



wwPDB EM Validation Summary Report ⓘ

Oct 19, 2024 – 04:48 PM EDT

PDB ID : 6B8H
EMDB ID : EMD-7067
Title : Mosaic model of yeast mitochondrial ATP synthase monomer
Authors : Guo, H.; Bueler, S.A.; Rubinstein, J.L.
Deposited on : 2017-10-07
Resolution : 3.60 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:

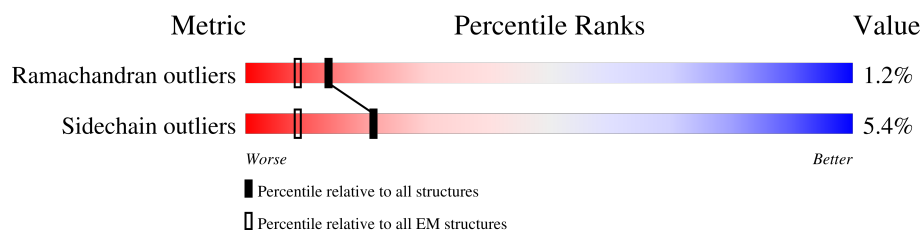
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	0	76	<div> <div>36%</div> <div>99%</div> </div>
1	1	76	<div> <div>33%</div> <div>99%</div> </div>
1	2	76	<div> <div>30%</div> <div>97%</div> </div>
1	3	76	<div> <div>20%</div> <div>96%</div> </div>
1	4	76	<div> <div>28%</div> <div>99%</div> </div>
1	5	76	<div> <div>29%</div> <div>97%</div> </div>
1	6	76	<div> <div>37%</div> <div>97%</div> </div>
1	7	76	<div> <div>66%</div> <div>96%</div> </div>
1	8	76	<div> <div>51%</div> <div>99%</div> </div>

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Mol	Chain	Length	Quality of chain
1	9	76	47%
1	J	76	97%
1	L	76	99%
1	M	76	99%
1	N	76	97%
1	P	76	96%
1	Q	76	99%
1	R	76	97%
1	S	76	96%
1	T	76	99%
1	U	76	97%
2	A	48	100%
2	V	48	96%
3	a	249	60%
3	p	249	100%
4	b	209	96%
4	q	209	93%
5	d	173	87%
5	r	173	88%
6	e	49	100%
6	s	49	100%
7	f	95	88%
7	t	95	85%
8	g	106	100%
8	u	106	99%

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Mol	Chain	Length	Quality of chain
9	i	59	100%
9	w	59	100%
10	k	68	16% 35% 65%
10	x	68	35% 65%
11	B	510	96% 89% 7%
11	C	510	98% 92% 6%
11	K	510	98% 94% 5%
11	W	510	96% 89% 7%
11	X	510	98% 92% 6%
11	n	510	98% 94% 5%
12	D	478	98% 94%
12	E	478	98% 92% 6%
12	F	478	98% 92% 5%
12	Y	478	98% 94%
12	Z	478	98% 92% 6%
12	c	478	98% 92% 5%
13	G	278	54% 83% 12% 5%
13	j	278	95% 83% 12% 5%
14	H	138	17% 72% 14% 14%
14	l	138	86% 72% 14% 14%
15	I	61	28% 62% 13% 21%
15	m	61	79% 62% 13% 21%
16	O	195	83% 78% 17%
16	o	195	83% 78% 17%
17	h	21	100%

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Mol	Chain	Length	Quality of chain
17	v	21	<div><div></div><div>100%</div></div> <div><div></div><div>100%</div></div>

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 75614 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 ATP synthase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	2	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	3	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	4	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	5	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	6	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	7	73	Total	C	N	O	S	0	0
			522	348	81	89	4		
1	8	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	9	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	0	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	L	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	M	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	N	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	P	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	Q	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	R	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	S	73	Total	C	N	O	S	0	0
			522	348	81	89	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	U	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	J	75	Total	C	N	O	S	0	0
			537	359	83	91	4		

- Molecule 2 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	48	Total	C	N	O	S	0	0
			410	287	59	60	4		
2	V	48	Total	C	N	O	S	0	0
			410	287	59	60	4		

- Molecule 3 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	249	Total	C	N	O	S	0	0
			1971	1338	296	326	11		
3	p	249	Total	C	N	O	S	0	0
			1971	1338	296	326	11		

- Molecule 4 is a protein called ATP synthase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	200	Total	C	N	O	S	0	0
			1153	715	210	227	1		
4	q	200	Total	C	N	O	S	0	0
			1153	715	210	227	1		

- Molecule 5 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	157	Total	C	N	O	S	0	0
			930	573	173	182	2		
5	r	157	Total	C	N	O	S	0	0
			930	573	173	182	2		

- Molecule 6 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	49	Total	C	N	O	0	0
			245	147	49	49		
6	s	49	Total	C	N	O	0	0
			245	147	49	49		

- Molecule 7 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	84	Total	C	N	O	S	0	0
			607	396	108	102	1		
7	t	84	Total	C	N	O	S	0	0
			607	396	108	102	1		

- Molecule 8 is a protein called AATP synthase subunit g.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	g	106	Total	C	N	O	0	0
			530	318	106	106		
8	u	106	Total	C	N	O	0	0
			530	318	106	106		

- Molecule 9 is a protein called ATP synthase subunit J, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	59	Total	C	N	O	S	0	0
			473	313	78	80	2		
9	w	59	Total	C	N	O	S	0	0
			473	313	78	80	2		

- Molecule 10 is a protein called ATP synthase subunit K, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	24	Total	C	N	O	S	0	0
			180	122	30	27	1		
10	x	24	Total	C	N	O	S	0	0
			180	122	30	27	1		

- Molecule 11 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	501	Total	C	N	O	S	0	0
			3745	2363	665	714	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	492	Total	C	N	O	S	0	0
			3700	2336	656	705	3		
11	C	500	Total	C	N	O	S	0	0
			3739	2359	664	713	3		
11	n	501	Total	C	N	O	S	0	0
			3745	2363	665	714	3		
11	W	492	Total	C	N	O	S	0	0
			3700	2336	656	705	3		
11	X	500	Total	C	N	O	S	0	0
			3739	2359	664	713	3		

- Molecule 12 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	470	Total	C	N	O	S	0	0
			3549	2250	604	689	6		
12	E	468	Total	C	N	O	S	0	0
			3536	2243	602	685	6		
12	F	469	Total	C	N	O	S	0	0
			3543	2247	603	687	6		
12	Y	470	Total	C	N	O	S	0	0
			3549	2250	604	689	6		
12	Z	468	Total	C	N	O	S	0	0
			3536	2243	602	685	6		
12	c	469	Total	C	N	O	S	0	0
			3543	2247	603	687	6		

- Molecule 13 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	265	Total	C	N	O	S	0	0
			2030	1277	355	388	10		
13	j	265	Total	C	N	O	S	0	0
			2030	1277	355	388	10		

- Molecule 14 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	119	Total	C	N	O	S	0	0
			751	470	133	146	2		
14	l	119	Total	C	N	O	S	0	0
			751	470	133	146	2		

- Molecule 15 is a protein called ATP synthase catalytic sector F1 epsilon subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	I	48	Total	C	N	O	0	0
			324	201	56	67		
15	m	48	Total	C	N	O	0	0
			324	201	56	67		

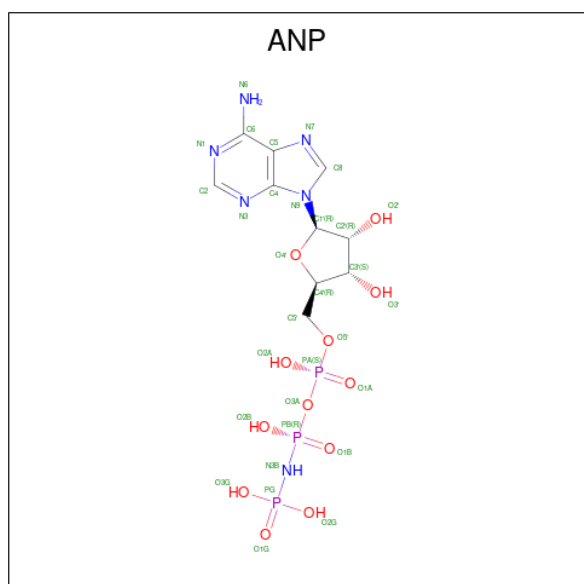
- Molecule 16 is a protein called ATP synthase subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	O	161	Total	C	N	O	0	0
			795	473	161	161		
16	o	161	Total	C	N	O	0	0
			795	473	161	161		

