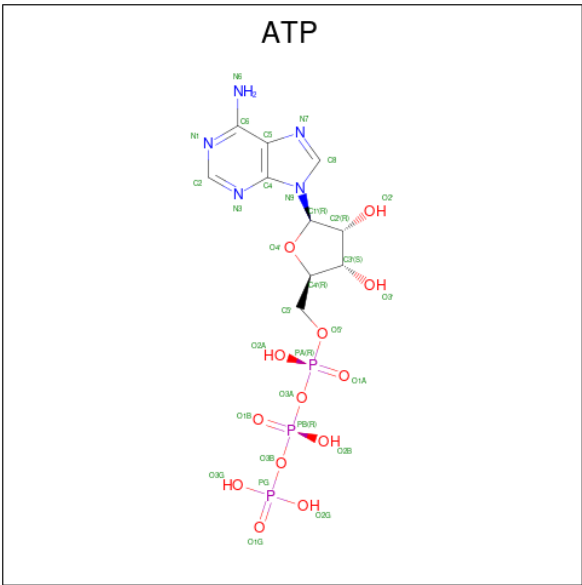
Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	117	Total	C	N	O	S	0	0
			993	614	191	186	2		

- Molecule 23 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



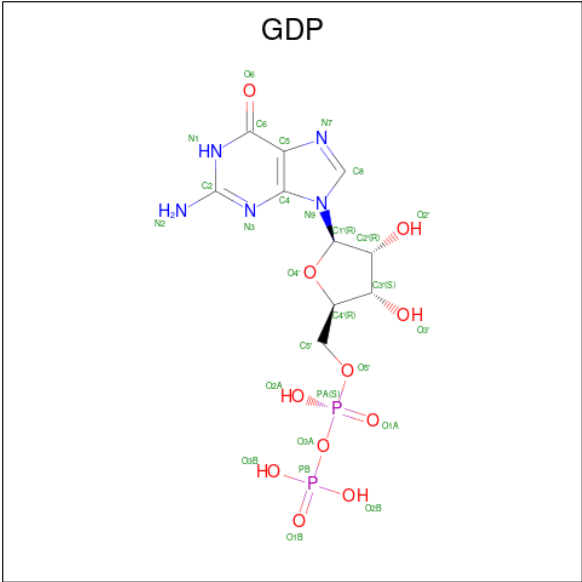
Mol	Chain	Residues	Atoms					AltConf
23	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
23	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

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



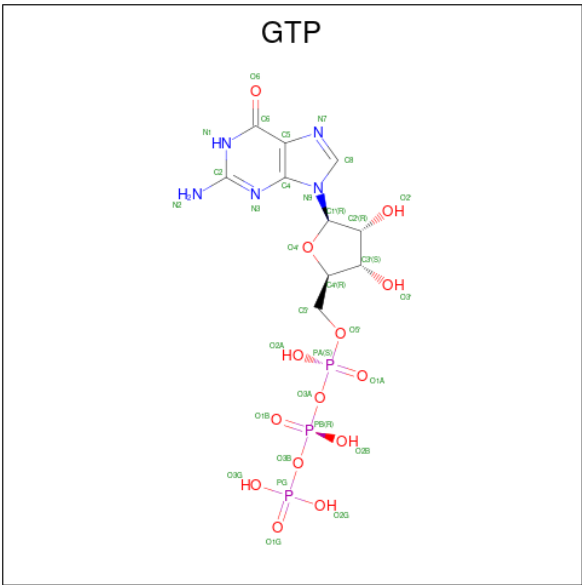
Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

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



Mol	Chain	Residues	Atoms					AltConf
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 (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

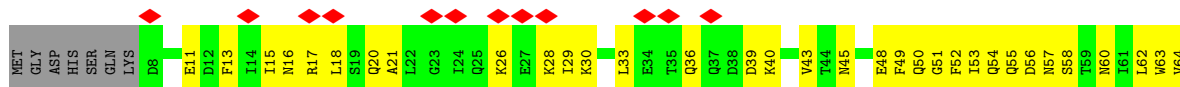
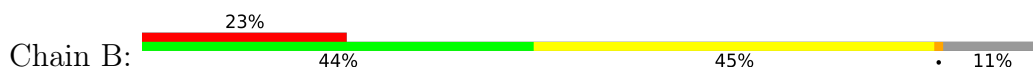
- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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





- Molecule 2: Outer arm dynein beta heavy chain

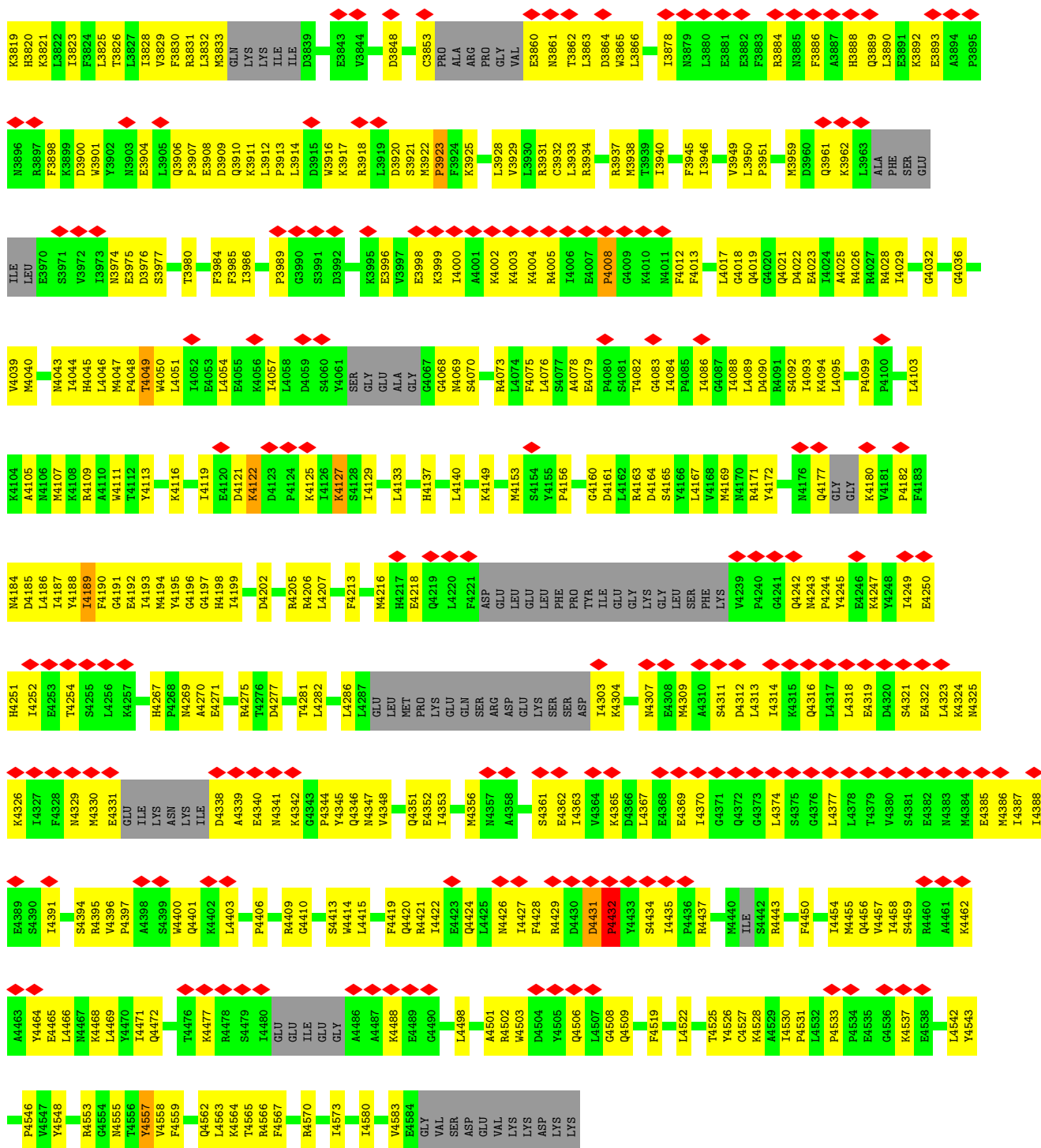


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N796	F797	N798	N799	K800	K801	K802	E803	N806	N810	P811	D812	D815	N819	N832	G833	N834	Q835	I836	Q837	K838	L839	K841	E842	N843	L844	N847	D850	K851	K852	Q853	N854	S855	K856	K857	N858	N859	N860	D861	P862	K863	N864	V865	I866	V867	S872	T873	A874	K875	K876	K877	L794	A795																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
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K640	K644	S651	S652	Q653	D654	L655	L656	K657	L661	C662	K663	E664	E665	N666	D667	K670	N671	N672	F673	D674	P675	S676	L677	K682	V686	P687	L688	R691	L692	T697	I701	K704	A705	E706	T707	Y708	R709	T710	Q711	I712	V713	A714	L715	D716	S632	K717	I718	W719	D720																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
L880	H881	L882	N883	E884	Q885	I886	N887	P888	V889	F890	P811	K892	R893	N894	D895	L899	F900	I901	R902	R903	L904	G907	Q908	S909	F913	D914	P915	E916	E917	G918	S921	L924	T925	V926	R927	P928	N929	I930	P931	P932	ASP	ASP	GLU	GLU	ASN	ASN	GLY	GLY	P952																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
K192	A193	H194	I195	F196	E197	G198	S199	I200	T201	T202	W203	T204	I207	K208	N209	V210	L211	K212	P215	E216	Q217	L218	L219	K220	Y221	P227	Q228	A229	E230	D231	F232	L233	L234	L235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	E1000	E1001
S865	G866	Q867	S868	E869	K870	C71	T72	F73	T74	TYR	GLY	Q77	D82	K83	F84	K85	K86	K87	G88	I89	A90	V91	I92	K93	L94	G95	L96	H97	K98	L99	T100	N101	E102	N103	I104	A105	V108	V109	V110	V111	E112	N115	N116	L117	L118	E119	H120	L121	L122	S123	V124	F125	N126	E127	I128	M129																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
S130	P131	V132	M133	Q134	N135	P136	L137	Q138	Q139	Q140	G141	G142	T143	D144	L145	V146	L147	K148	M151	E152	K153	F154	N155	N156	Y157	V158	A159	Q160	H161	Y162	V163	L164	L165	G166	Q167	I168	K169	G170	K171	THR	M173	L174	P175	L176	P177	S178	H179	K180	L181	S184	D185	T186	T187	P188	D189	K190	D191																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							

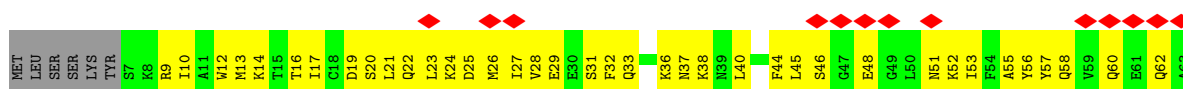
ARG	GLY	R1093	P1155	F1229	L1290	Y1362	E1424	K1488	K1557	L1634	L1701	R1767	ARG	N1850
GLN	ASP	W1094	R1156	M1230	Q1291	N1363	N1426	S1489	D1586	G1635	E1702	L1768	THR	K1851
THR	ASP	W1097	R1157	K1231	K1292	I1365	I1427	Q1490	M1580	D1636	G1703	E1769	LEU	I1852
ARG	GLY	V1098	T1160	E1232	S1293	V1366	N1428	G1491	P1567	C1637	A1704	N1770	THR	I1853
PHE	GLY	T1099	T1161	V1233	E1234	E1367	E1429	Y1493	S1568	F1638	K1705	L1771	ARG	I1854
PRO	ASN	D1100	M1164	E1235	N1294	E1368	I1430	Y1494	V1569	D1639	N1706	L1772	GLY	I1855
TRP	THR	F1101	M1167	S1236	K1368	V1369	V1431	E1495	V1570	G1640	T1707	K1773	GLU	V1856
LYS	GLU	F1102	M1167	F1236	K1296	K1370	D1432	F1496	E1571	L1641	A1708	K1774	ASP	D1857
ASN	LYS	V1103	M1167	K1237	C1301	N1371	A1434	Y1497	A1572	T1644	L1709	V1775	ASP	F1858
LYS	GLN	V1104	K1170	K1238	M1302	G1372	K1435	D1498	C1573	T1645	L1710	G1777	LYS	W1859
LYS	N1034	N1104	L1171	E1239	L1305	I1371	K1436	R1500	T1574	L1644	G1713	D1778	LYS	R1860
P1035	P1035	Q1105	K1172	F1240	K1306	LEU	K1437	R1501	I1575	F1646	G1714	L1779	LYS	R1861
L1036	L1036	R1107	K1173	M1241	N1307	VAL	E1437	E1502	E1576	E1647	D1715	H1780	LYS	
L1037	L1037	T1109	H1174	Q1242	K1308	PRO	A1438	D1503	V1582	P1648	K1716	I1781		
K1038	K1038	Q1110	N1175	K1243	L1309	LEU	K1439	W1504	G1583	P1649	P1717	L1782		
G1040	G1040	Q1111	V1176	Q1244	K1309	VAL	I1440	E1506	W1584	A1650	R1718	E1783		
R1041	R1041	P1177	P1177	L1244	L1310	SER	E1441	K1507	S1585	N1651	E1719	R1784		
A1042	A1042	K1111	F1178	P1245	M1311	A1381	K1442	L1508	Q1586	P1652	E1720	K1786		
K1043	K1043	N1112	T1179	F1246	A1314	L1382	K1443	G1509	I1588	A1653	V1722	I1787		
I1044	I1044	L1113	T1179	D1247	I1315	H1383	K1444	R1510	K1589	E1654	E1723	I1788		
P1045	P1045	L1114	E1180	Y1248	A1316	S1384	L1444	V1511	C1590	T1655	G1724	I1789		
N1046	N1046	D1115	K1181	Y1249	I1317	E1385	K1445	V1514	C1591	S1656	Y1725	I1791		
L1047	L1047	F1116	G1182	E1250	I1318	F1386	N1446	V1519	L1595	V1658	G1726	I1792		
D1048	D1048	I1117	T1183	S1251	I1319	M1387	I1447	L1514	E1600	G1659	A1727	I1793		
		E1118	D1184	M1252	F1320	E1388	E1448	L1519	E1595	I1659	Q1728	V1795		
D1051	D1051	K1119	P1185	Y1253	Q1321	I1388	Q1449	Q1522	E1600	G1661	I1729	H1796		
E1052	E1052	T1120	P1186	Q1253	N1323	I1399	W1450	K1523	E1600	G1662	A1730	I1797		
K1053	K1053	K1121	L1187	Y1254	D1324	R1390	W1451	W1524	K1603	I1662	L1731	S1797		
I1054	I1054	D1122	Q1188	E1255	K1325	H1391	K1452	W1525	K1604	I1663	K1732	R1798		
T1055	T1055	G1123	Q1189	N1256	K1326	W1392	K1454	K1526	SER	I1664	T1733	D1799		
H1056	H1056	I1190	I1199	I1257	T1327	L1395	Q1455	I1527	F1606	S1664	V1736	V1800		
L1057	L1057	K1125	M1196	Y1258	K1328	Q1397	F1456	L1528	R1607	K1665	I1742	V1801		
		K1126	F1197	N1259	K1332	I1398	E1457	L1530	Y1610	D1666	G1743	E1802		
Q1061	Q1061		N1197	M1258	I1333	T1399	Y1461	F1531	S1613	E1668	R1744	V1806		
			F1199	A1260	I1200	G1400	K1462	L1532	N1614	K1669	A1745	I1806		
I1064	I1064	A1129	I1198	A1260	D1262	T1401	E1463	L1534	Q1615	V1670	F1746	Q1807		
S1065	S1065	H1131	E1199	Y1261	T1263	V1402	T1466	S1535	S1616	K1671	E1747	V1809		
K1068	K1068	E1132	R1203	M1264	T1341	F1403	S1469	R1539	S1617	F1672	D1748	S1810		
T1069	T1069	N1133	V1204	M1265	M1342	D1404	L1470	L1542	L1617	S1673	L1749	E1811		
P1070	P1070	H1135	V1207	V1266	K1343	H1405	D1471	T1546	L1618	S1674	A1750	E1812		
E1071	E1071	K1136	K1208	Y1267	T1344	N1406	M1472	T1548	L1619	F1675	K1675	E1813		
D1072	D1072	K1137	K1208	Y1268	L1345	S1407	M1473	K1547	T1619	F1676	G1678	E1814		
T1073	T1073	K1138	I1212	H1269	G1346	L1408	M1474	V1548	S1622	I1677	G1751	F1815		
S1074	S1074	L1139	P1213	K1270	I1349	S1409	M1474	F1549	N1623	C1622	G1752	A1816		
W1075	W1075	Q1215	Q1215	L1271	L1352	F1410	V1476	F1549	N1623	N1626	G1753	W1817		
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R1077	R1077	M1141	S1142	E1275	K1354	F1412	K1478	G1551	A1627	I1680	T1755			
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K1084	K1084	S1148	D1226	E1280	F1360	L1420	L1484		C1631		E1759			
R1090	R1090	D1149	D1227	Y1281	G1361	Y1423	M1485		Y1633		C1760			
V1091	V1091	V1150	I1228	N1283			G1486				Q1761			
T1092	T1092	K1151	D1152	E1285							L1763			
		V1153	K1286	L1287							E1765			
		E1154	F1288	E1289							V1766			

G2805	G2806	F2807	P2808	G2809	T2810	E2811	N2812	L2813	L2814	L2817	L2818	L2819	G2820	T2821	G2822	F2823	V2824	A2825	H2827	GLN	LEU	ASP	GLN	GLN	TYR	T2835	Q2836	C2837	T2838	T2839	V2841	L2842	K2843	R2844	V2845	L2846	D2847	D2848	K2849	E2851	E2852	E2855	V2863	L2864	F2865	Q2866	Q2867	A2868	M2869	K2874							
P2730	S2731	K2732	K2733	R2734	Y2737	Q2738	T2739	N2740	E2743	V2747	C2748	E2749	G2750	I2751	C2752	P2756	G2757	Q2758	Y2759	S2760	G2761	G2762	D2763	Q2764	A2771	K2772	H2773	E2774	M2775	K2776	R2777	T2778	F2779	E2780	D2781	R2782	F2783	I2784	A2785	H2788	V2789	R2793	K2794	T2795	E2798	A2799	L2800	S2801	K2802	C2803	L2804						
G2659	S2660	F2661	L2666	L2667	Q2668	R2669	N2670	F2671	F2672	V2673	F2674	S2680	S2681	D2682	K2685	T2686	I2687	F2688	G2689	S2690	L2691	L2692	N2693	A2694	H2695	L2696	S2697	T2698	L2699	D2700	D2701	K2702	A2703	Q2704	K2705	M2706	A2707	F2708	K2709	L2710	V2711	A2712	E2713	T2714	Y2715	F2716	D2719	K2720	K2723	N2724	THR	THR	ALA	F2728			
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I3742	I3742	I3742	I3742	K3467	K3467	GLU	GLU	GLU	GLU	GLU	M3029	T2948	T2948
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• Molecule 3: Dynein heavy chain, outer arm protein

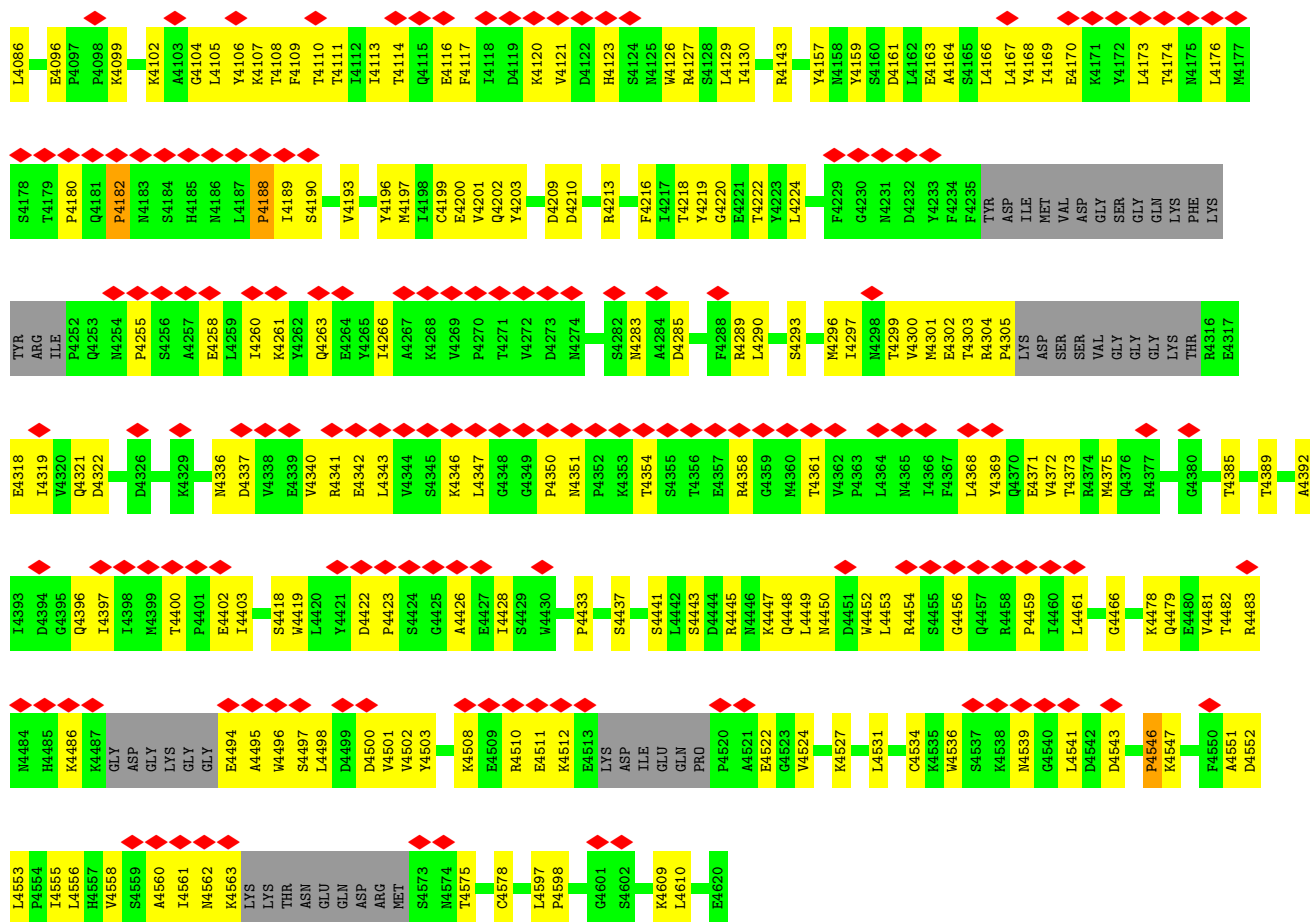




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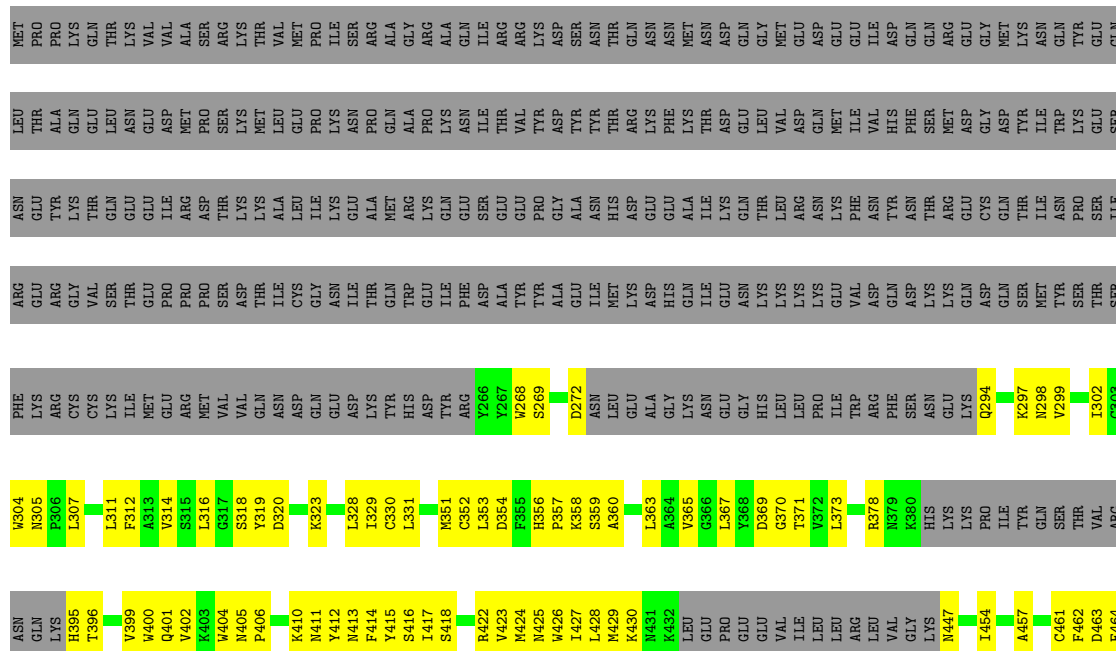
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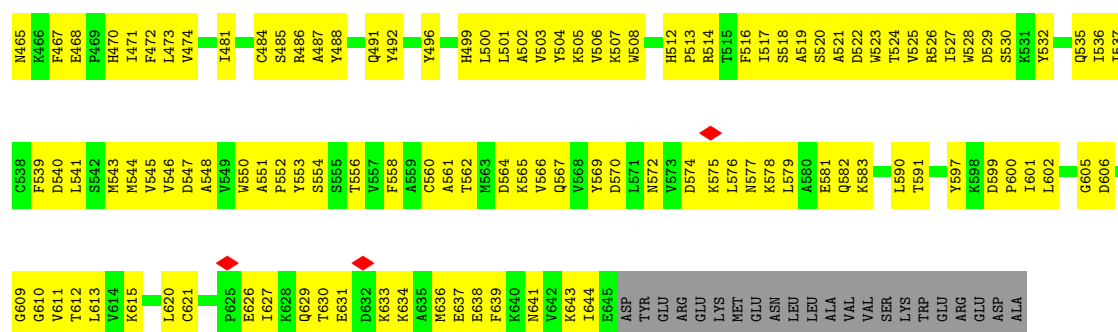
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ARG	VAL	PHE	ASN	LYS	GLY	LYS	ALA	VAL	PHE	LEU	LYS	ALA	GLN	THR	LYS	GLY	THR	LEU	GLY	ASP	THR	ILE	VAL	GLY	THR	GLY	THR	LYS	ASN	THR	VAL	GLY	ASP	THR	GLY	GLN	ALA	ILE	LEU	GLU	PRO	LEU	ASN	GLN	SER	ALA	ARG	GLU								
ILE	SER	LEU	LYS	GLU	GLU	ILE	GLN	LEU	ASN	GLU	ALA	THR	LYS	GLU	THR	LYS	LEU	LEU	LEU	GLY	THR	ILE	VAL	GLY	THR	GLY	THR	LYS	ASN	THR	VAL	GLY	ASP	THR	GLY	GLN	ALA	ILE	LEU	GLU	PRO	LEU	ASN	GLN	SER	ALA	ARG	GLU								



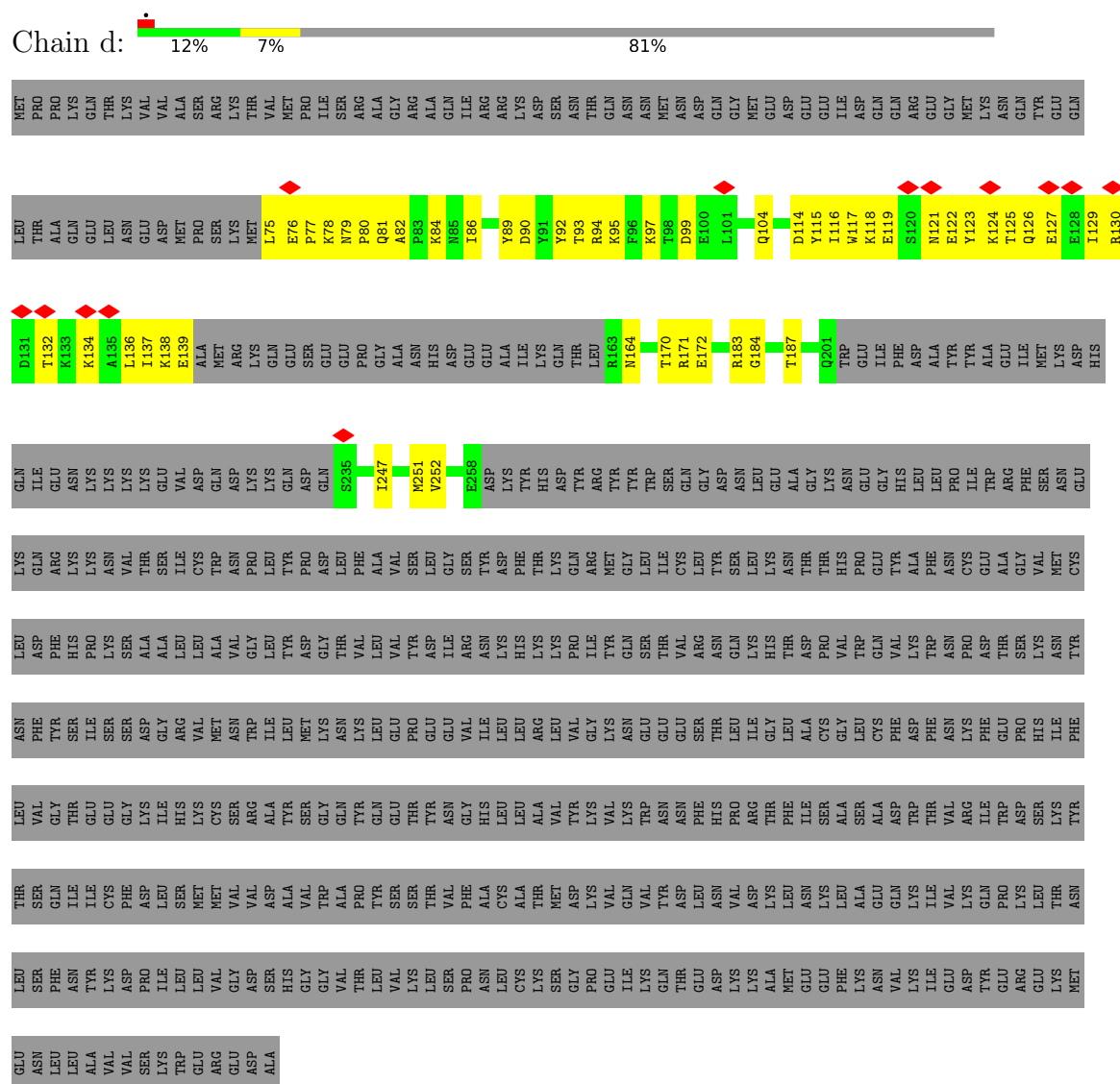
• Molecule 4: Dynein intermediate chain 2

Chain D: 21% 28% 50%

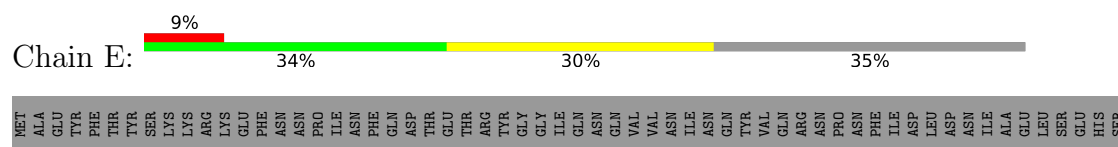




• Molecule 4: Dynein intermediate chain 2



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

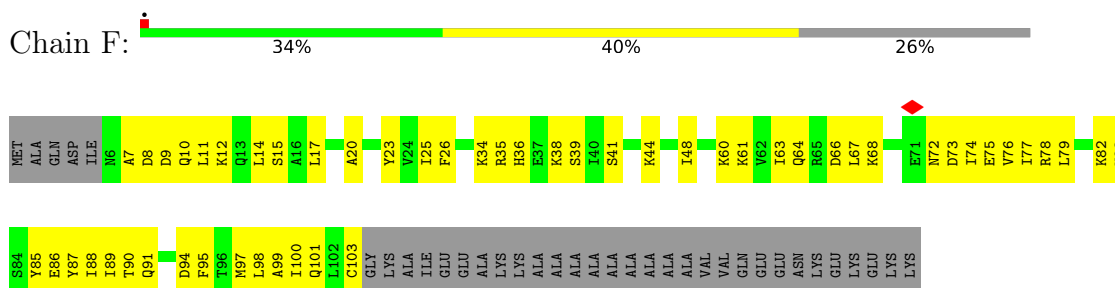


- Molecule 5: Flagellar outer dynein arm intermediate protein, putative

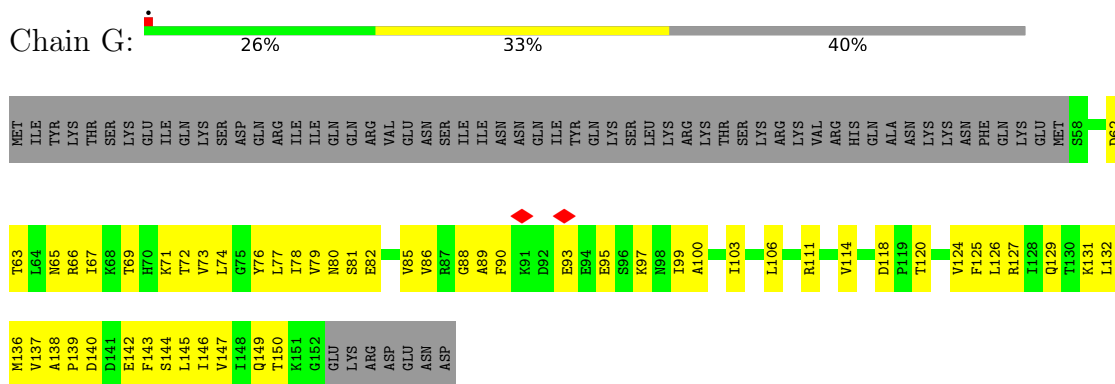
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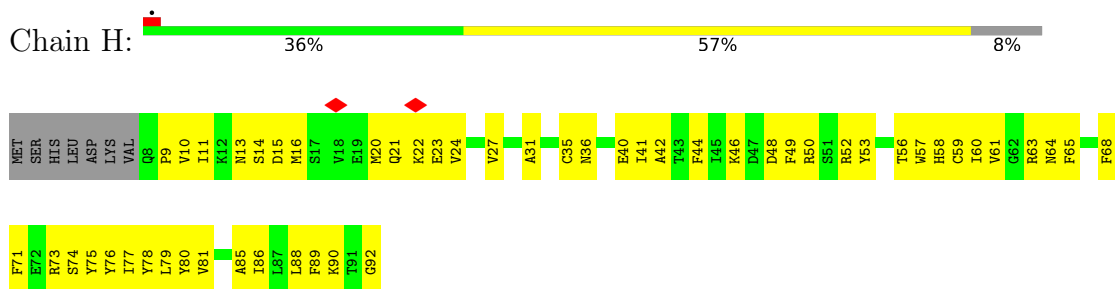
- Molecule 6: Dynein light chain roadblock-type 2 protein



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

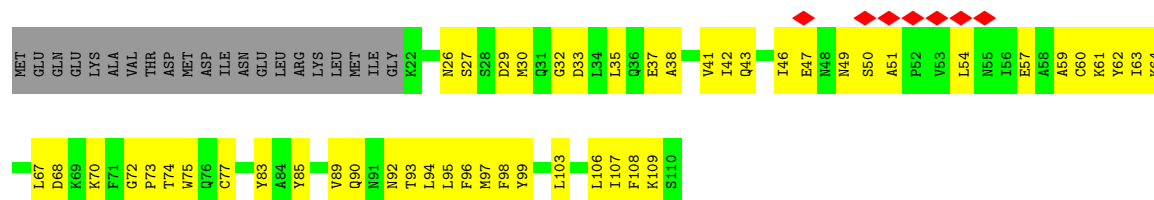


- Molecule 8: Dynein light chain



- Molecule 9: Dynein light chain

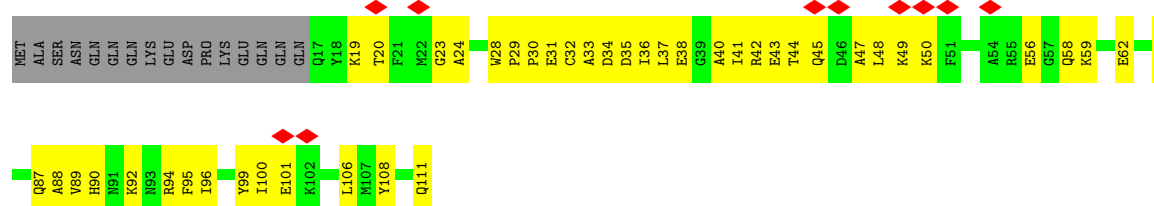




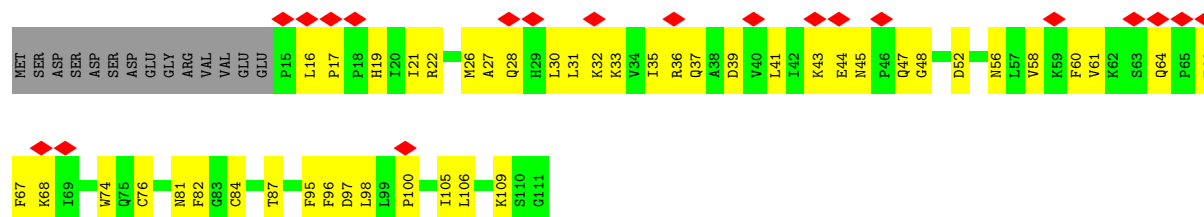
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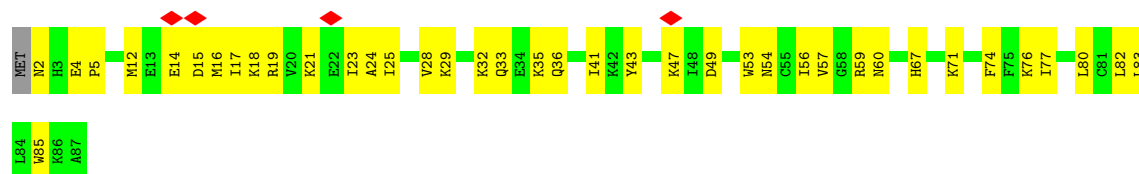
• Molecule 11: Dynein light chain