- Molecule 17 is a protein called ATP synthase subunit h.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	h	21	Total	C	N	O	0	0
			105	63	21	21		
17	v	21	Total	C	N	O	0	0
			105	63	21	21		

- Molecule 18 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
18	K	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	B	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	C	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	D	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	F	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	n	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	W	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	X	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	Y	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	c	1	Total	C	N	O	P	0
			31	10	6	12	3	

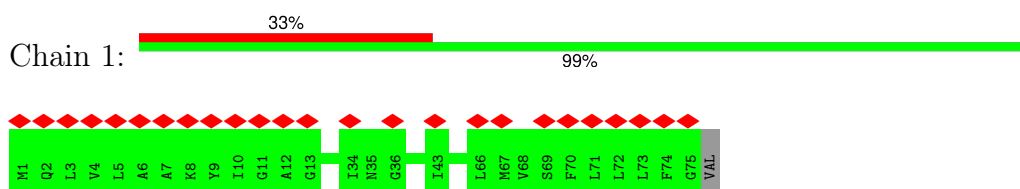
- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
19	K	1	Total	Mg	0
			1	1	
19	B	1	Total	Mg	0
			1	1	
19	C	1	Total	Mg	0
			1	1	
19	D	1	Total	Mg	0
			1	1	
19	F	1	Total	Mg	0
			1	1	
19	n	1	Total	Mg	0
			1	1	
19	W	1	Total	Mg	0
			1	1	
19	X	1	Total	Mg	0
			1	1	
19	Y	1	Total	Mg	0
			1	1	
19	c	1	Total	Mg	0
			1	1	

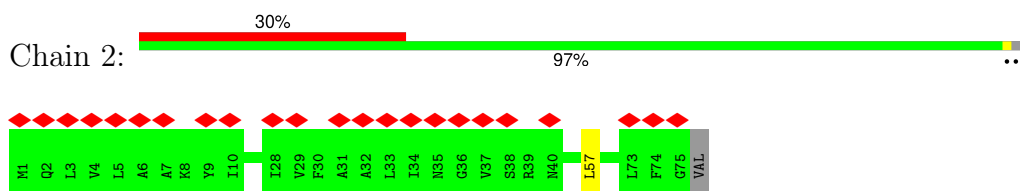
3 Residue-property plots [i](#)

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.

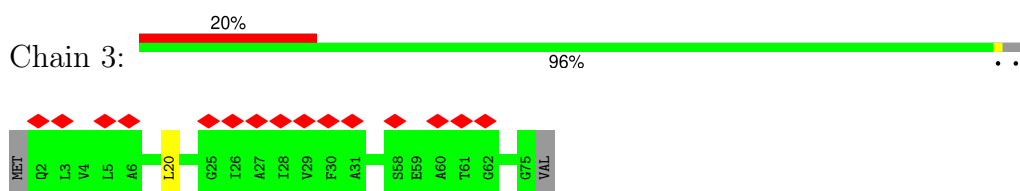
- Molecule 1: ATP synthase subunit 9, mitochondrial



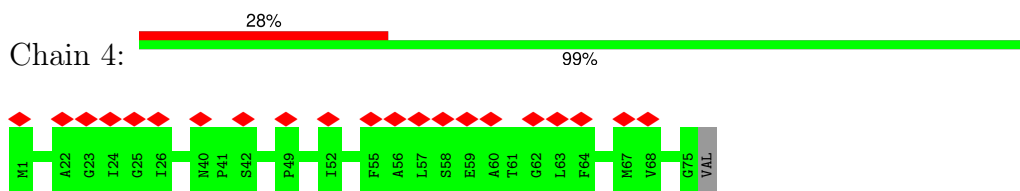
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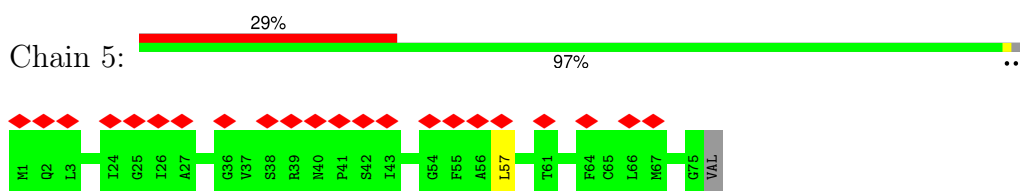
- Molecule 1: ATP synthase subunit 9, mitochondrial



- Molecule 1: ATP synthase subunit 9, mitochondrial

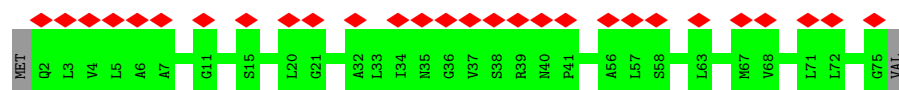


- Molecule 1: ATP synthase subunit 9, mitochondrial



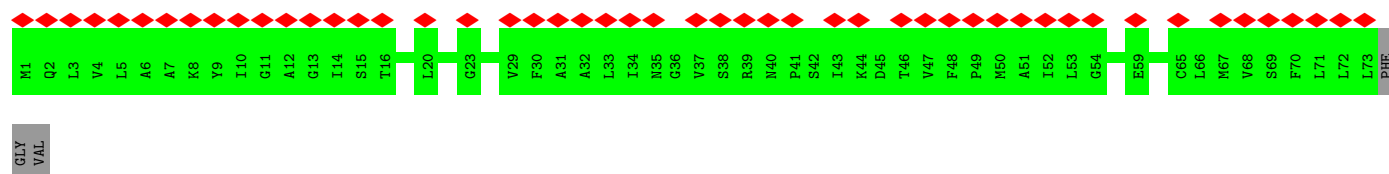
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 6: 



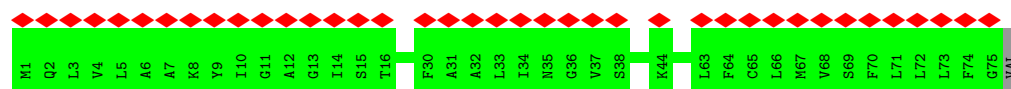
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Chain 7: 



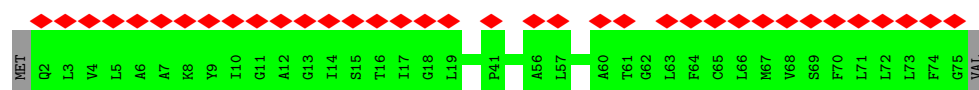
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 8: 



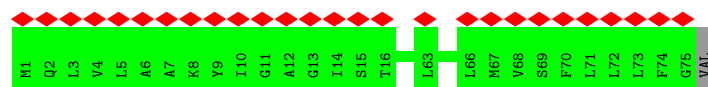
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 9: 



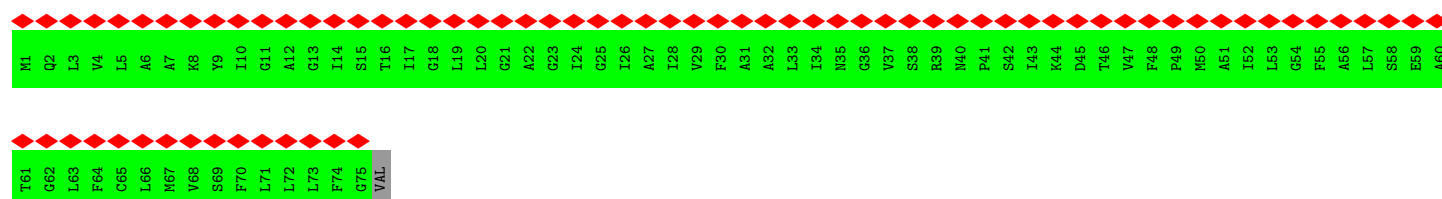
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 0: 