• Molecule 12: Dynein light chain

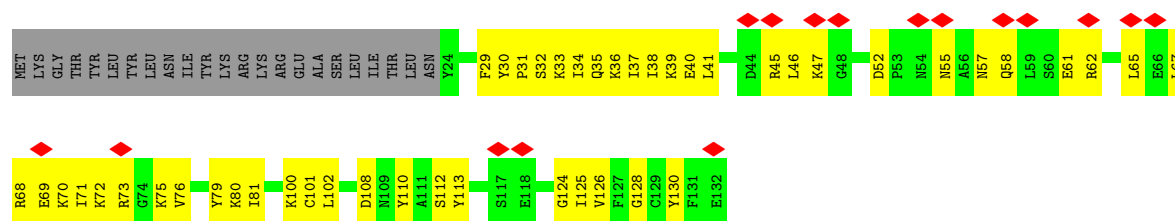


• Molecule 13: Dynein light chain

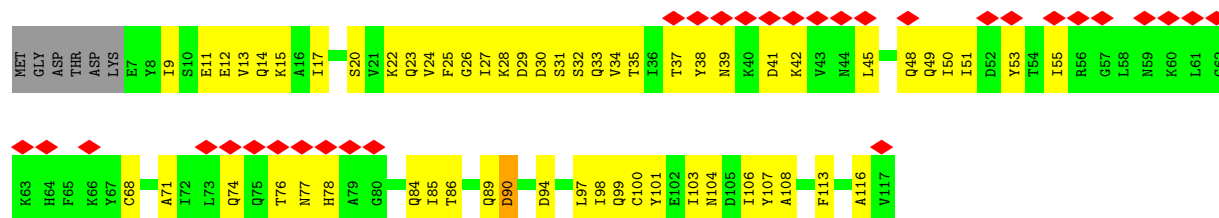


• Molecule 14: Dynein light chain 2A

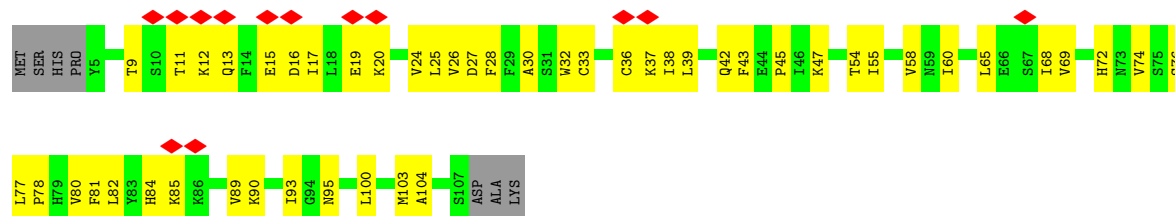




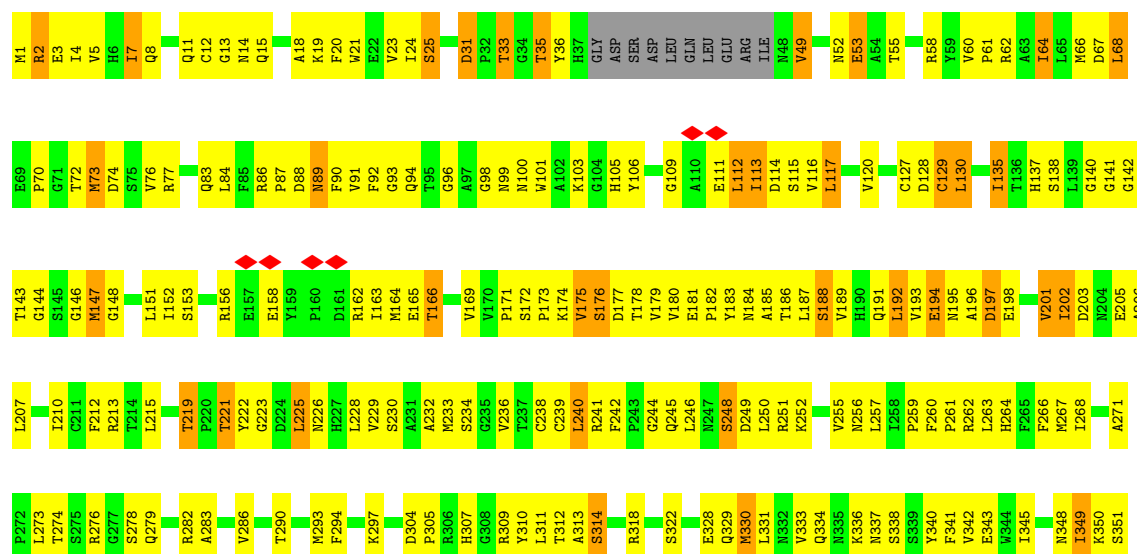
• Molecule 15: Dynein light chain tctex-type 1 protein

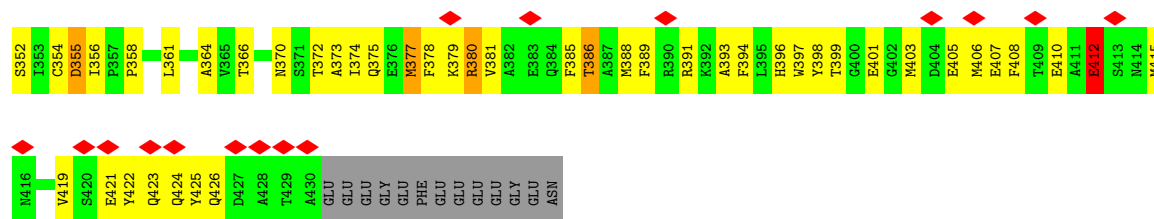


• Molecule 16: Thioredoxin

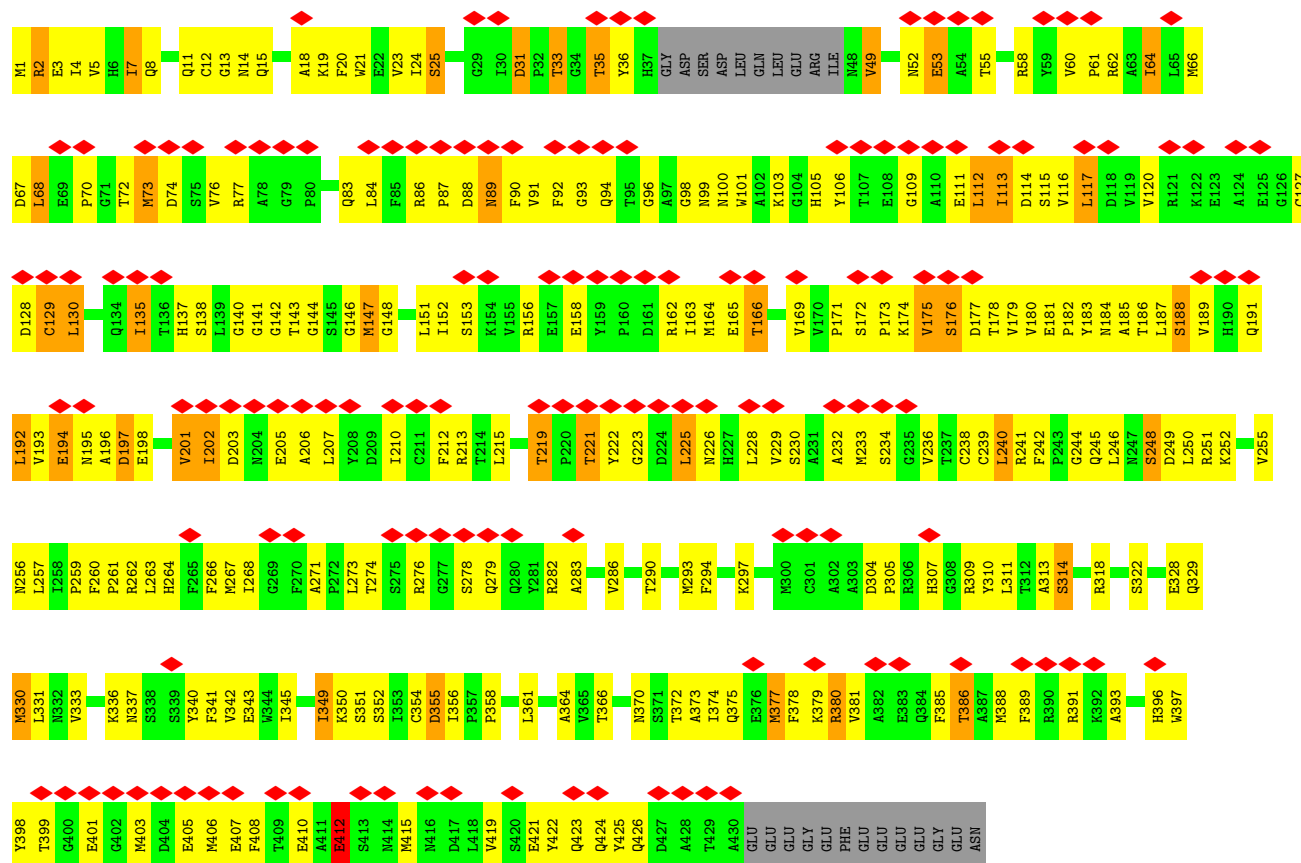


• Molecule 17: Tubulin beta chain

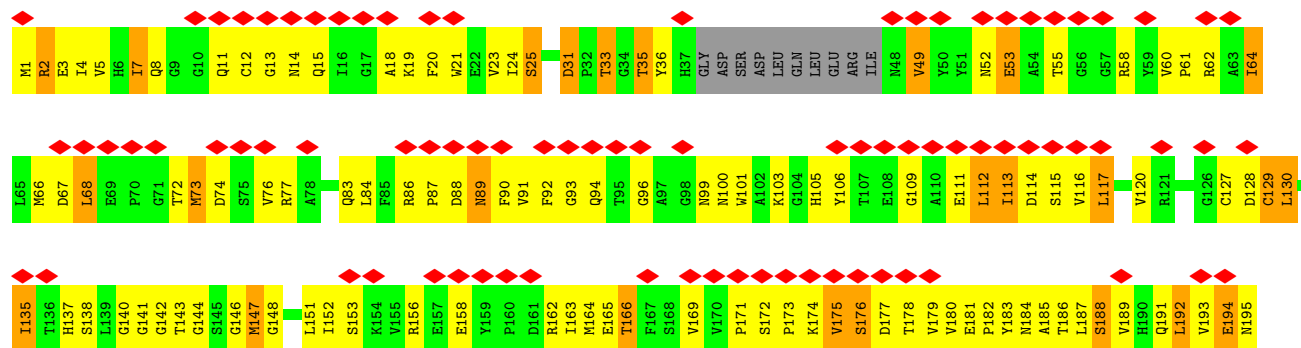
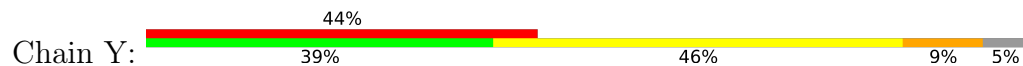


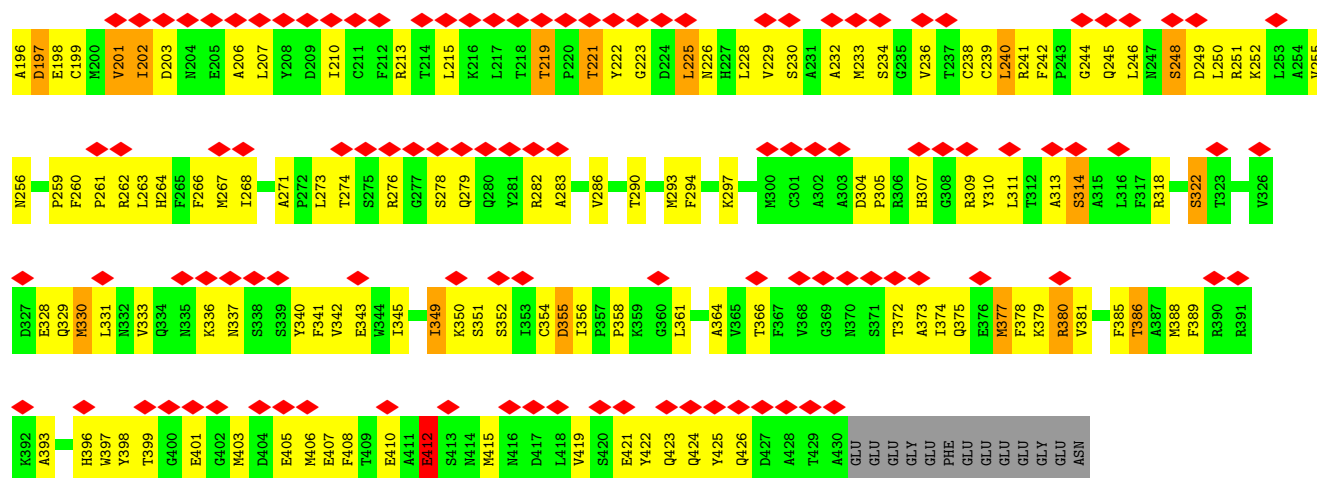


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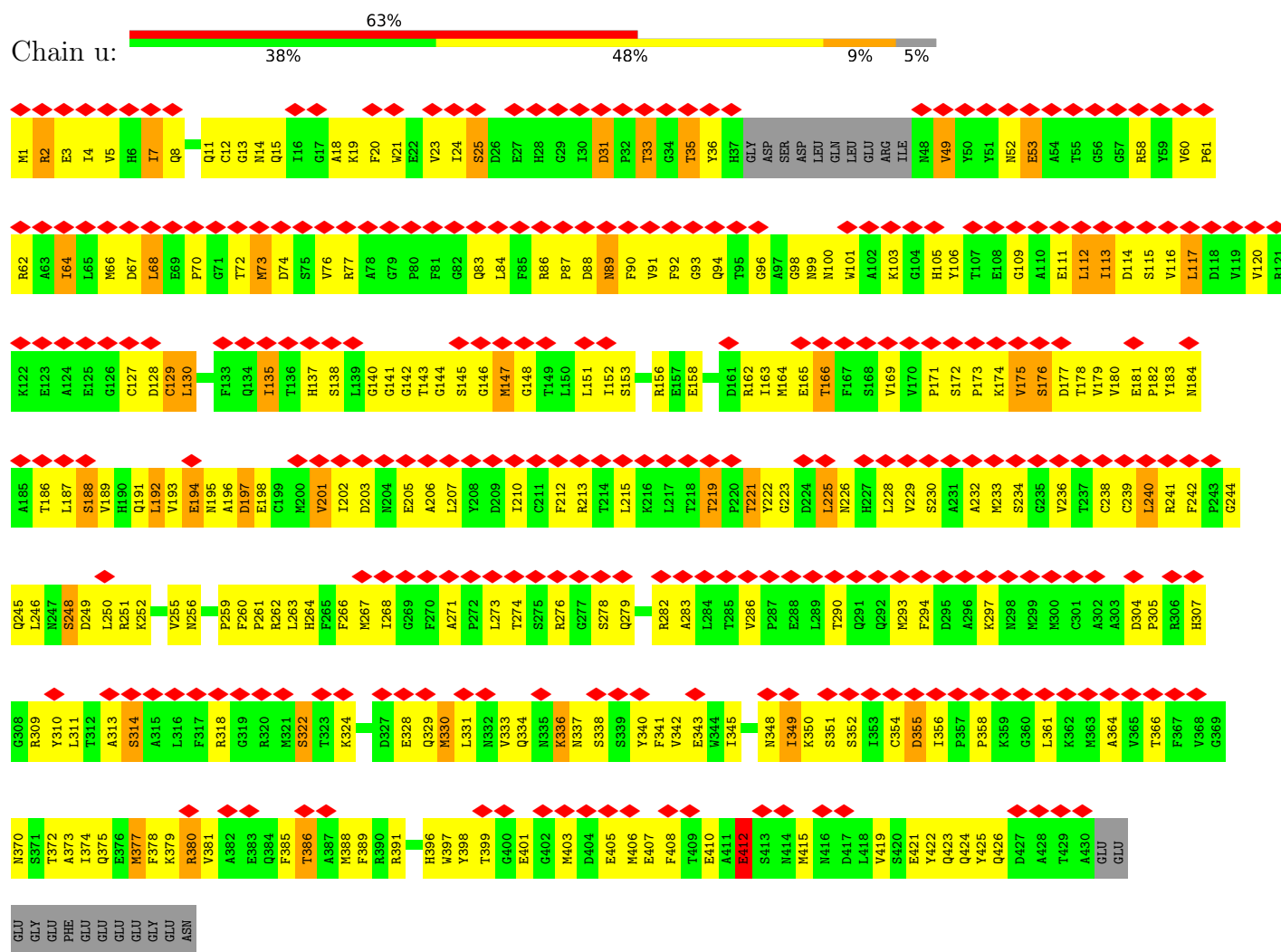


• Molecule 17: Tubulin beta chain



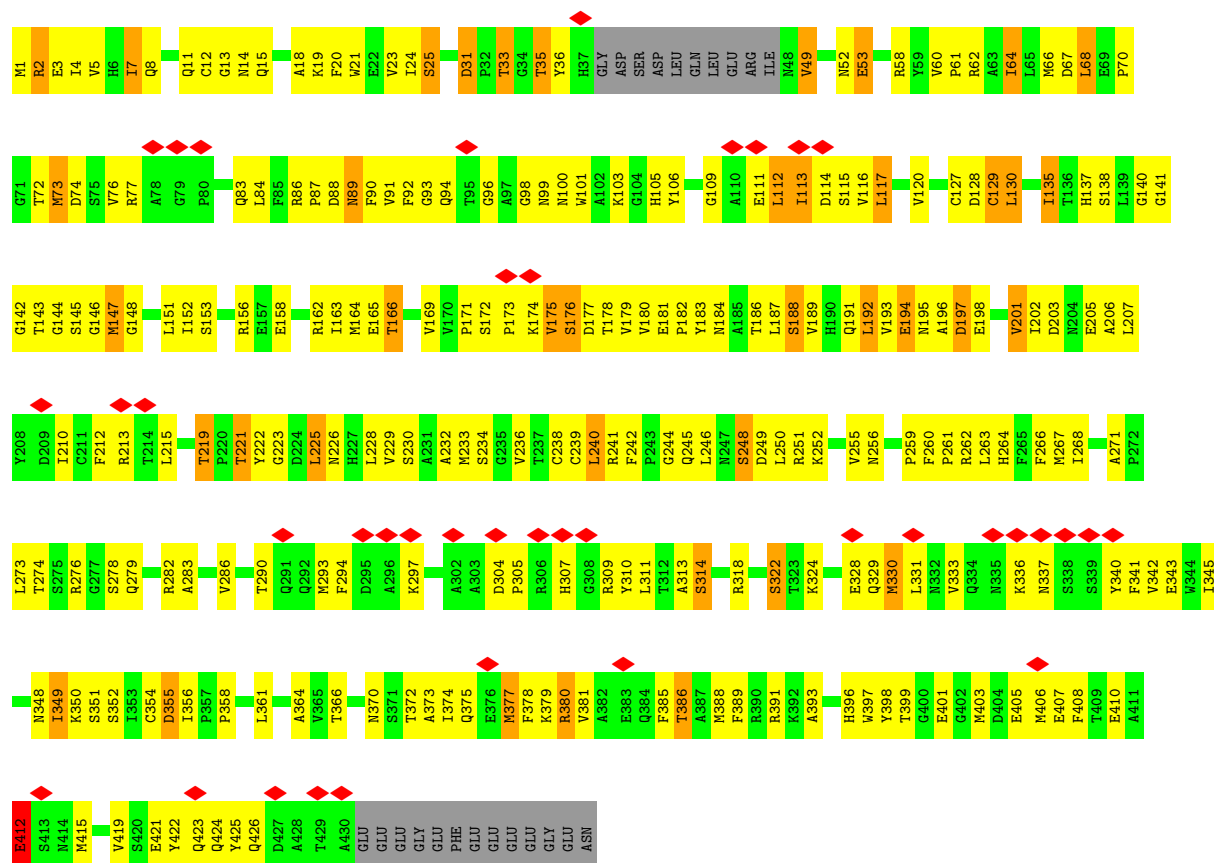


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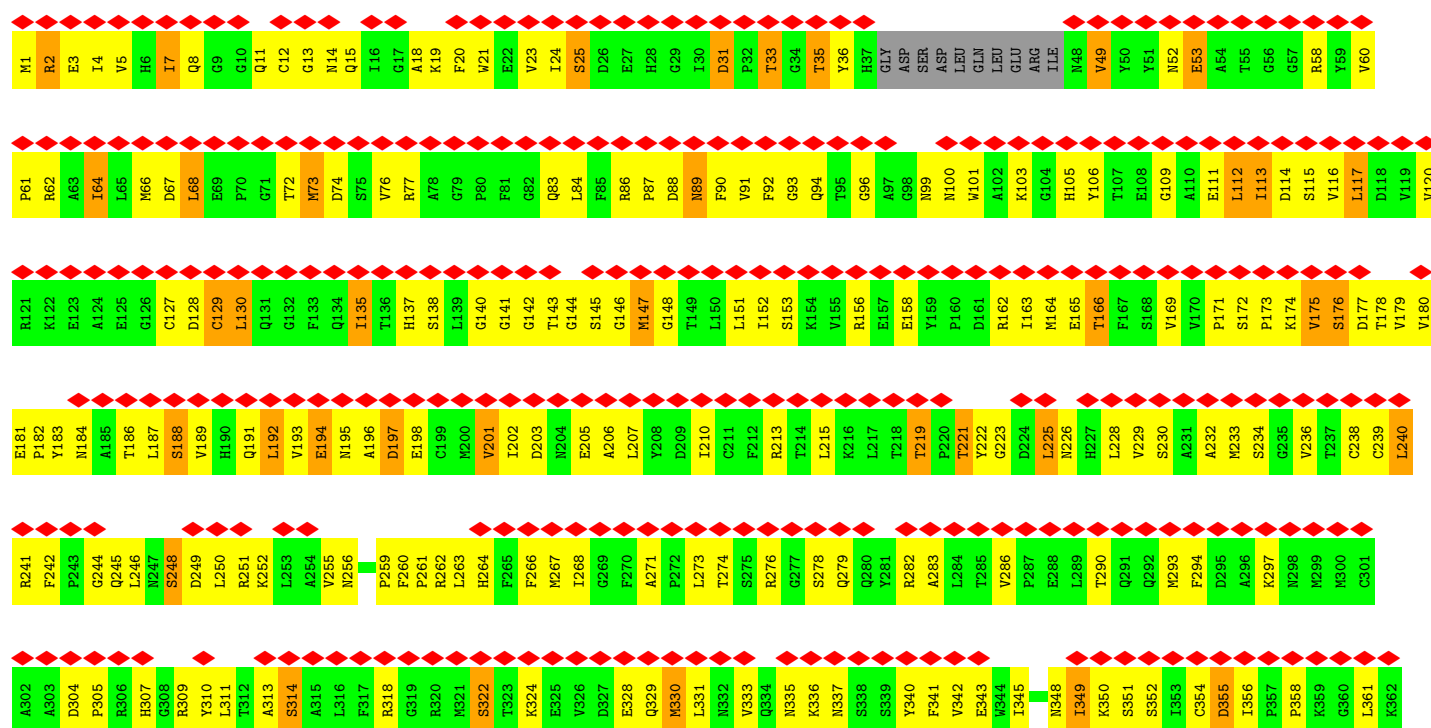
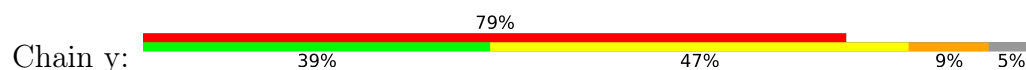


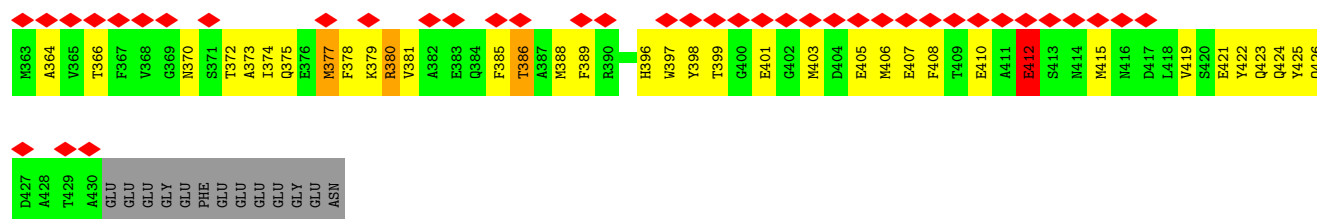
• Molecule 17: Tubulin beta chain



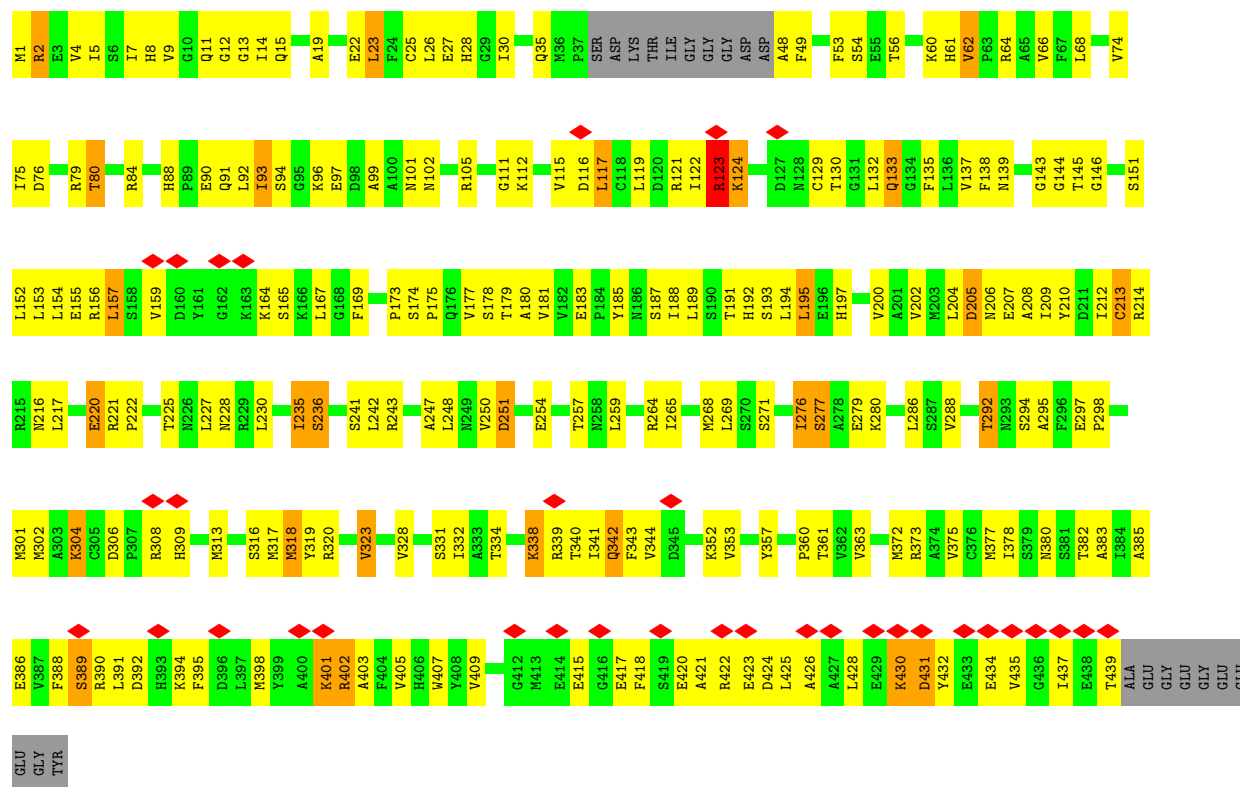


• Molecule 17: Tubulin beta chain

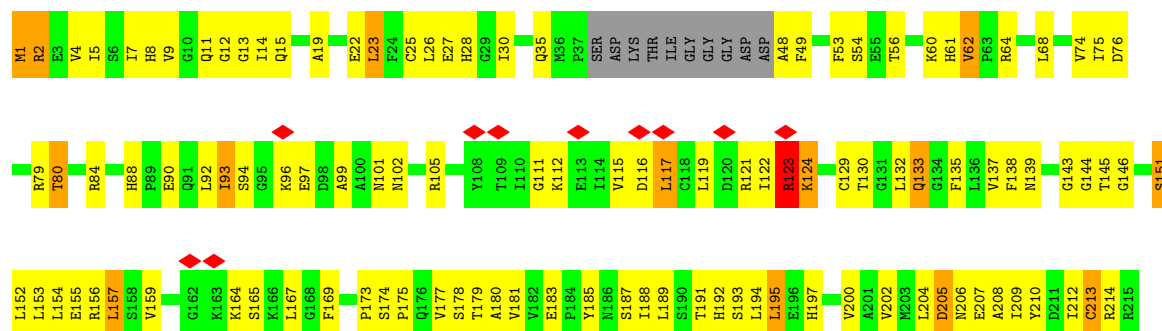


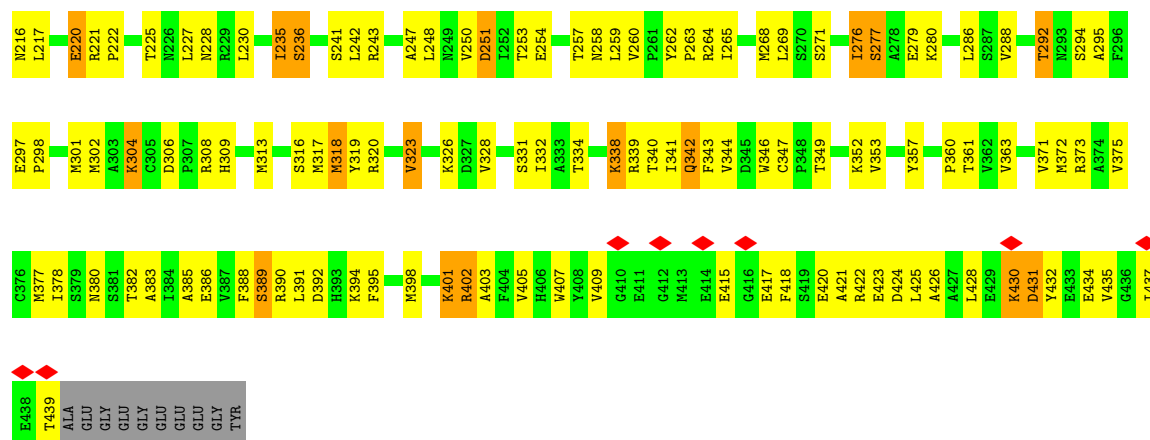


• Molecule 18: Tubulin alpha chain

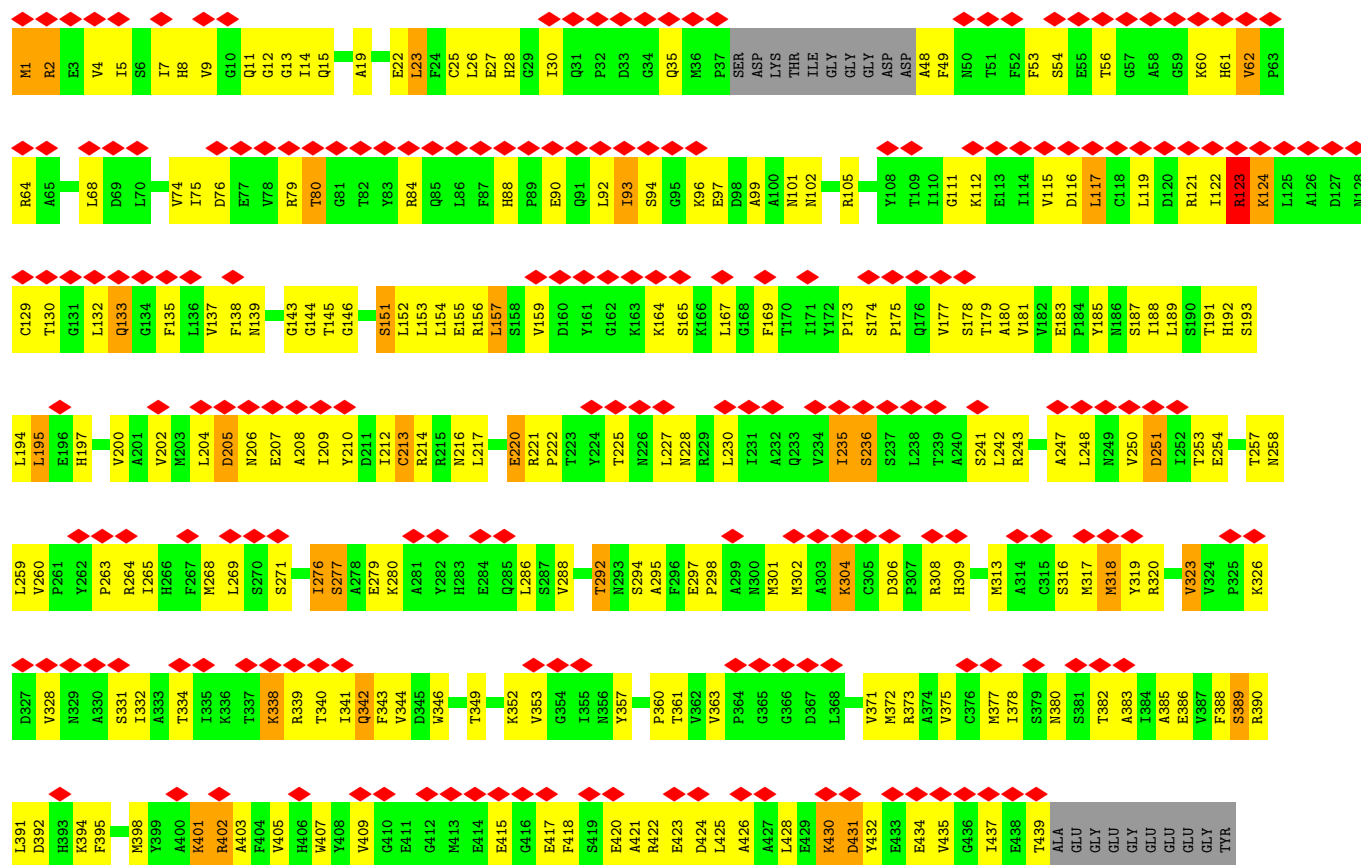


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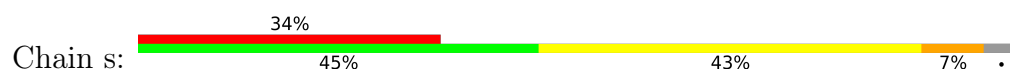


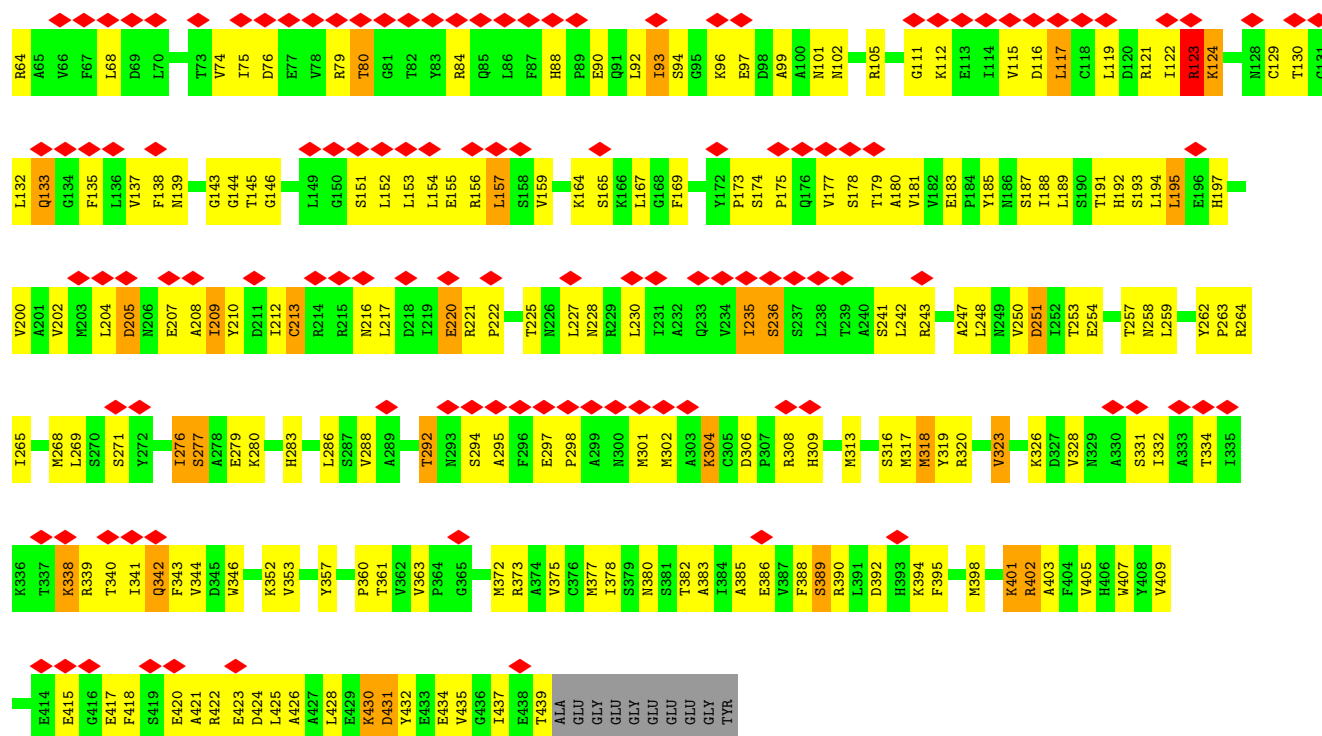


• Molecule 18: Tubulin alpha chain

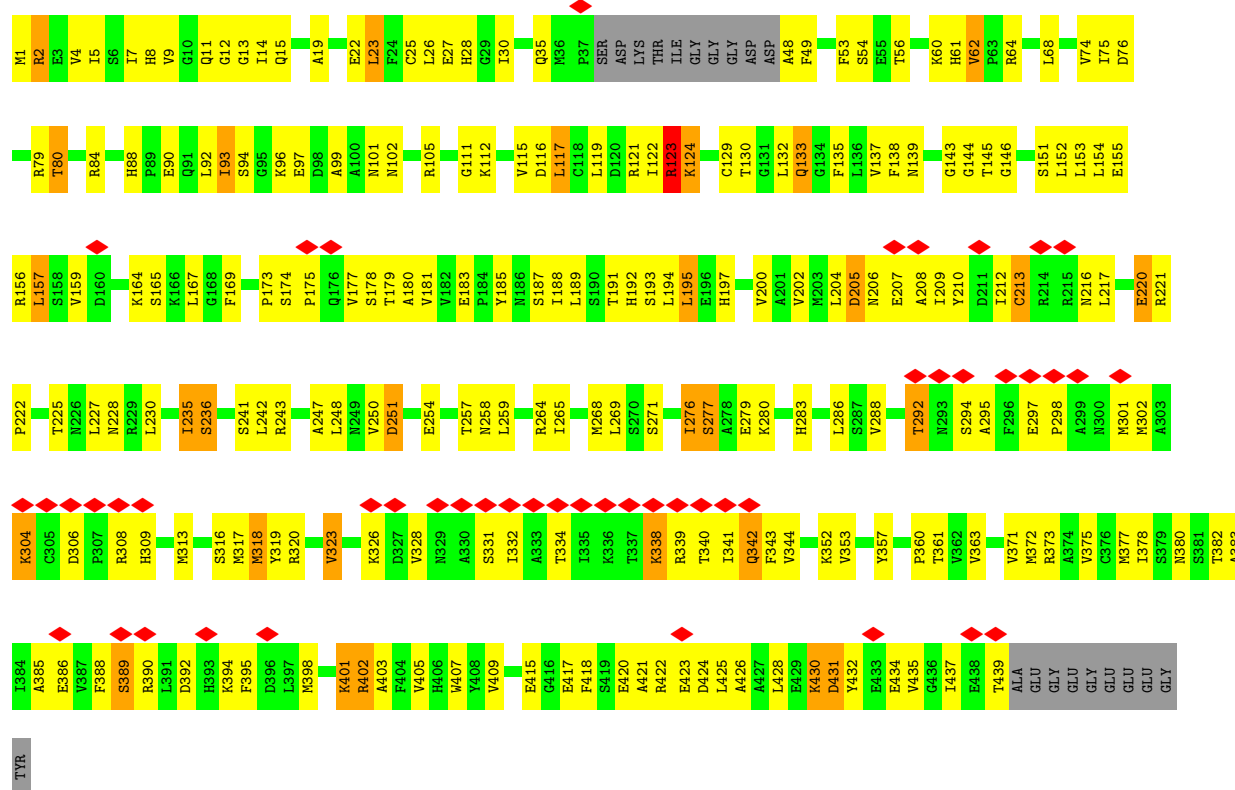


• Molecule 18: Tubulin alpha chain

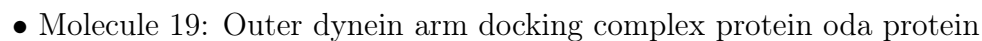




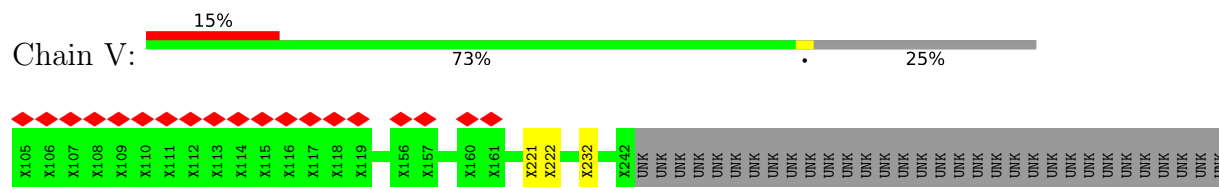
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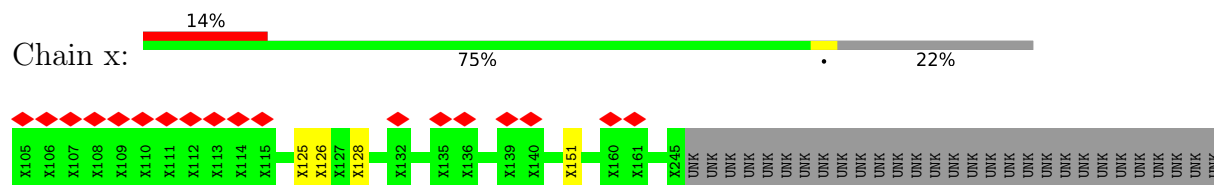
• Molecule 18: Tubulin alpha chain