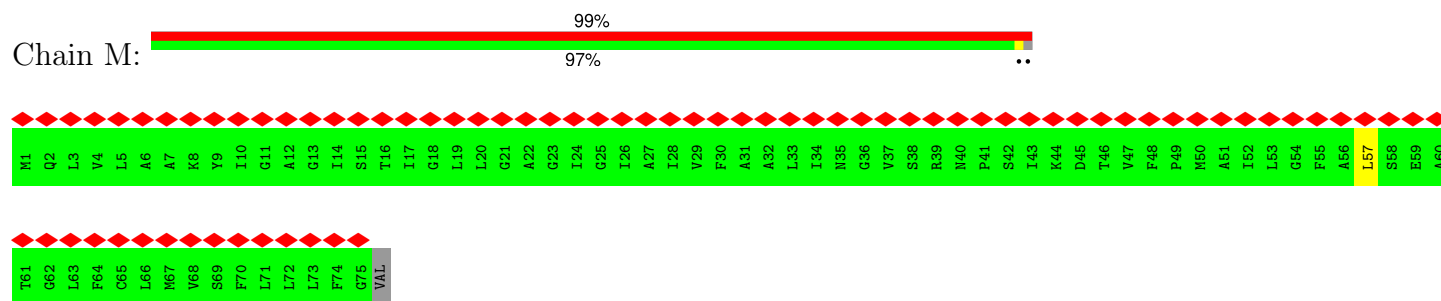


- Molecule 1: ATP synthase subunit 9, mitochondrial

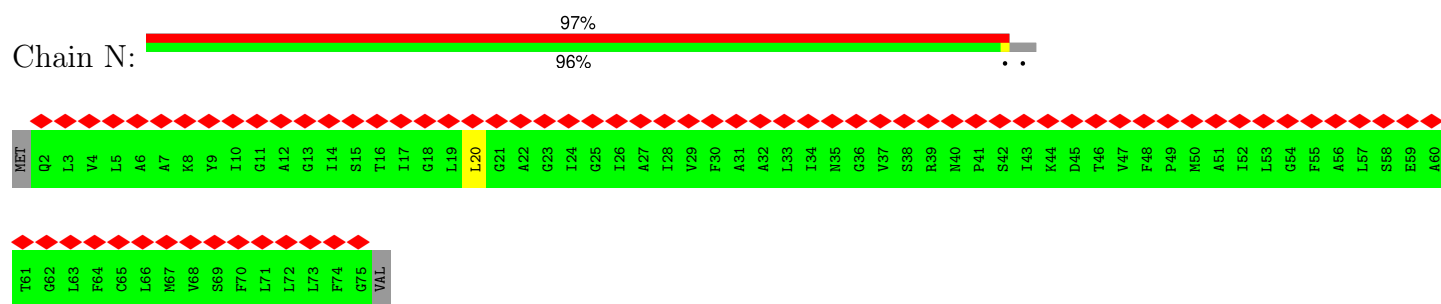
Chain L: 



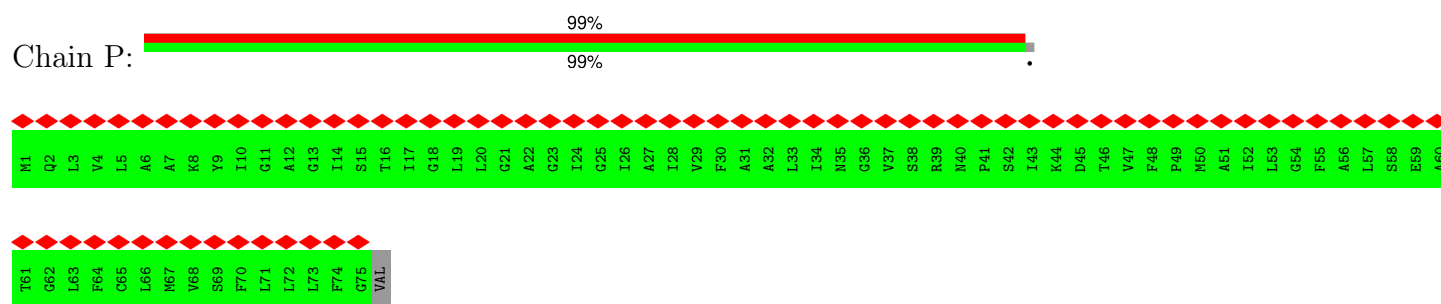
- Molecule 1: ATP synthase subunit 9, mitochondrial



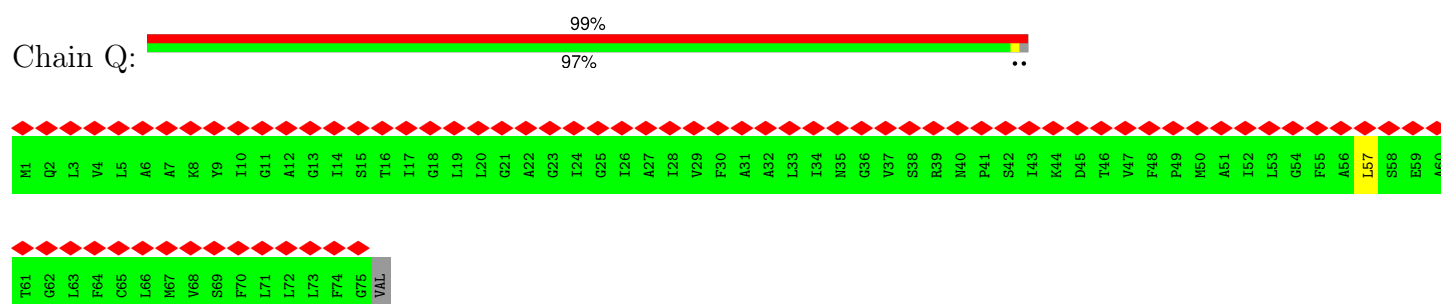
- Molecule 1: ATP synthase subunit 9, mitochondrial



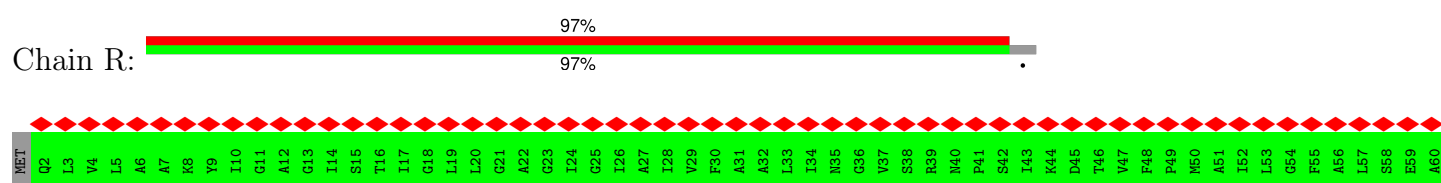
- Molecule 1: ATP synthase subunit 9, mitochondrial

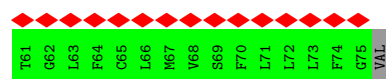


- Molecule 1: ATP synthase subunit 9, mitochondrial

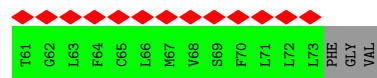
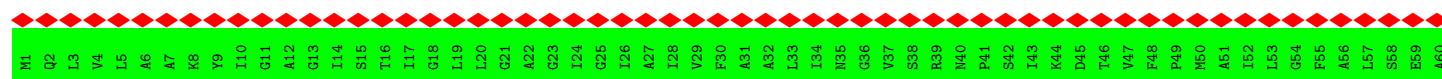


- Molecule 1: ATP synthase subunit 9, mitochondrial

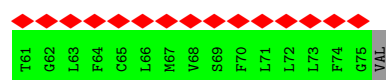
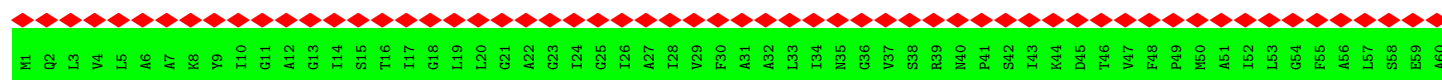




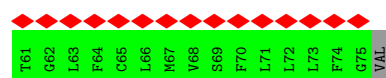
- Molecule 1: ATP synthase subunit 9, mitochondrial



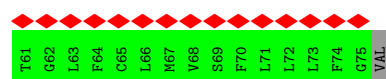
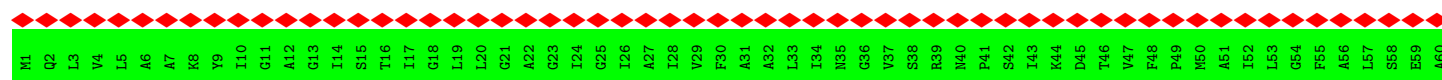
- Molecule 1: ATP synthase subunit 9, mitochondrial



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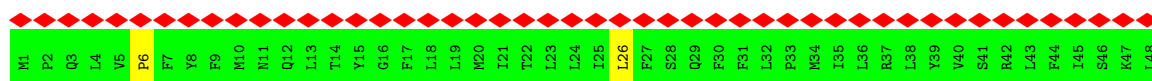