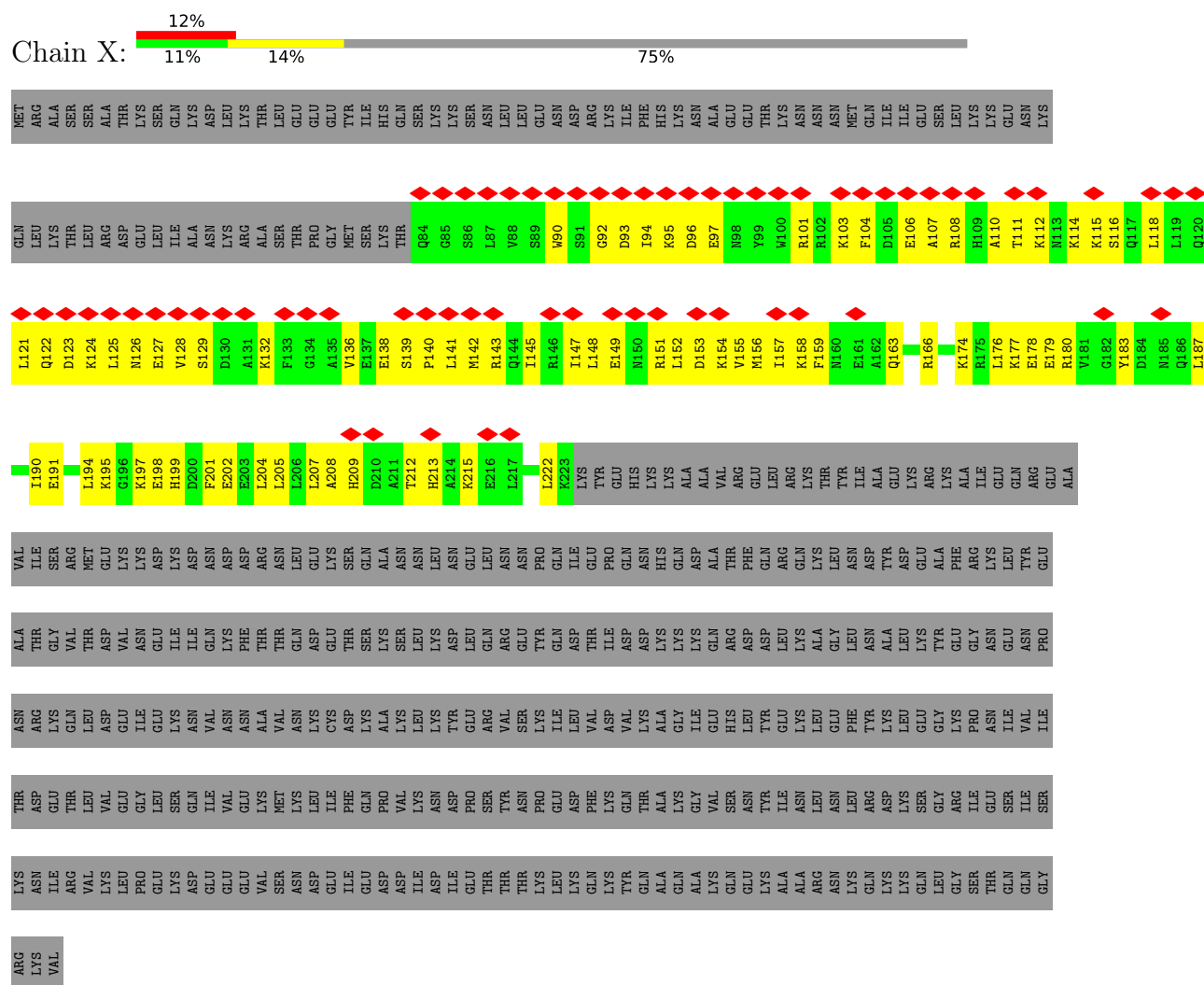
- Molecule 20: Docking complex 1/2 protein



- Molecule 20: Docking complex 1/2 protein



- Molecule 21: Docking complex 1 protein



- Molecule 22: Outer dynein arm docking complex protein oda protein



[illegible]

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 (Å)	313.95, 232.05, 461.37	wwPDB
Map dimensions	169, 85, 115	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.73, 2.73, 2.73	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.22	0/2778	0.59	1/3776 (0.0%)
2	B	0.25	1/33725 (0.0%)	0.54	17/45530 (0.0%)
3	C	0.21	1/34189 (0.0%)	0.49	16/46162 (0.0%)
4	D	0.23	0/2737	0.51	0/3707
4	d	0.24	0/973	0.51	0/1319
5	E	0.24	0/3334	0.52	3/4523 (0.1%)
5	e	0.22	0/687	0.72	2/940 (0.2%)
6	F	0.22	0/793	0.54	0/1070
7	G	0.19	0/751	0.45	0/1014
8	H	0.16	0/718	0.37	0/965
9	I	0.19	0/705	0.45	0/954
10	J	0.15	0/723	0.41	0/966
11	K	0.24	0/828	0.59	0/1114
12	L	0.18	0/790	0.44	0/1063
13	M	0.19	0/743	0.42	0/996
14	N	0.26	0/915	0.58	0/1229
15	O	0.18	0/891	0.47	0/1209
16	P	0.22	0/866	0.46	0/1171
17	Q	0.26	0/3359	0.64	1/4546 (0.0%)
17	U	0.26	0/3359	0.64	1/4546 (0.0%)
17	Y	0.26	0/3359	0.64	1/4546 (0.0%)
17	q	0.26	0/3359	0.64	1/4546 (0.0%)
17	u	0.26	0/3359	0.64	1/4546 (0.0%)
17	y	0.26	0/3359	0.64	1/4546 (0.0%)
18	R	0.25	0/3413	0.58	1/4625 (0.0%)
18	S	0.25	0/3413	0.58	1/4625 (0.0%)
18	W	0.25	0/3413	0.58	1/4625 (0.0%)
18	r	0.25	0/3413	0.58	1/4625 (0.0%)
18	s	0.25	0/3413	0.58	1/4625 (0.0%)
18	w	0.24	0/3413	0.58	1/4625 (0.0%)
19	T	0.19	0/1070	0.44	0/1436
21	X	0.20	0/1164	0.49	0/1556

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	Z	0.21	0/998	0.53	0/1323
All	All	0.24	2/131010 (0.0%)	0.55	51/177049 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	77	GLN	N-CA	10.07	1.65	1.46
3	C	2876	LEU	C-N	5.23	1.41	1.33

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	106	PRO	N-CA-CB	13.37	110.41	102.92
2	B	3951	PRO	N-CA-CB	10.73	110.00	102.81
2	B	4432	PRO	N-CA-CB	10.36	114.13	103.25
2	B	1330	TRP	CA-CB-CG	9.31	131.29	113.60
2	B	2455	SER	N-CA-C	-8.34	100.15	110.41

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	ARG	Peptide

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Mol	Chain	Res	Type	Group
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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2698	0	2574	196	0
2	B	33080	0	33110	2062	0
3	C	33529	0	33455	1646	0
4	D	2669	0	2619	189	0
4	d	957	0	836	72	0
5	E	3264	0	3004	253	0
5	e	684	0	481	40	0
6	F	781	0	791	48	0
7	G	744	0	771	43	0
8	H	702	0	686	57	0
9	I	694	0	684	47	0
10	J	702	0	671	27	0
11	K	803	0	766	83	0
12	L	773	0	806	50	0
13	M	726	0	726	35	0
14	N	897	0	911	75	0
15	O	878	0	868	55	0
16	P	847	0	836	48	0
17	Q	3287	0	3180	240	0
17	U	3287	0	3180	229	0
17	Y	3287	0	3180	212	0
17	q	3287	0	3180	224	0
17	u	3287	0	3180	223	0
17	y	3287	0	3180	214	0
18	R	3342	0	3289	176	0
18	S	3342	0	3289	208	0
18	W	3342	0	3289	198	0
18	r	3342	0	3289	179	0
18	s	3342	0	3289	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	w	3342	0	3289	191	0
19	T	1057	0	1032	35	0
20	V	490	0	102	4	0
20	x	505	0	105	7	0
21	X	1149	0	1162	241	0
22	Z	993	0	1031	228	0
23	C	54	0	19	31	0
24	C	31	0	9	3	0
25	Q	28	0	12	3	0
25	U	28	0	12	3	0
25	Y	28	0	12	3	0
25	q	28	0	12	3	0
25	u	28	0	12	3	0
25	y	28	0	12	3	0
26	R	32	0	12	5	0
26	S	32	0	12	5	0
26	W	32	0	12	5	0
26	r	32	0	12	5	0
26	s	32	0	12	5	0
26	w	32	0	12	5	0
27	R	1	0	0	0	0
27	S	1	0	0	0	0
27	W	1	0	0	0	0
27	r	1	0	0	0	0
27	s	1	0	0	0	0
27	w	1	0	0	0	0
All	All	129847	0	127013	7395	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 29.

The worst 5 of 7395 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)
21:X:197:LYS:CD	22:Z:192:MET:HB2	1.28	1.58
21:X:201:PHE:CZ	22:Z:195:ILE:HD12	1.38	1.58
21:X:204:LEU:CD1	22:Z:199:ALA:HB2	1.26	1.54
21:X:180:ARG:CZ	22:Z:171:ARG:CD	1.83	1.51
21:X:180:ARG:NH2	22:Z:171:ARG:HD2	1.20	1.49

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	36	72
2	B	4037/4594 (88%)	3637 (90%)	384 (10%)	16 (0%)	30	67
3	C	4127/4620 (89%)	3813 (92%)	305 (7%)	9 (0%)	43	78
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%)	12	49
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	7	38
21	X	138/555 (25%)	133 (96%)	5 (4%)	0	100	100
22	Z	113/538 (21%)	110 (97%)	1 (1%)	2 (2%)	6	34
All	All	15928/24065 (66%)	14686 (92%)	1211 (8%)	31 (0%)	44	78

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 ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/3691 (8%)	291 (100%)	0	100	100
2	B	3646/4145 (88%)	3629 (100%)	17 (0%)	81	83
3	C	3699/4196 (88%)	3689 (100%)	10 (0%)	86	86
4	D	297/609 (49%)	297 (100%)	0	100	100
4	d	89/609 (15%)	89 (100%)	0	100	100
5	E	322/597 (54%)	321 (100%)	1 (0%)	86	86
5	e	42/597 (7%)	42 (100%)	0	100	100
6	F	87/109 (80%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	86/149 (58%)	86 (100%)	0	100	100
8	H	76/83 (92%)	76 (100%)	0	100	100
9	I	76/95 (80%)	76 (100%)	0	100	100
10	J	74/82 (90%)	74 (100%)	0	100	100
11	K	81/97 (84%)	81 (100%)	0	100	100
12	L	86/99 (87%)	86 (100%)	0	100	100
13	M	77/78 (99%)	77 (100%)	0	100	100
14	N	96/119 (81%)	96 (100%)	0	100	100
15	O	98/104 (94%)	97 (99%)	1 (1%)	68	78
16	P	97/104 (93%)	97 (100%)	0	100	100
17	Q	356/376 (95%)	283 (80%)	73 (20%)	1	7
17	U	356/376 (95%)	283 (80%)	73 (20%)	1	7
17	Y	356/376 (95%)	283 (80%)	73 (20%)	1	7
17	q	356/376 (95%)	283 (80%)	73 (20%)	1	7
17	u	356/376 (95%)	283 (80%)	73 (20%)	1	7
17	y	356/376 (95%)	283 (80%)	73 (20%)	1	7
18	R	363/376 (96%)	308 (85%)	55 (15%)	3	12
18	S	363/376 (96%)	308 (85%)	55 (15%)	3	12
18	W	363/376 (96%)	308 (85%)	55 (15%)	3	12
18	r	363/376 (96%)	308 (85%)	55 (15%)	3	12
18	s	363/376 (96%)	308 (85%)	55 (15%)	3	12
18	w	363/376 (96%)	308 (85%)	55 (15%)	3	12
19	T	118/271 (44%)	118 (100%)	0	100	100
21	X	122/502 (24%)	122 (100%)	0	100	100
22	Z	108/491 (22%)	108 (100%)	0	100	100
All	All	13982/21339 (66%)	13185 (94%)	797 (6%)	20	40

5 of 797 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	s	402	ARG
18	r	235	ILE
17	u	33	THR

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Mol	Chain	Res	Type
18	s	389	SER
17	u	273	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 375 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	36	GLN
18	W	216	ASN
15	O	48	GLN
18	S	8	HIS
17	Y	191	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
26	GTP	W	501	27	33,34,34	0.96	1 (3%)	50,54,54	1.54	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	GTP	r	501	27	33,34,34	0.97	1 (3%)	50,54,54	1.54	8 (16%)
26	GTP	S	501	27	33,34,34	0.96	1 (3%)	50,54,54	1.54	8 (16%)
24	ATP	C	4702	-	32,33,33	1.40	4 (12%)	48,52,52	1.78	9 (18%)
25	GDP	u	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
26	GTP	s	501	27	33,34,34	0.96	1 (3%)	50,54,54	1.55	8 (16%)
26	GTP	w	501	27	33,34,34	0.96	2 (6%)	50,54,54	1.54	8 (16%)
25	GDP	Q	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
23	ADP	C	4701	-	28,29,29	1.49	6 (21%)	43,45,45	3.20	16 (37%)
25	GDP	U	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
25	GDP	Y	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
25	GDP	y	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
23	ADP	C	4703	-	28,29,29	2.09	9 (32%)	43,45,45	3.78	22 (51%)
25	GDP	q	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
26	GTP	R	501	27	33,34,34	0.96	1 (3%)	50,54,54	1.54	8 (16%)

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
26	GTP	W	501	27	-	3/22/38/38	0/3/3/3
26	GTP	r	501	27	-	3/22/38/38	0/3/3/3
26	GTP	S	501	27	-	3/22/38/38	0/3/3/3
24	ATP	C	4702	-	-	0/22/38/38	0/3/3/3
25	GDP	u	501	-	-	2/16/32/32	0/3/3/3
26	GTP	s	501	27	-	3/22/38/38	0/3/3/3
26	GTP	w	501	27	-	3/22/38/38	0/3/3/3
25	GDP	Q	501	-	-	2/16/32/32	0/3/3/3
23	ADP	C	4701	-	-	5/16/32/32	0/3/3/3
25	GDP	U	501	-	-	2/16/32/32	0/3/3/3
25	GDP	Y	501	-	-	2/16/32/32	0/3/3/3
25	GDP	y	501	-	-	2/16/32/32	0/3/3/3
23	ADP	C	4703	-	-	5/16/32/32	0/3/3/3
25	GDP	q	501	-	-	2/16/32/32	0/3/3/3
26	GTP	R	501	27	-	3/22/38/38	0/3/3/3

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	4703	ADP	C5-C4	6.69	1.51	1.39
23	C	4701	ADP	C5-C4	5.07	1.48	1.39
24	C	4702	ATP	C5-C4	4.66	1.47	1.39
23	C	4703	ADP	O4'-C4'	3.86	1.53	1.45
23	C	4703	ADP	C8-N7	3.19	1.37	1.31

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	4703	ADP	O4'-C1'-C2'	-9.55	86.18	106.62
23	C	4701	ADP	O3A-PA-O1A	-9.11	83.30	110.70
23	C	4703	ADP	O4'-C1'-N9	9.00	125.37	108.09
23	C	4701	ADP	O5'-PA-O1A	-8.44	75.47	108.94
23	C	4703	ADP	C2'-C3'-C4'	-8.43	86.32	102.61

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'
23	C	4703	ADP	O4'-C4'-C5'-O5'
23	C	4703	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

15 monomers are involved in 82 short contacts:

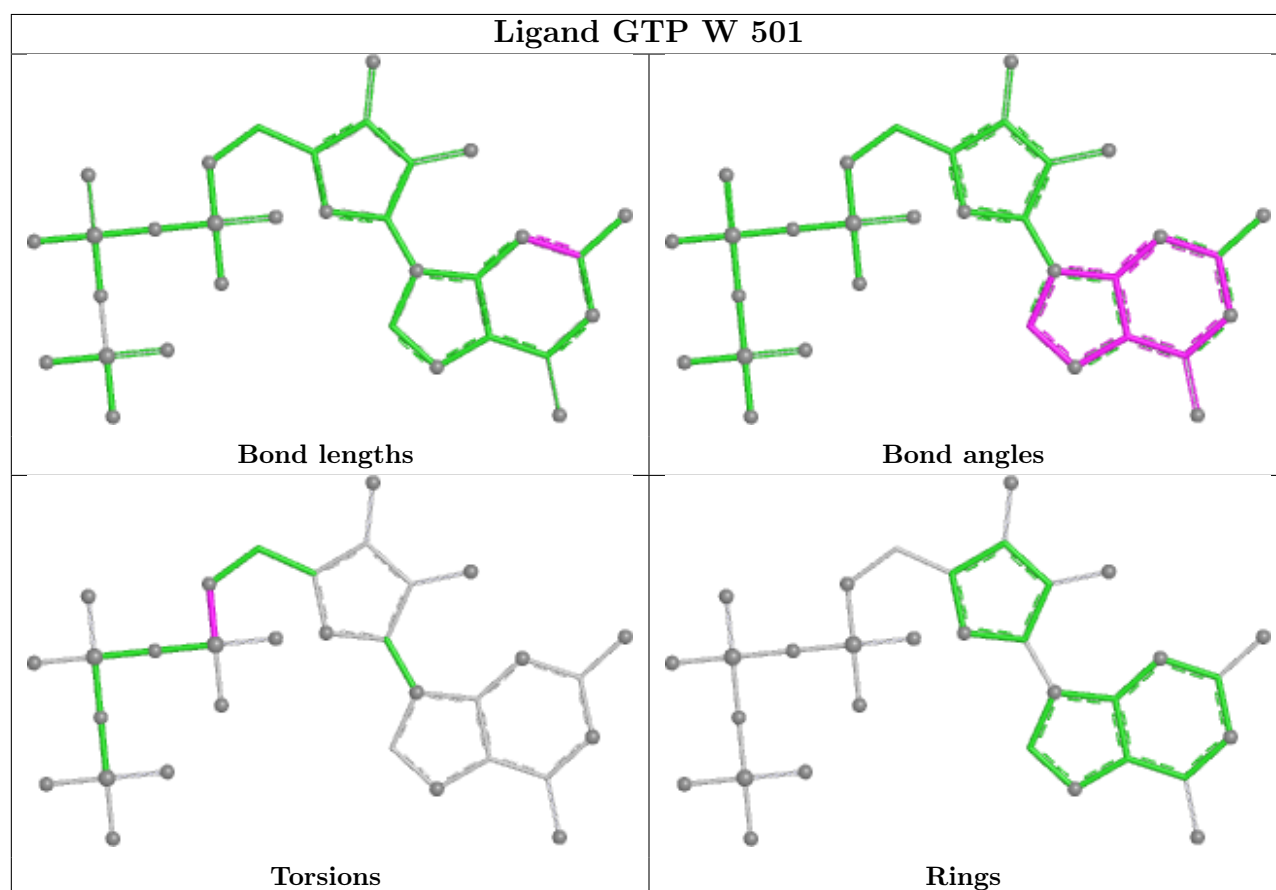
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	W	501	GTP	5	0
26	r	501	GTP	5	0
26	S	501	GTP	5	0
24	C	4702	ATP	3	0
25	u	501	GDP	3	0
26	s	501	GTP	5	0
26	w	501	GTP	5	0
25	Q	501	GDP	3	0
23	C	4701	ADP	7	0
25	U	501	GDP	3	0
25	Y	501	GDP	3	0

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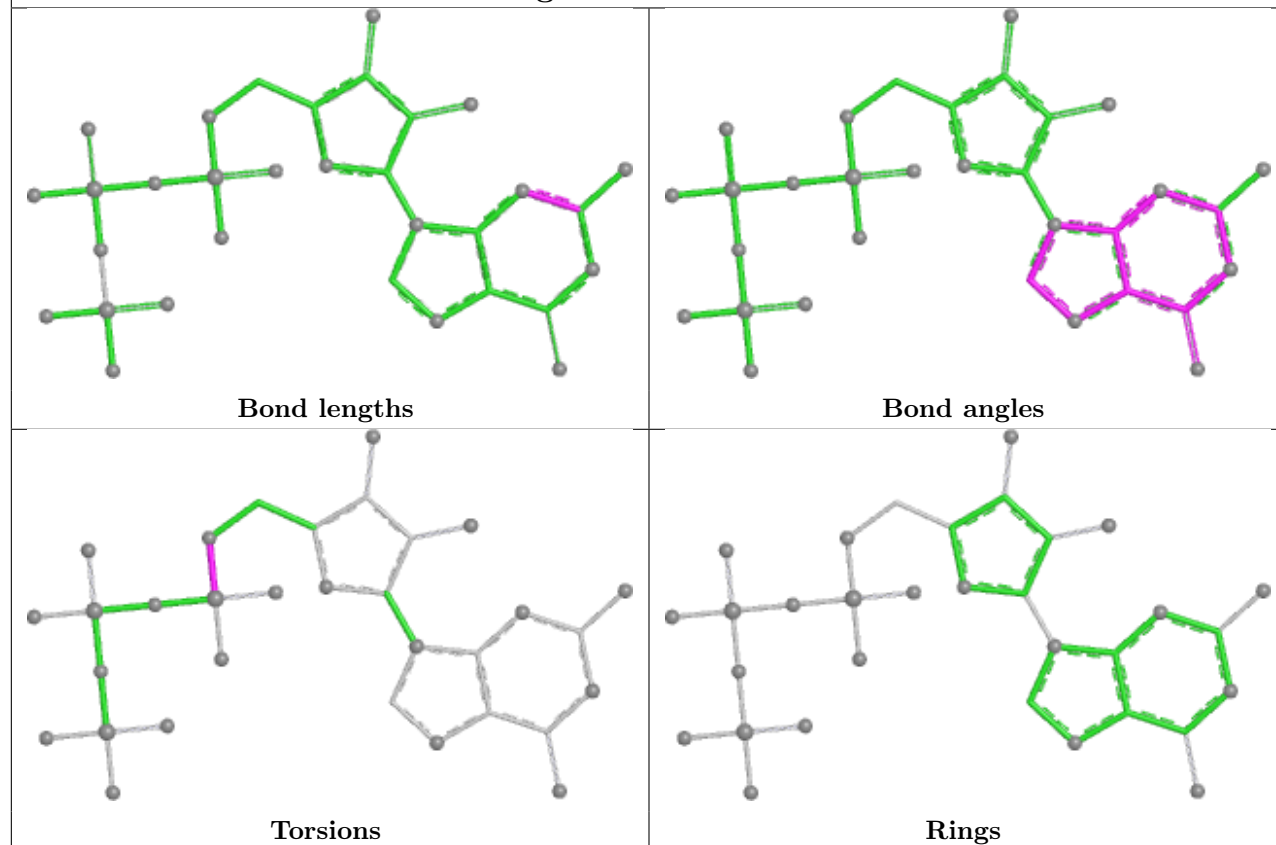
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	y	501	GDP	3	0
23	C	4703	ADP	24	0
25	q	501	GDP	3	0
26	R	501	GTP	5	0

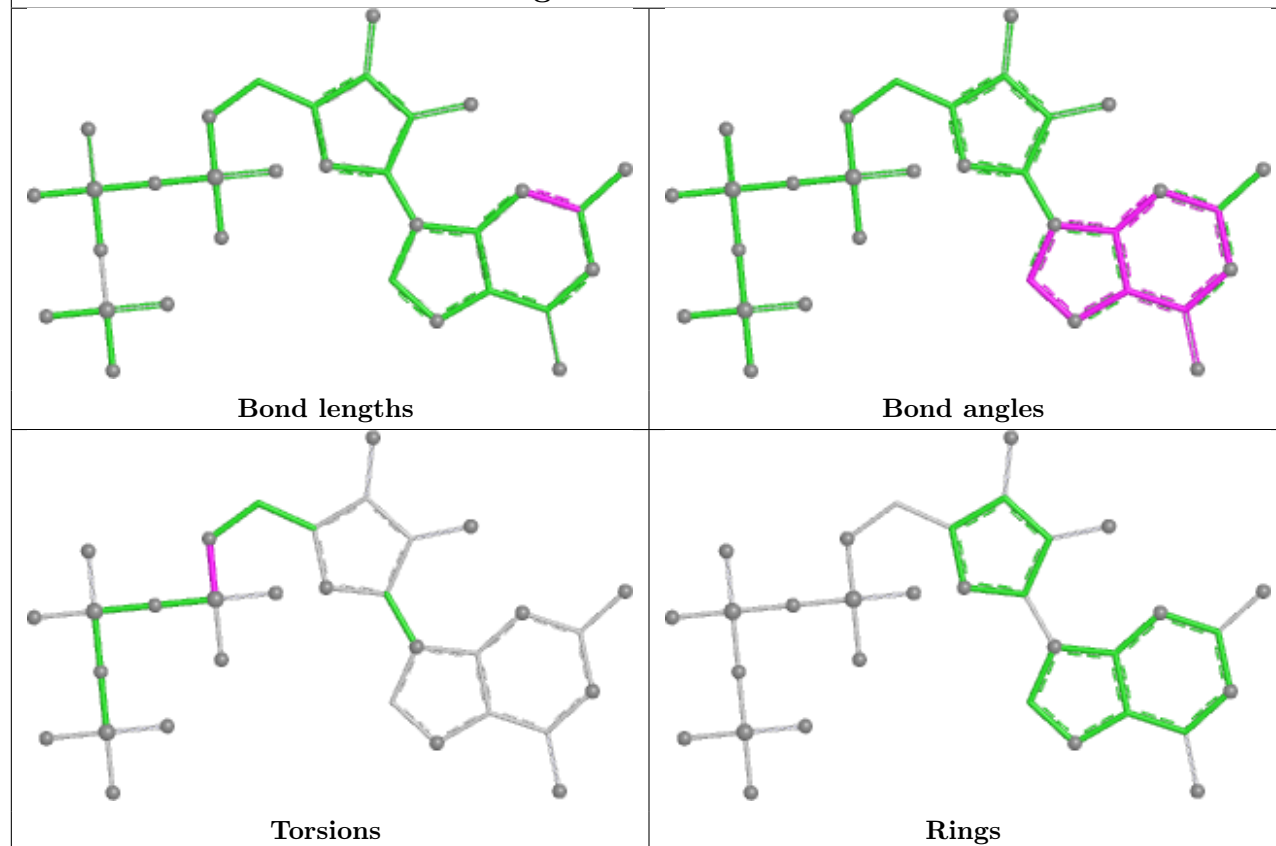
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

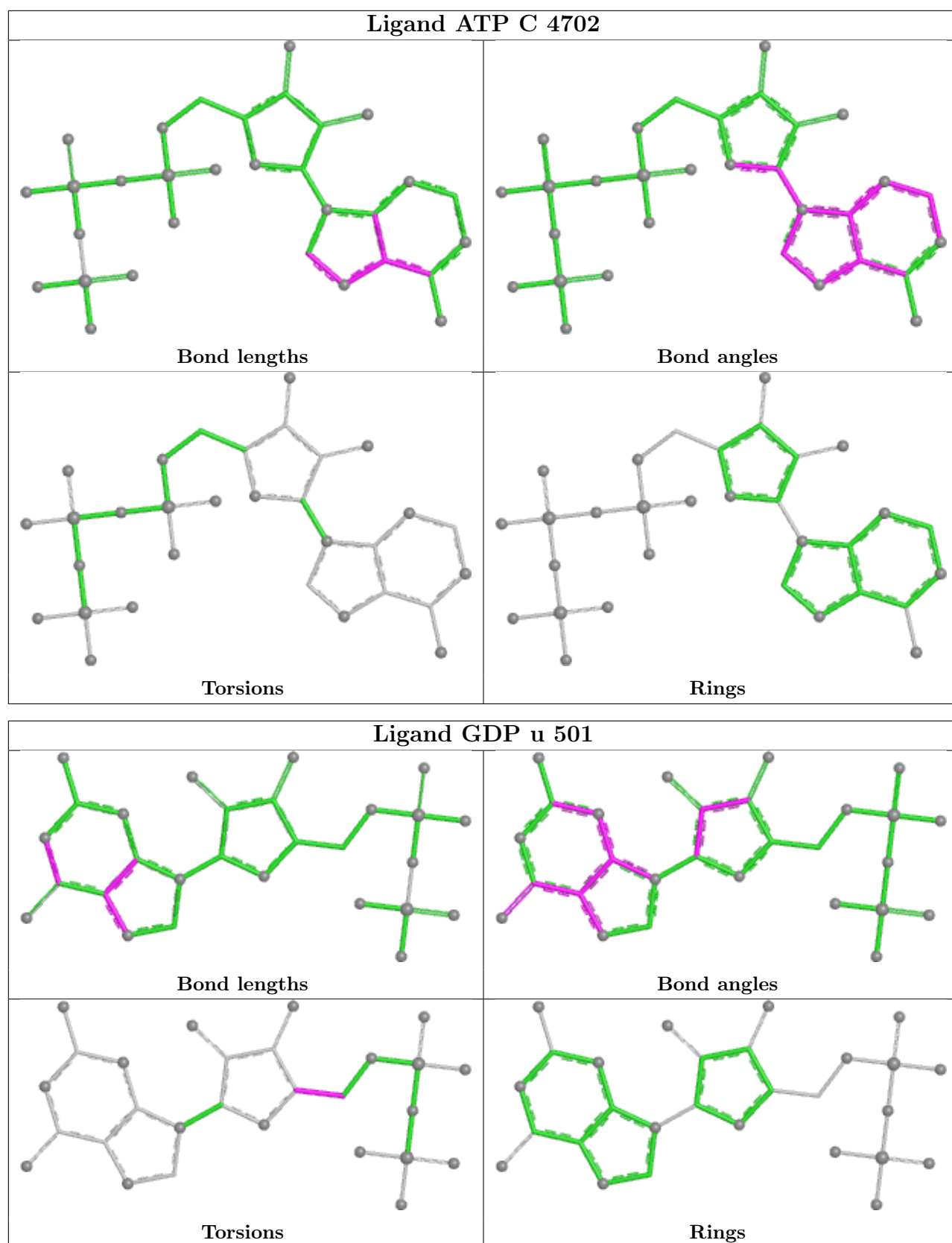


Ligand GTP r 501

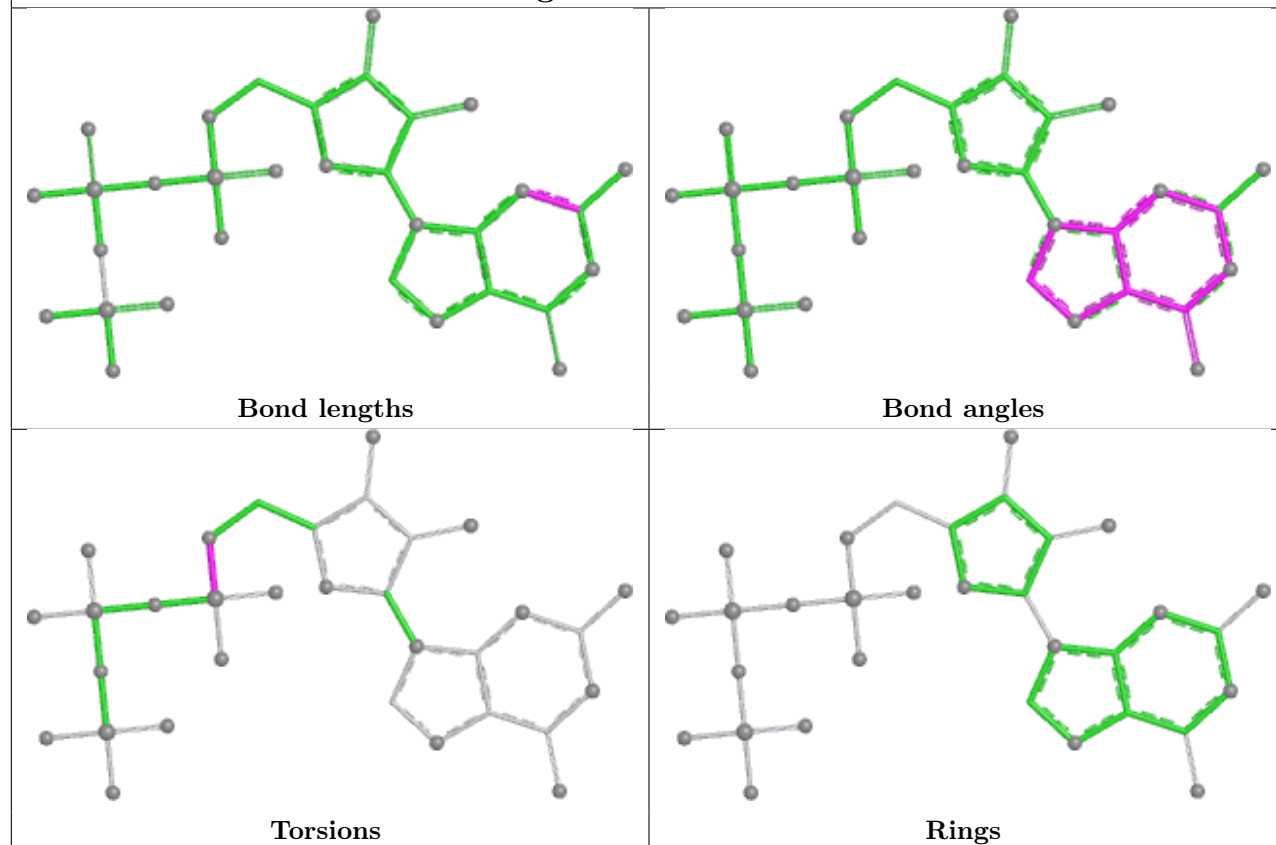


Ligand GTP S 501

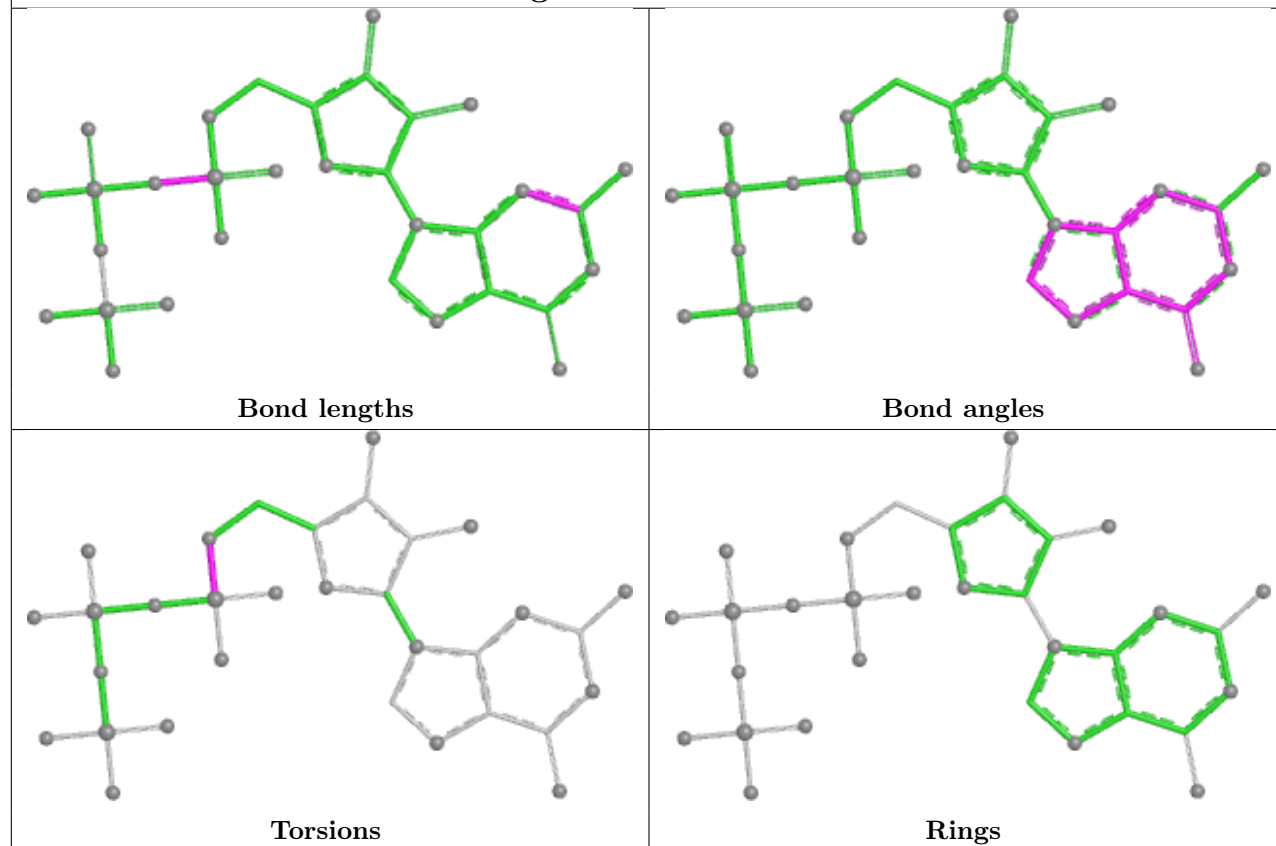


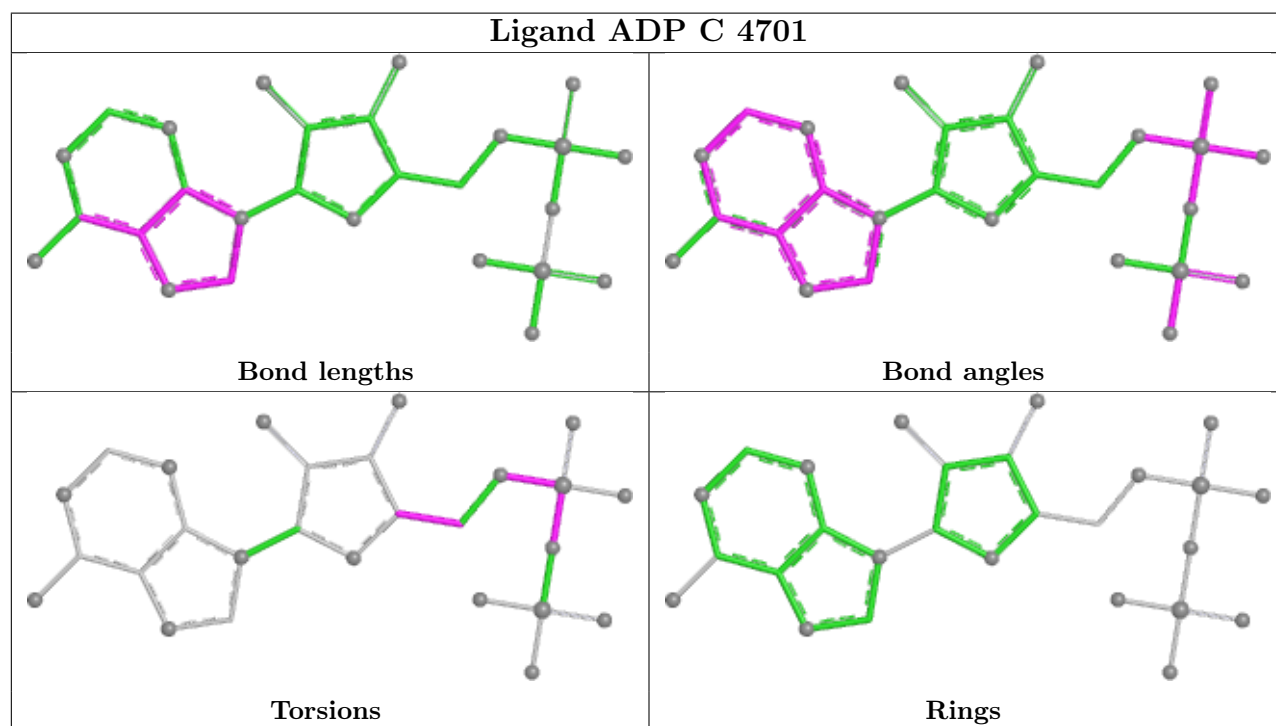
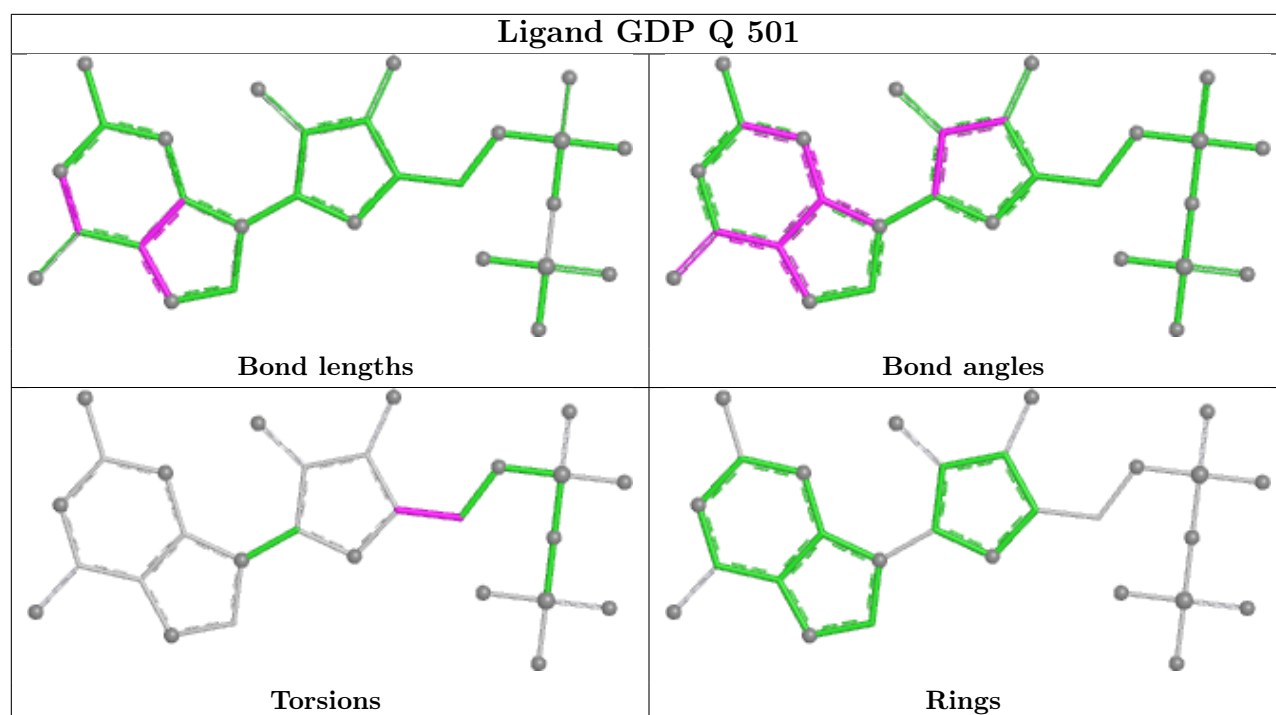