- Molecule 1: ATP synthase subunit 9, mitochondrial

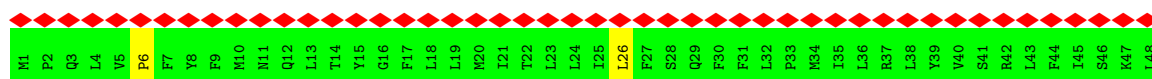


- Molecule 2: ATP synthase protein 8

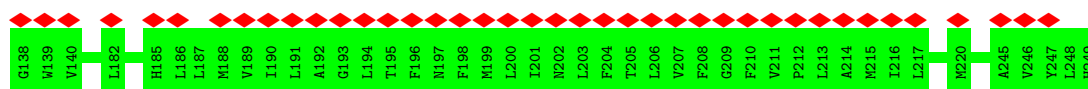
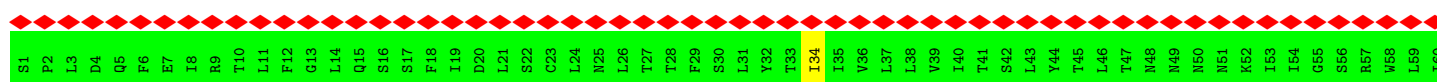




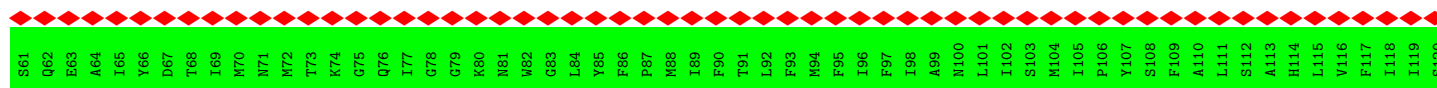
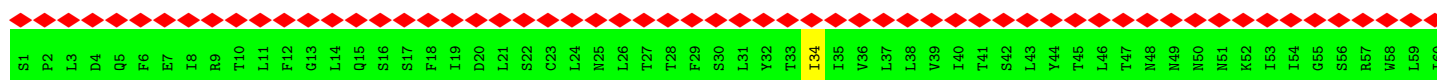
• Molecule 2: ATP synthase protein 8



• Molecule 3: ATP synthase subunit a

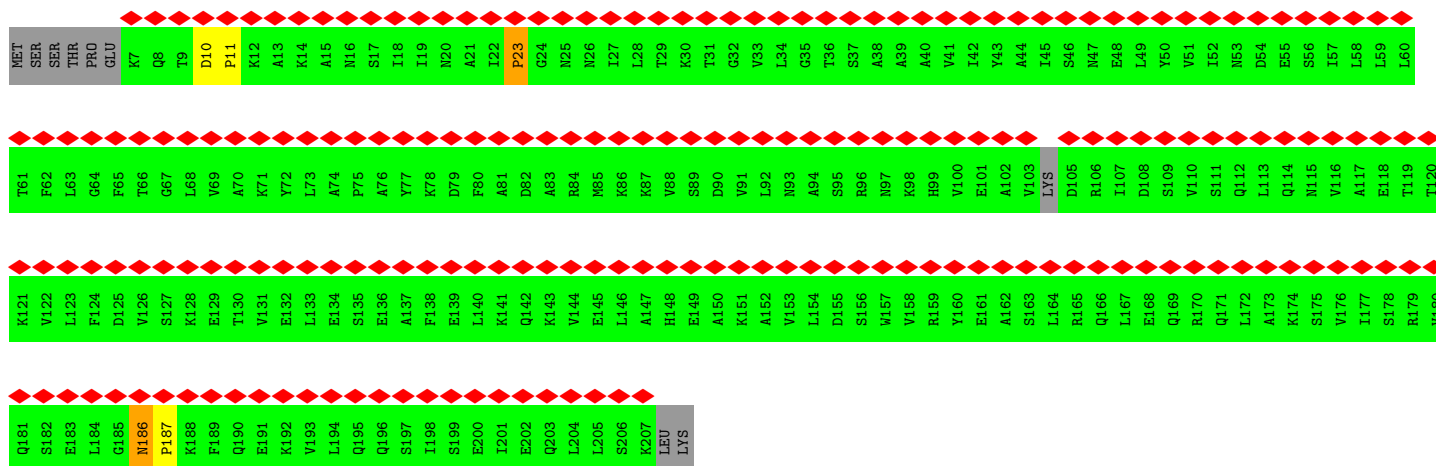


• Molecule 3: ATP synthase subunit a

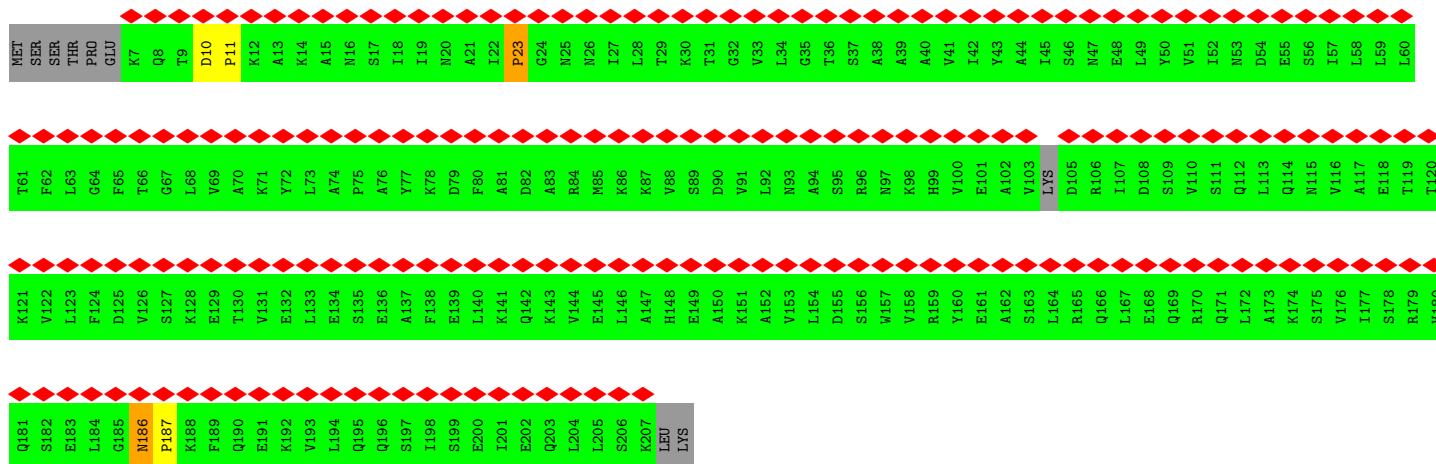
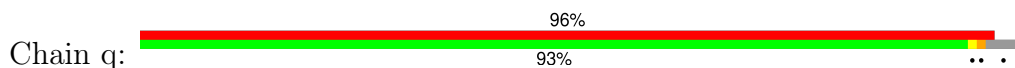


• Molecule 4: ATP synthase subunit 4, mitochondrial

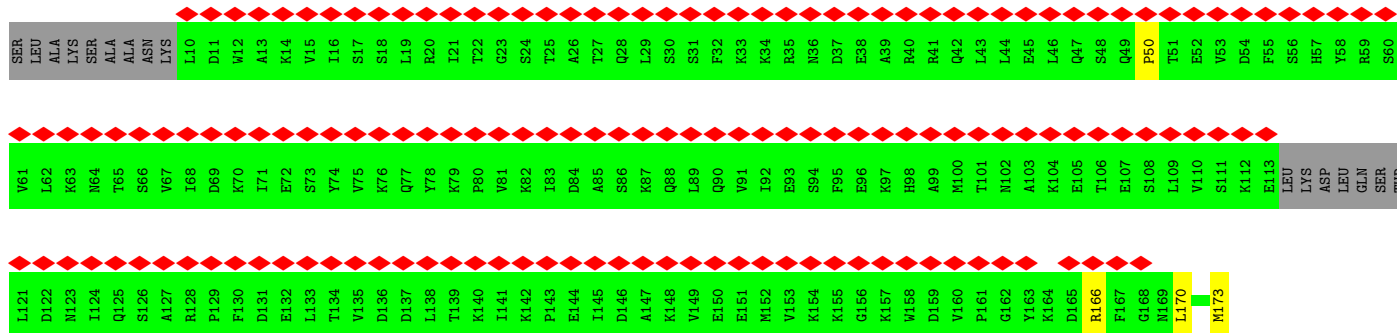
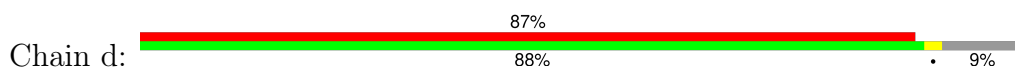




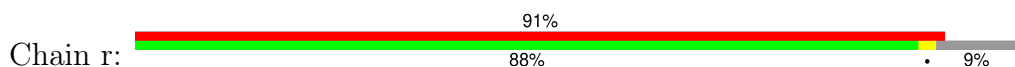
• Molecule 4: ATP synthase subunit 4, mitochondrial

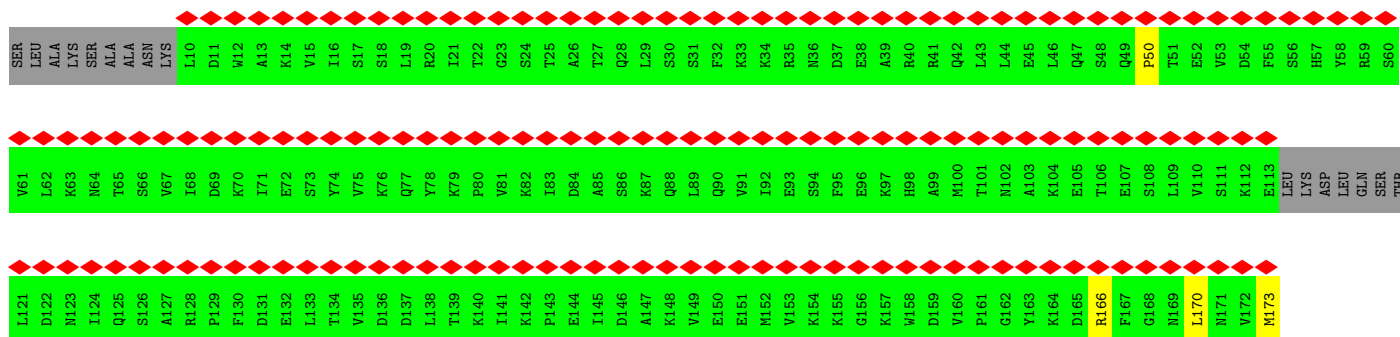


• Molecule 5: ATP synthase subunit d, mitochondrial

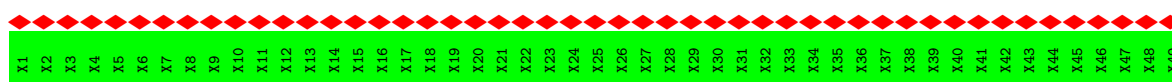


• Molecule 5: ATP synthase subunit d, mitochondrial

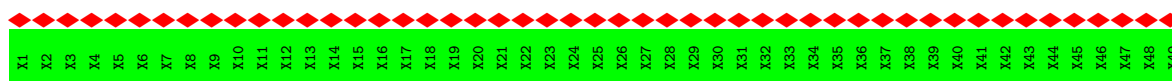




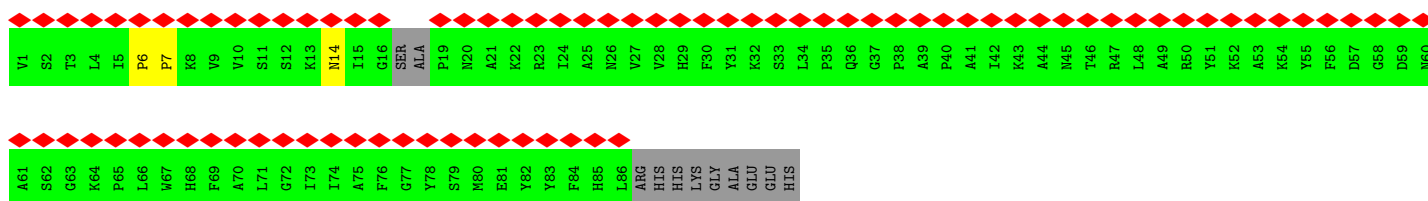
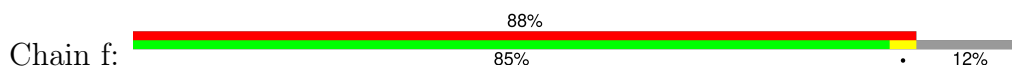
- Molecule 6: ATP synthase subunit e, mitochondrial



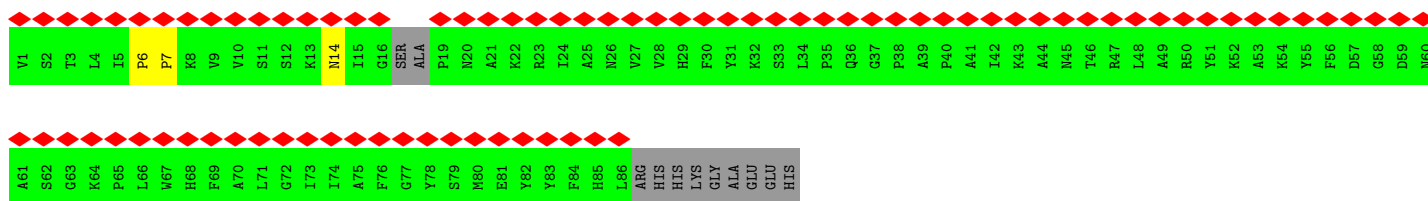
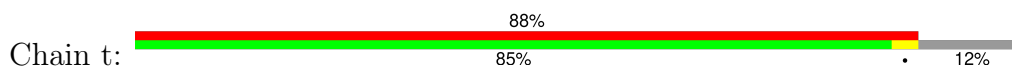
- Molecule 6: ATP synthase subunit e, mitochondrial



- Molecule 7: ATP synthase subunit f, mitochondrial

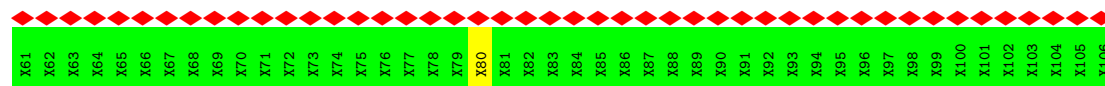
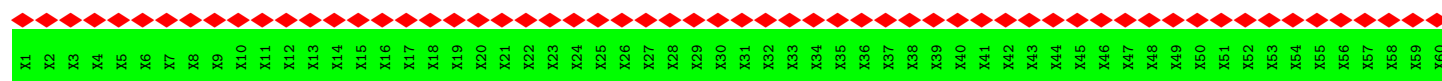


- Molecule 7: ATP synthase subunit f, mitochondrial

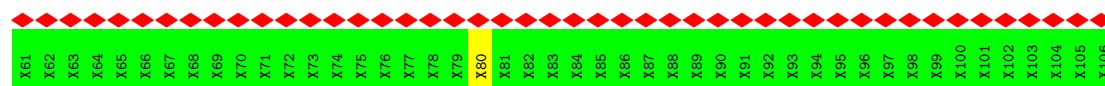
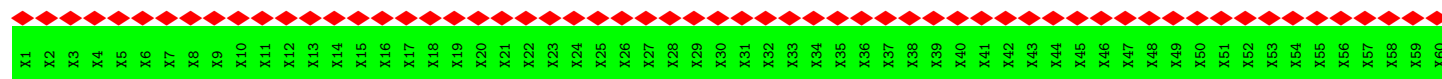


- Molecule 8: AATP synthase subunit g





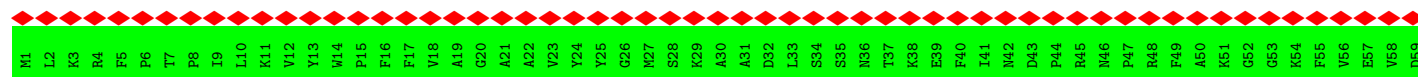
• Molecule 8: AATP synthase subunit g



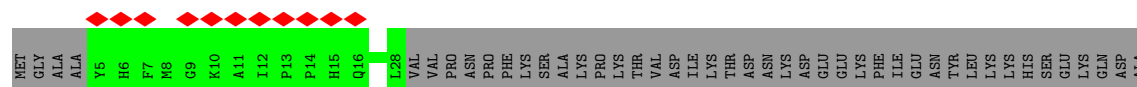
• Molecule 9: ATP synthase subunit J, mitochondrial