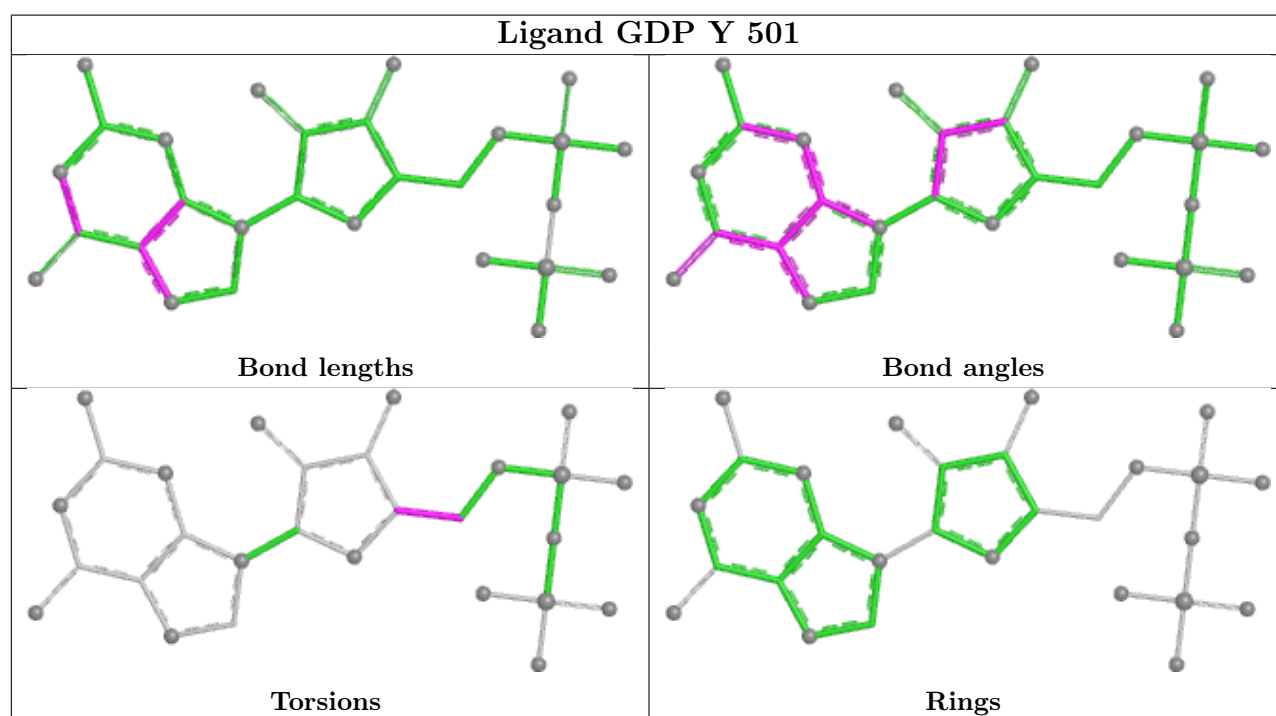
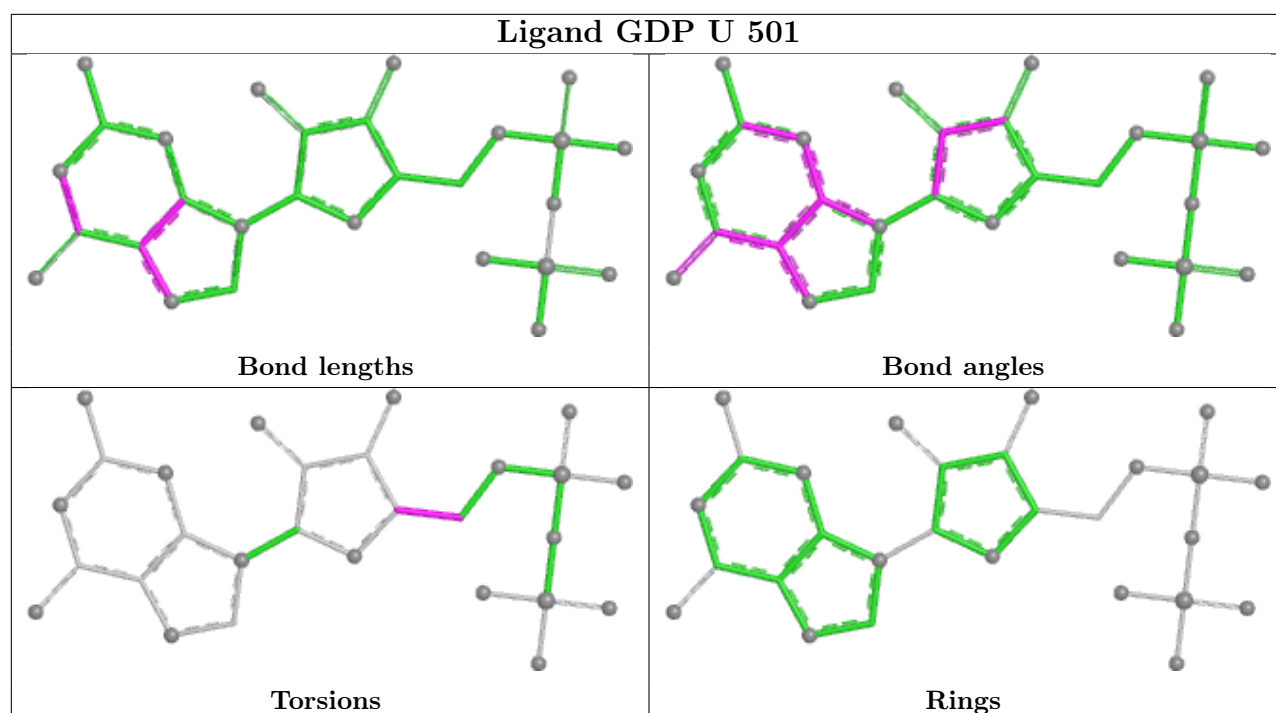
Ligand GTP s 501

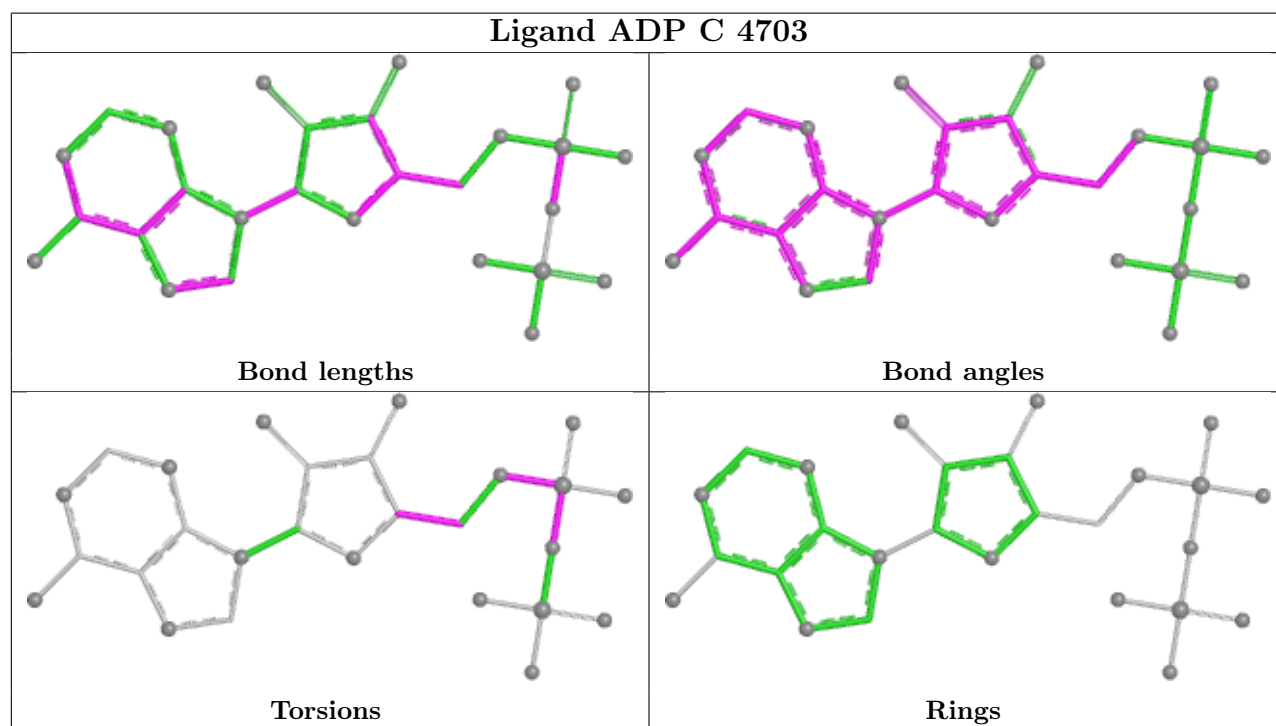
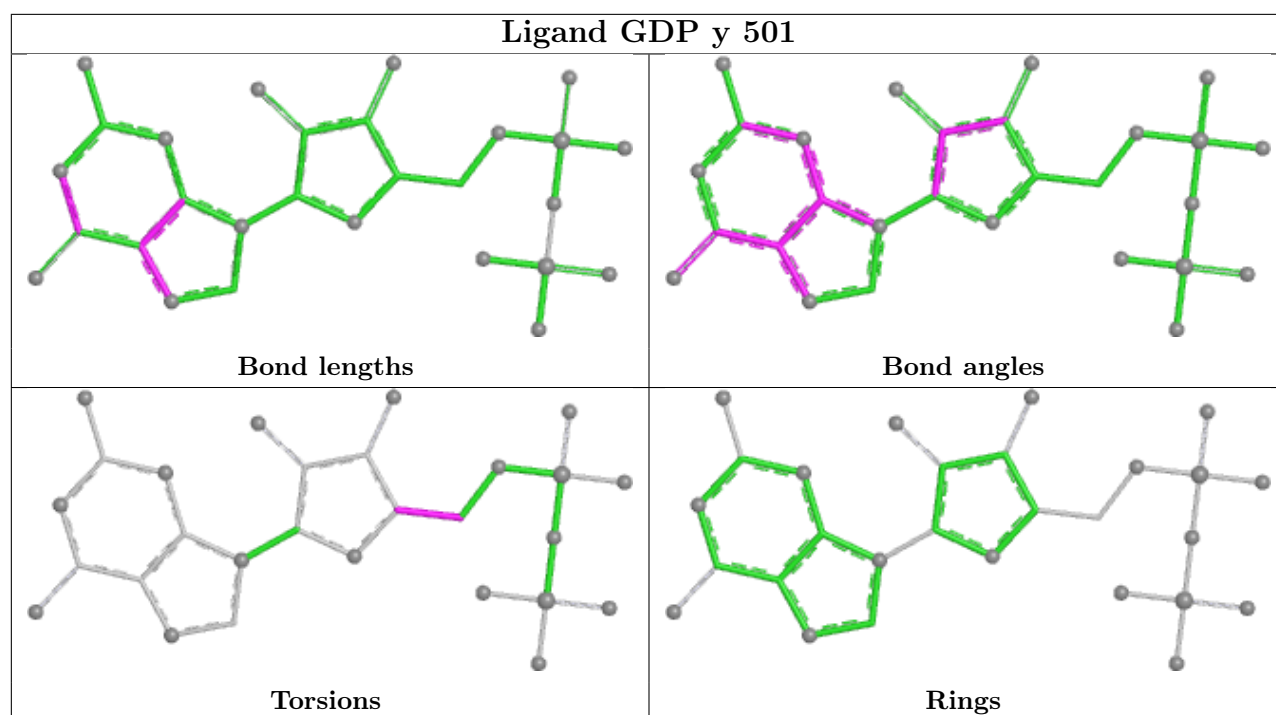


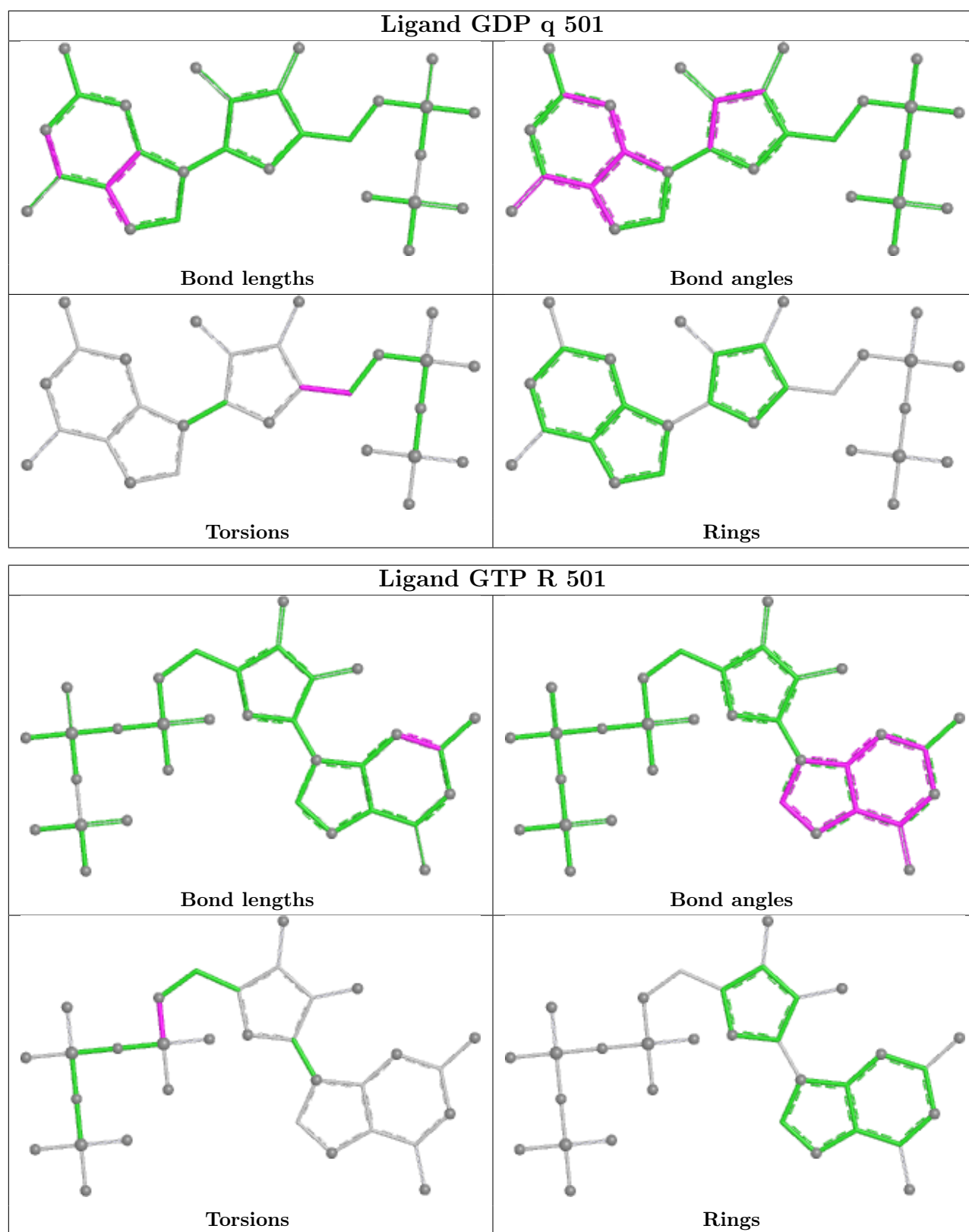
Ligand GTP w 501











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

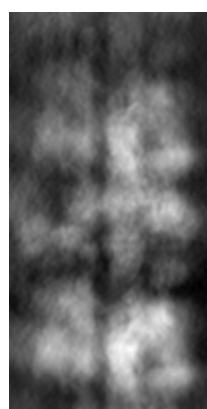
6 Map visualisation [i](#)

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.

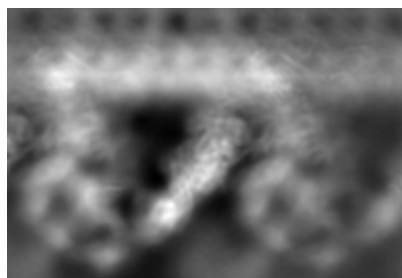
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

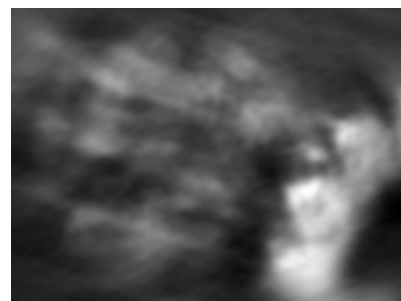
6.1.1 Primary map



X



Y

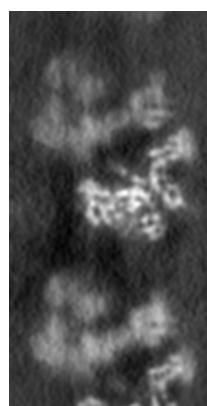


Z

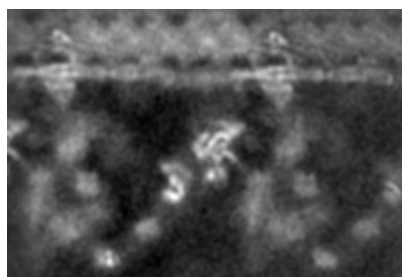
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

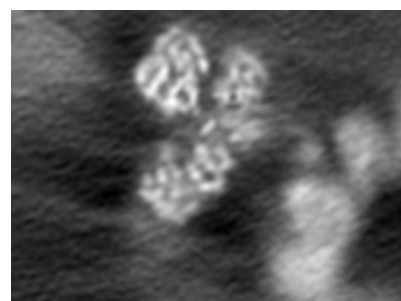
6.2.1 Primary map



X Index: 57



Y Index: 42



Z Index: 84

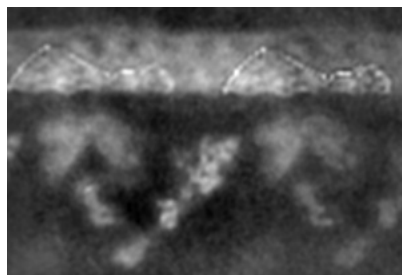
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

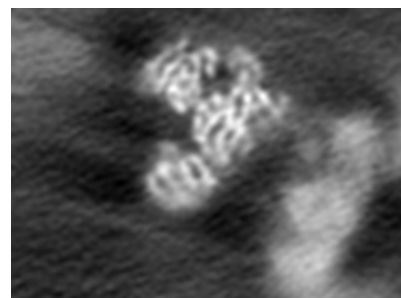
6.3.1 Primary map



X Index: 86



Y Index: 32

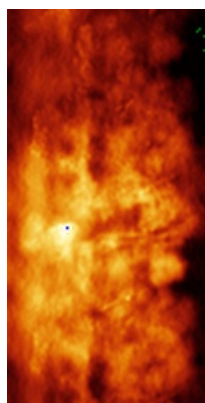


Z Index: 88

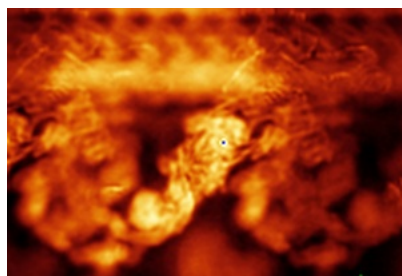
The images above show the largest variance slices of the map in three orthogonal directions.