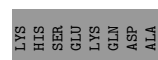
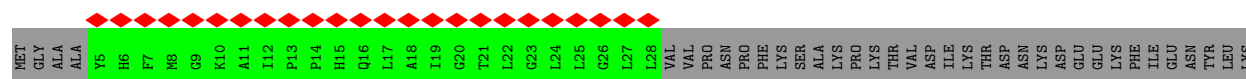
• Molecule 9: ATP synthase subunit J, mitochondrial



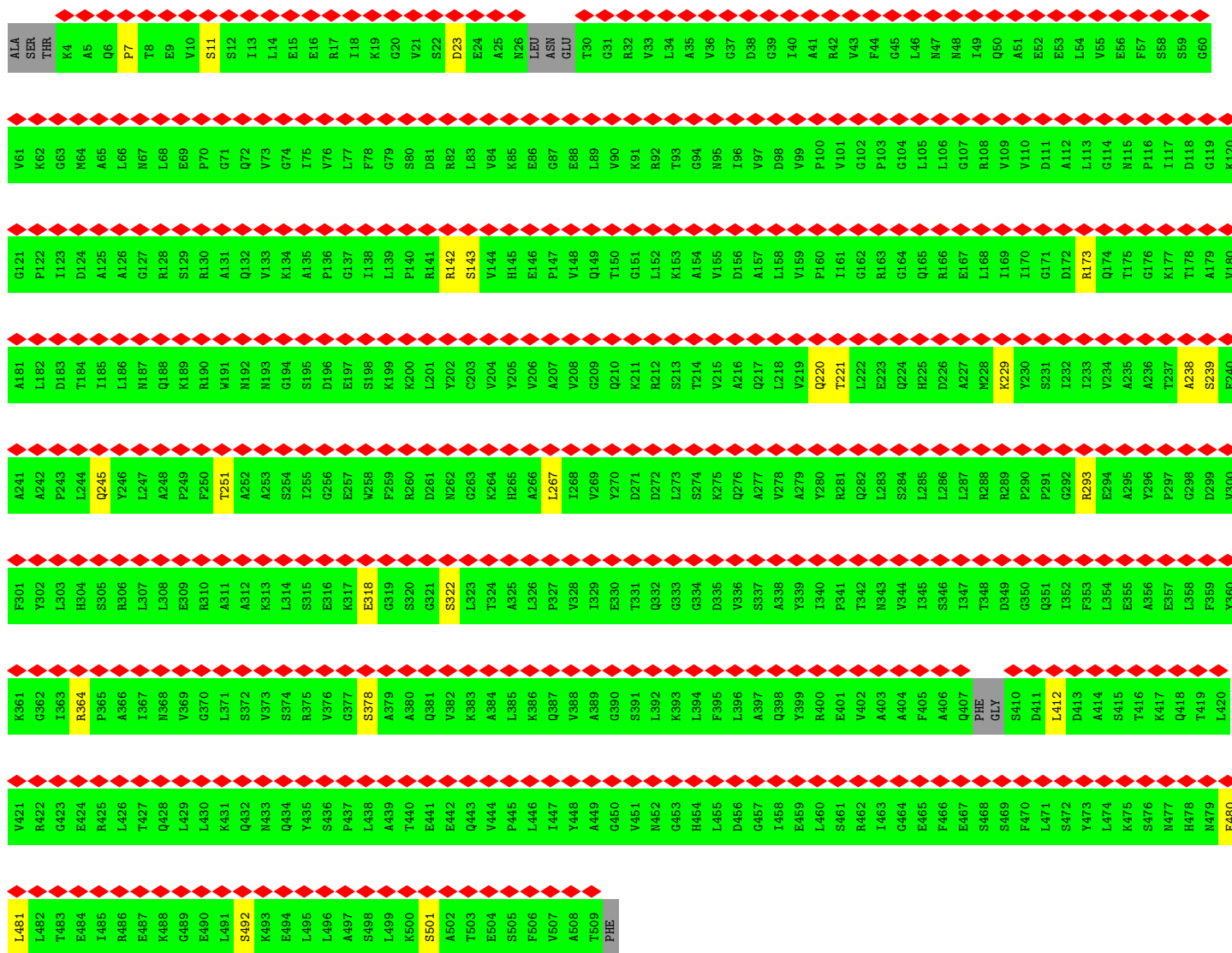
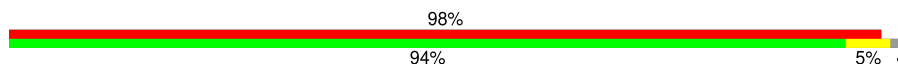
• Molecule 10: ATP synthase subunit K, mitochondrial



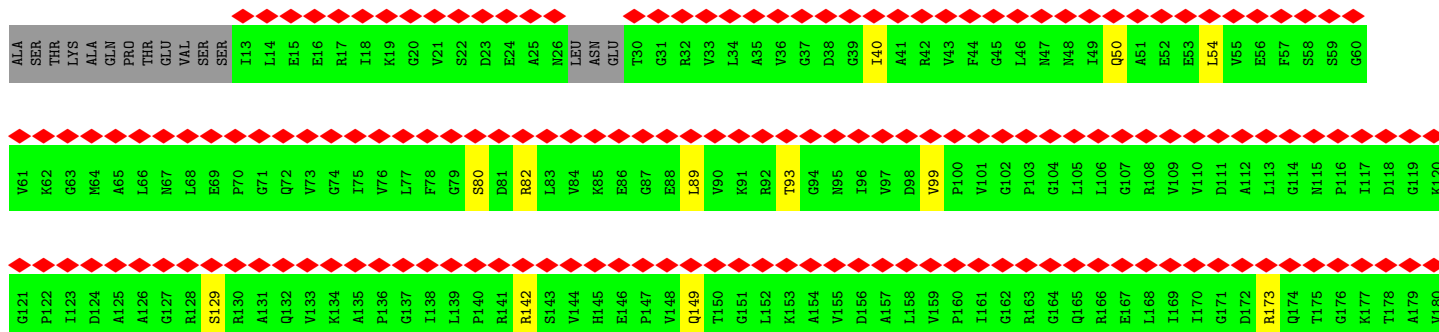
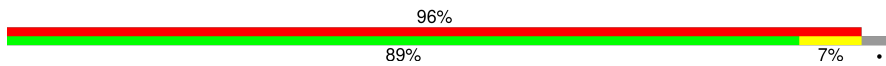
• Molecule 10: ATP synthase subunit K, mitochondrial



Chain K:

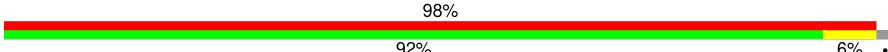


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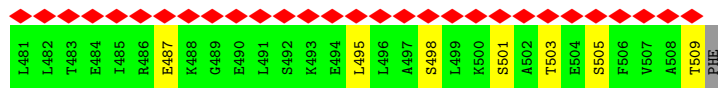
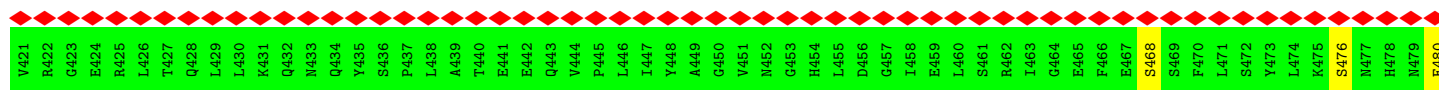