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

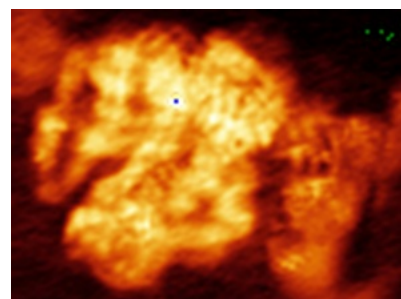
6.4.1 Primary map



X



Y

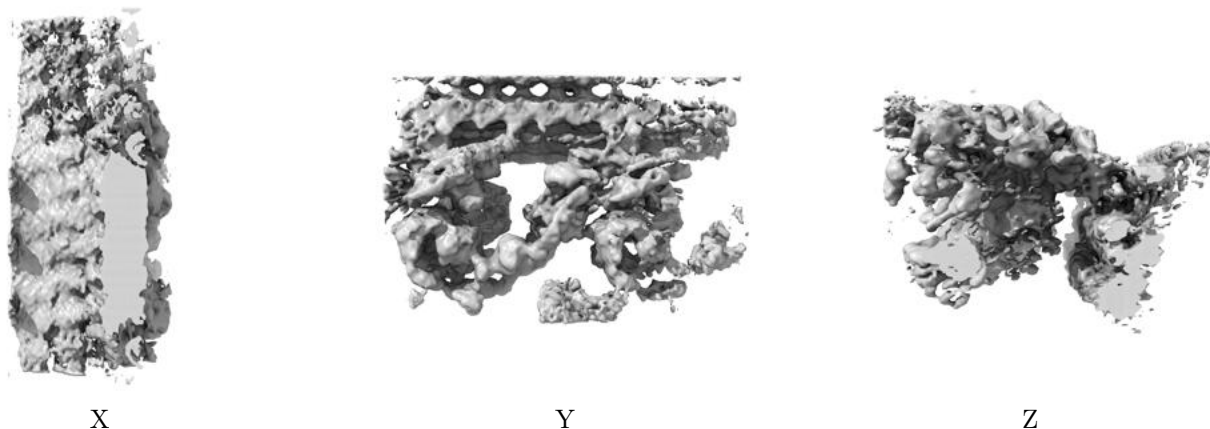


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

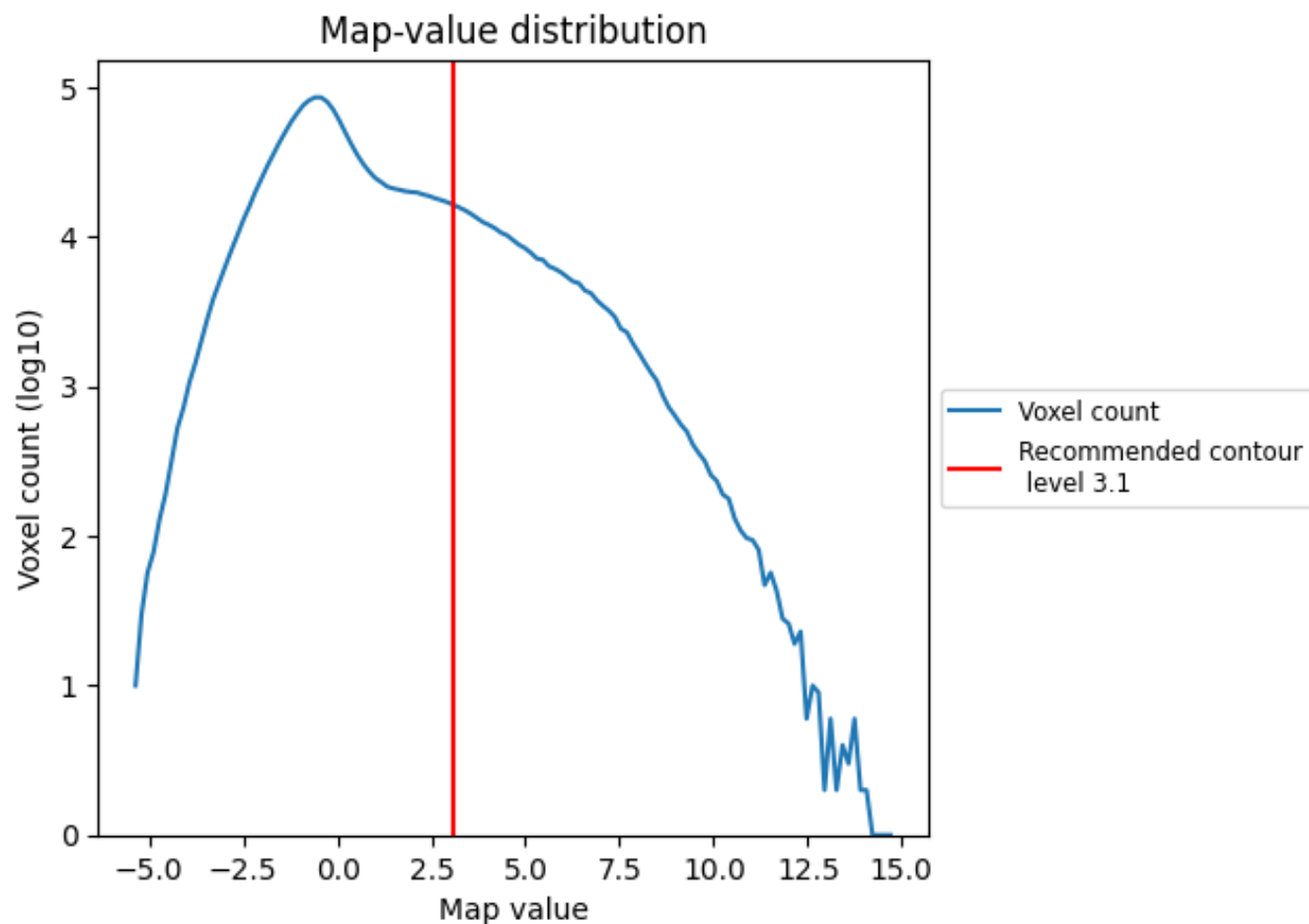
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

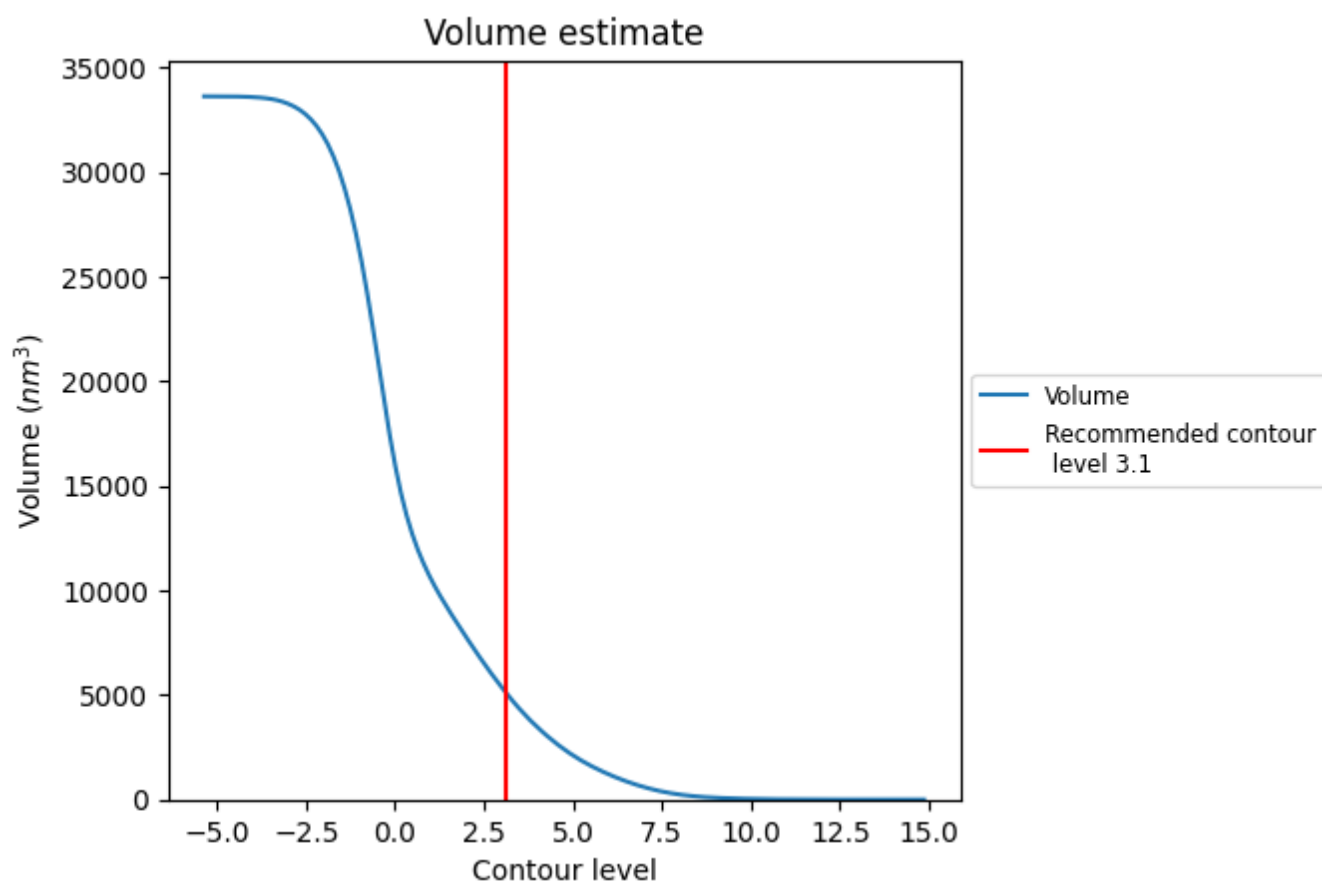
This section contains the results of statistical analysis of the map.

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.

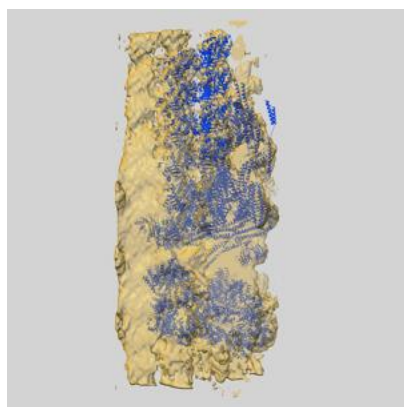
8 Fourier-Shell correlation

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

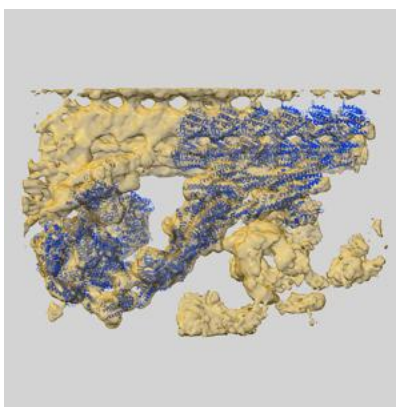
9 Map-model fit [i](#)

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](#).

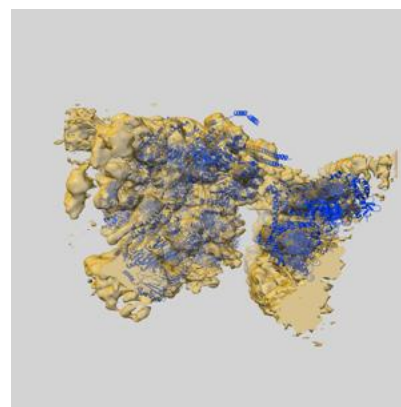
9.1 Map-model overlay [i](#)



X



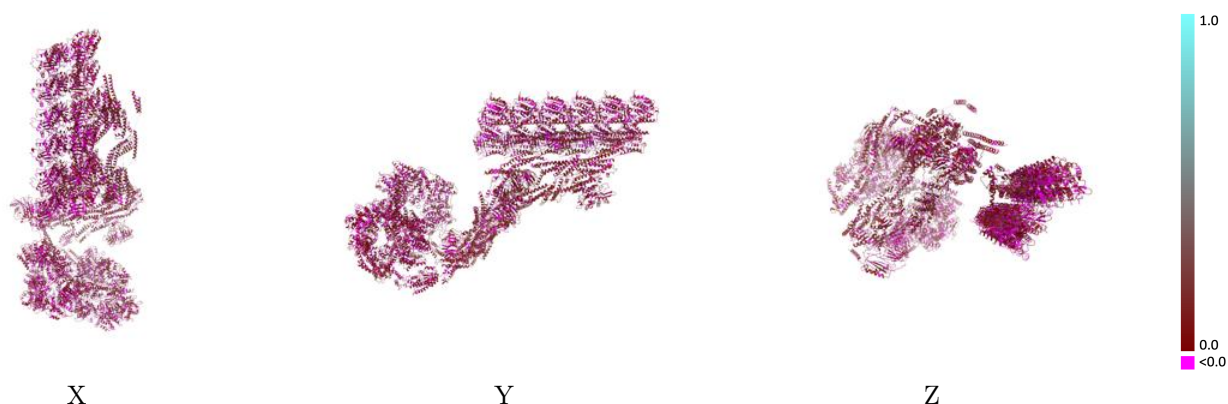
Y



Z

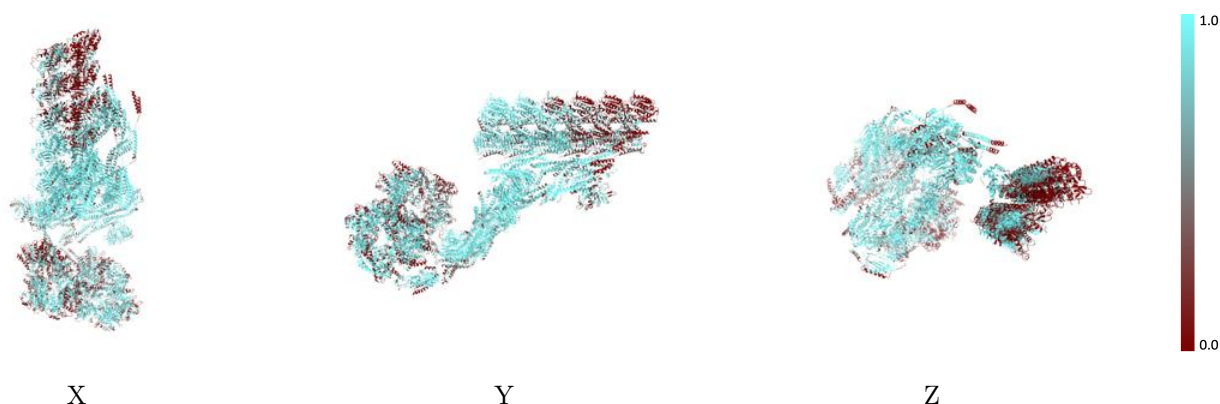
The images above show the 3D surface view of the map at the recommended contour level 3.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



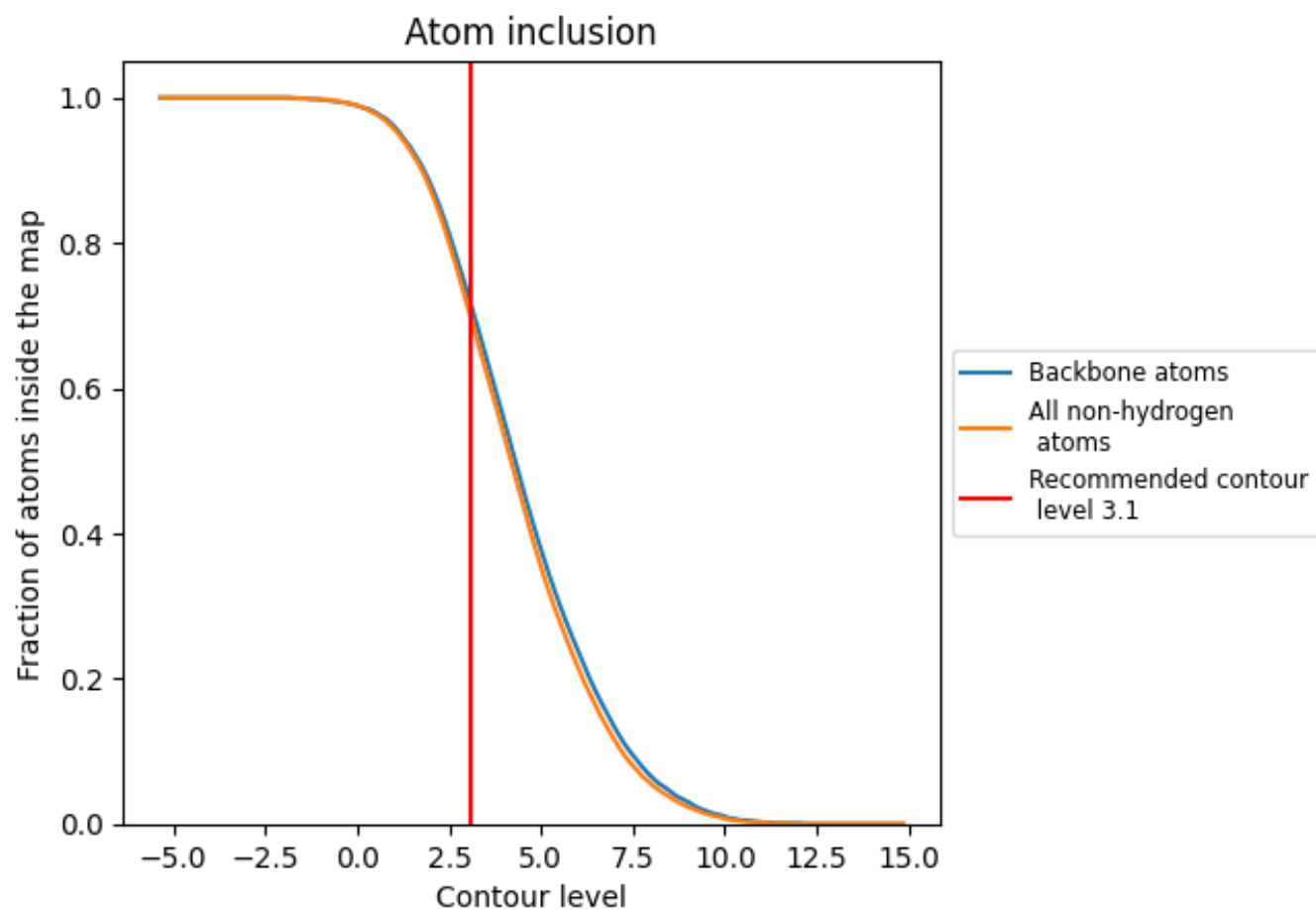
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.6960	 0.0670
A	 0.9340	 0.0870
B	 0.7120	 0.0750
C	 0.6660	 0.0700
D	 0.9630	 0.1060
E	 0.8600	 0.0950
F	 0.9780	 0.1290
G	 0.9440	 0.1420
H	 0.9360	 0.1260
I	 0.9010	 0.1210
J	 0.8900	 0.0960
K	 0.8680	 0.0410
L	 0.7710	 0.0560
M	 0.9290	 0.0870
N	 0.8140	 0.0540
O	 0.6940	 0.0750
P	 0.8550	 0.0730
Q	 0.9430	 0.0300
R	 0.9130	 0.0270
S	 0.9420	 0.0250
T	 0.8720	 0.0870
U	 0.6190	 0.0270
V	 0.8160	 0.1200
W	 0.4650	 0.0350
X	 0.4590	 0.1170
Y	 0.4900	 0.0460
Z	 0.4940	 0.1210
d	 0.8630	 0.0940
e	 0.8420	 0.1200
q	 0.8910	 0.0480
r	 0.8680	 0.0360
s	 0.6110	 0.0400
u	 0.3230	 0.0620
w	 0.2130	 0.0700
x	 0.8180	 0.1580
y	 0.1660	 0.0460