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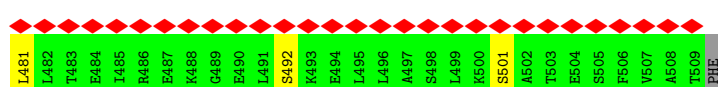
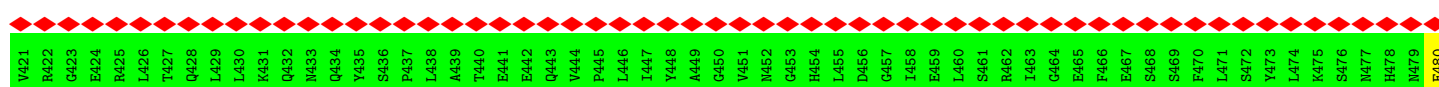
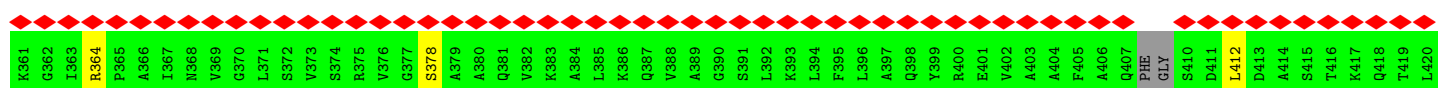
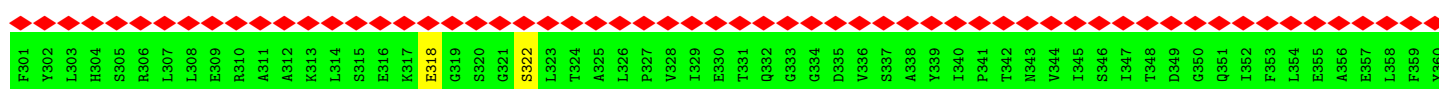
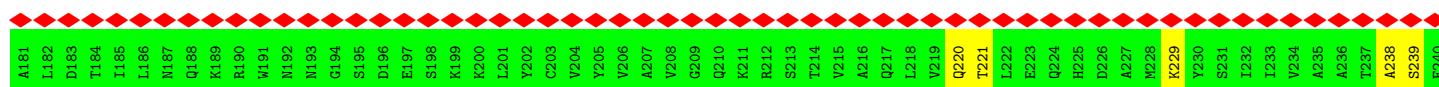
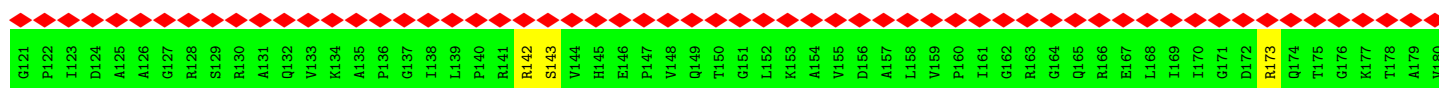
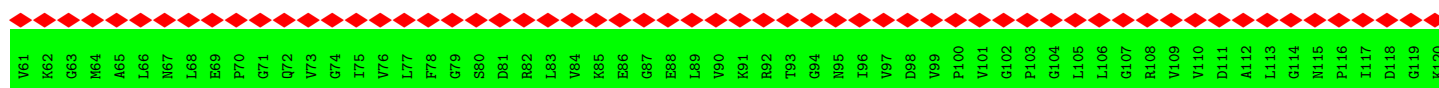
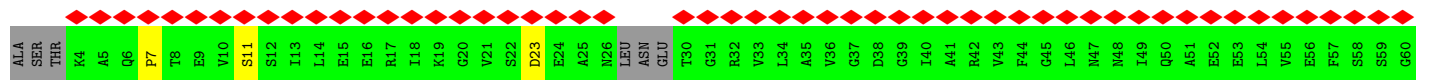
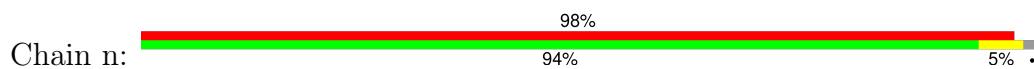
• Molecule 11: ATP synthase subunit alpha, mitochondrial

Chain C: 

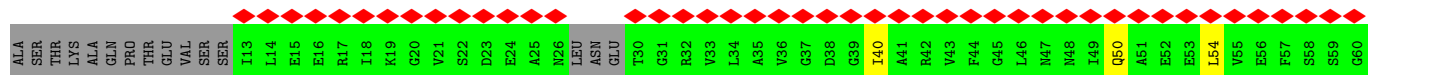
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V61	K62	G63	H64	A65	L66	N67	L68	E69	P70	G71	Q72	V73	G74	I75	V76	L77	F78	G79	S80	D81	L82	L83	H84	K85	E86	G87	E88	L89	V90	K91	L92	K93	G94	N95	I96	V97	D98	V99	P100	V101	G102	P103	G104	L105	L106	G107	R108	V109	I110	D111	A112	L113	G114	N115	P116	I117	D118	G119	K120
G121	P122	I123	D124	A125	A126	G127	R128	S129	R130	A131	Q132	V133	K134	A135	P136	G137	I138	L139	P140	R141	L142	S143	V144	H145	E146	P147	V148	Q149	T150	G151	L152	K153	A154	V155	D156	A157	L158	V159	P160	I161	G162	R163	G164	Q165	R166	E167	L168	I169	T170	G171	D172	R173	Q174	T175	G176	K177	T178	A179	V180
A181	L182	D183	T184	L185	L186	M187	Q188	R189	R190	M191	N192	M193	G194	S195	D196	E197	S198	K199	K200	L201	L202	C203	V204	V205	V206	A207	V208	G209	Q210	R211	R212	S213	T214	V215	A216	Q217	L218	V219	Q220	T221	L222	E223	Q224	H225	D226	A227	H228	K229	V230	S231	I232	I233	V234	A235	A236	T237	A238	S239	E240
A241	A242	P243	L244	Q245	Y246	L247	A248	P249	P250	T251	A252	A253	S254	I255	G256	E257	W258	F259	R260	L261	N262	G263	K264	H265	A266	L267	V268	V269	D270	D271	D272	L273	S274	K275	Q276	A277	V278	A279	Y280	R281	Q282	L283	S284	H285	L286	L287	R288	R289	P290	P291	Q292	R293	E294	A295	Y296	P297	Q298	D299	V300
F301	Y302	L303	H304	S305	R306	L307	L308	S309	R310	A311	A312	K313	L314	S315	E316	K317	E318	G319	S320	S321	S322	L323	T324	A325	L326	P327	V328	I329	E330	T331	Q332	G333	G334	D335	V336	S337	A338	Y339	I340	P341	T342	N343	V344	I345	S346	I347	T348	G349	S410	D411	L412	I413	L414	E415	T416	K417	Q418	T419	L420
K361	G362	I363	R364	P365	A366	I367	N368	V369	G370	L371	S372	V373	S374	R375	V376	G377	S378	A379	A380	K381	N382	G383	A384	L385	K386	Q387	V388	A389	S390	T391	Q392	G393	L394	F395	L396	A397	Q398	Y399	R400	E401	V402	A403	A404	F405	A406	Q407	F408	G409	S410	D411	L412	D413	A414	S415	T416	K417	Q418	T419	L420

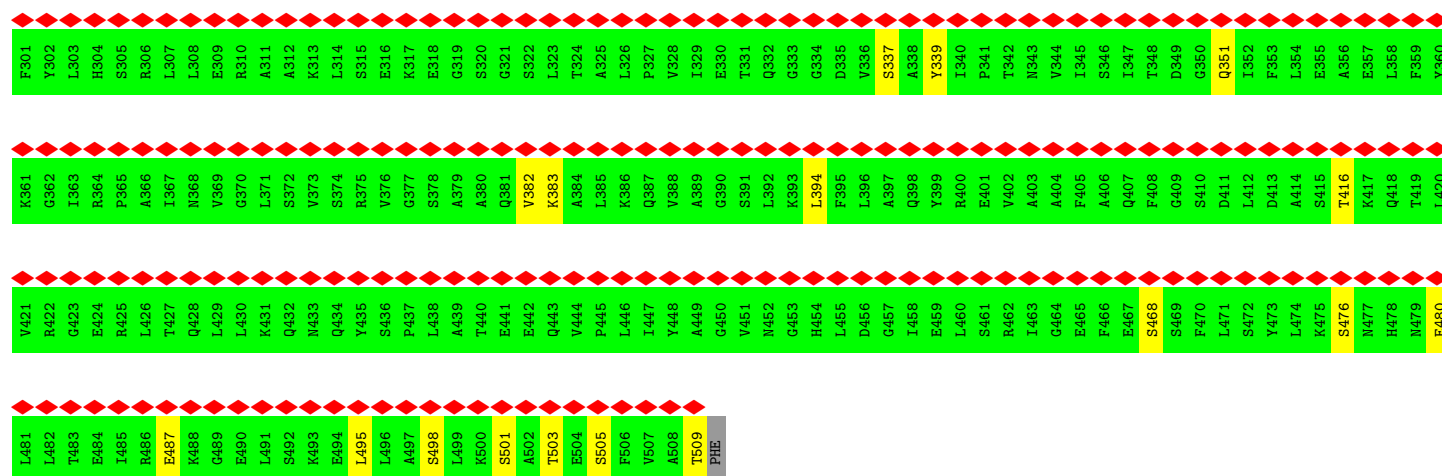


• Molecule 11: ATP synthase subunit alpha, mitochondrial

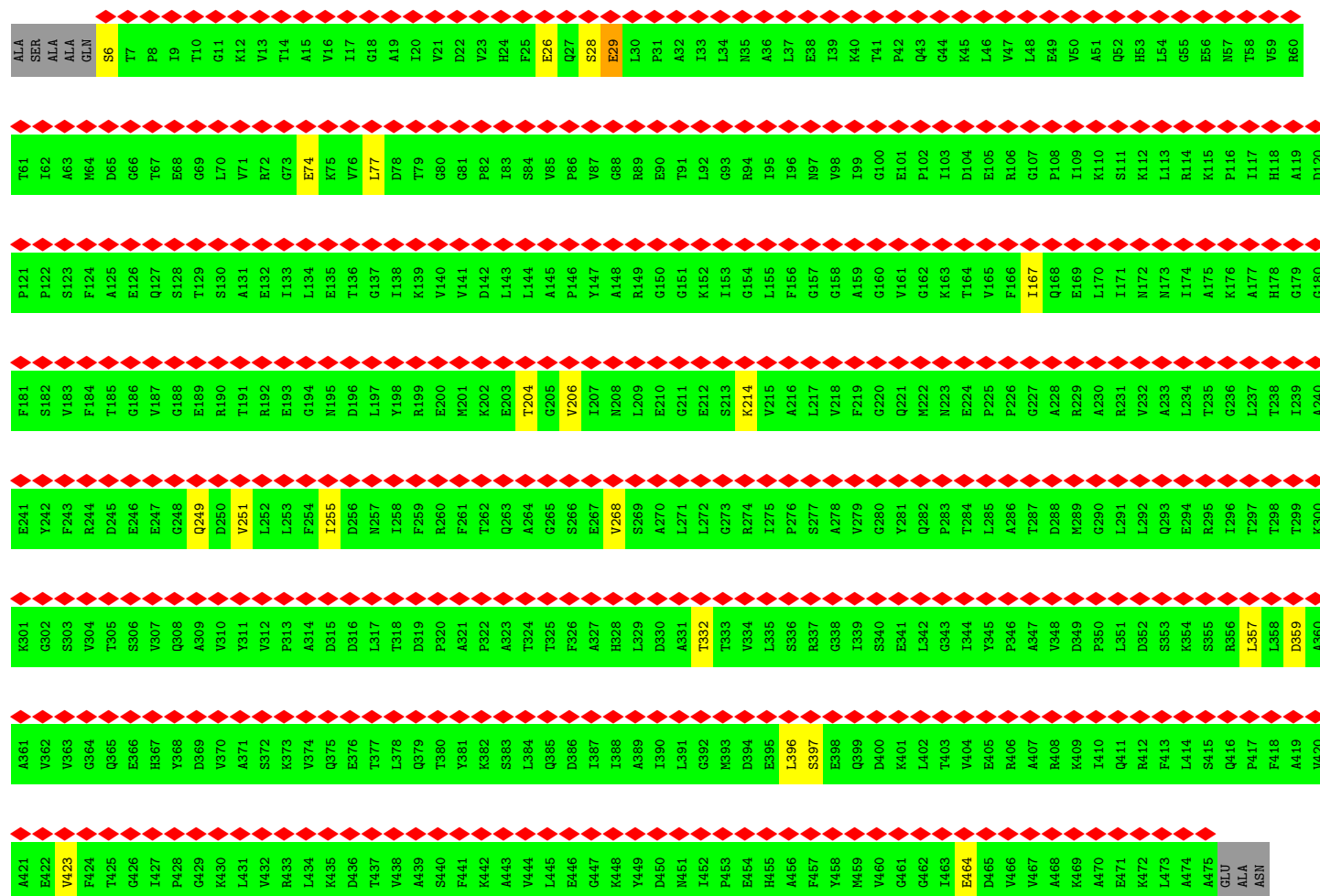


• Molecule 11: ATP synthase subunit alpha, mitochondrial

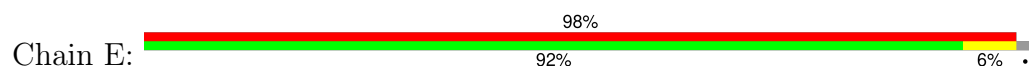




• Molecule 12: ATP synthase subunit beta, mitochondrial

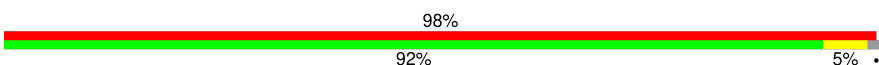


• Molecule 12: ATP synthase subunit beta, mitochondrial

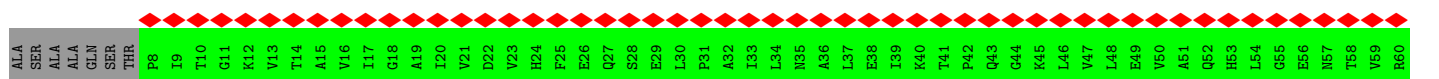


ALA	SER	ALA	ALA	GLN	SER	THR	P8	I9	T10	G11	K12	V13	T14	A15	V16	I17	G18	A19	I20	V21	D22	V23	H24	F25	E26	Q27	S28	E29	L30	P31	A32	L33	L34	N35	A36	L37	E38	I39	K40	T41	P42	Q43	O44	K45	L46	V47	L48	E49	V50	A51	Q52	H53	L54	G55	E56	N57	V58	V59	R60
T61	I62	A63	M64	D65	G66	T67	E68	G69	L70	V71	R72	G73	E74	K75	V76	L77	D78	T79	G80	G81	P82	H83	S84	V85	P86	V87	R88	R89	E90	T91	L92	G93	R94	I95	I96	N97	V98	I99	G100	E101	P102	I103	D104	E105	R106	G107	P108	I109	A51	Q52	H53	L54	G55	E56	N57	T58	V59	R60	
P121	P122	S123	F124	I125	E126	Q127	S128	T129	S130	A131	E132	I133	L134	E135	T136	G137	I138	K139	V140	V141	D142	L143	L144	A145	P146	Y147	R148	G149	G150	G151	K152	I153	G154	L155	F156	G157	G158	A159	G160	V161	G162	K163	T164	V165	F166	I167	Q168	E169	L170	I171	N172	N173	I174	A175	K176	I177	H178	G179	G180
F181	S182	V183	F184	T185	G186	V187	G188	E189	R190	T191	R192	E193	G194	N195	D196	L197	Y198	R199	E200	M201	K202	E203	T204	G205	V206	I207	N208	L209	E210	G211	E212	S213	K214	V215	A216	L217	V218	F219	G220	Q221	M222	N223	E224	P225	P226	G227	A228	R229	A230	R231	V232	A233	L234	T235	Q236	L237	T238	I239	A240
E241	Y242	F243	R244	D245	E246	E247	G248	Q249	D250	V251	L252	L253	F254	L255	D256	N257	I258	F259	R260	F261	T262	Q263	A264	G265	S266	E267	V268	S269	A270	L271	L272	G273	R274	L275	P276	S277	A278	V279	G280	Y281	Q282	P283	T284	L285	A286	T287	D288	M289	Q290	L291	L292	Q293	E294	R295	I296	T297	T298	T299	K300
K301	G302	S303	V304	T305	S306	V307	Q308	A309	V310	Y311	V312	P313	A314	D315	D316	L317	T318	D319	P320	A321	K322	Q323	T324	T325	F326	A327	H328	L329	D330	A331	K332	T333	V334	L335	S336	R337	G338	I339	S340	E341	L342	G343	I344	Y345	P346	A347	V348	D349	P350	L351	D352	S353	K354	S355	R356	L357	D358	D359	A360
A361	V362	V363	G364	Q365	E366	H367	Q368	D369	V370	A371	S372	K373	V374	Q375	E376	T377	L378	Q379	T380	F381	K382	S383	L384	Q385	D386	I387	L388	A389	I390	L391	K392	M393	D394	E395	L396	S397	E398	Q399	D400	K401	L402	T403	V404	E405	R406	A407	R408	K409	L410	Q411	R412	F413	L414	S415	Q416	P417	F418	A419	V420
A421	E422	V423	F424	T425	Q426	L427	P428	G429	L430	A431	V432	R433	L434	K435	D436	T437	V438	A439	S440	F441	K442	A443	V444	L445	E446	G447	K448	Y449	D450	M451	L452	P453	A454	H455	A456	F457	M458	M459	V460	G461	G462	I463	E464	D465	V466	V467	A468	K469	A470	E471	L472	L473	A474	A475	GLU	ALA	ASN		

• Molecule 12: ATP synthase subunit beta, mitochondrial

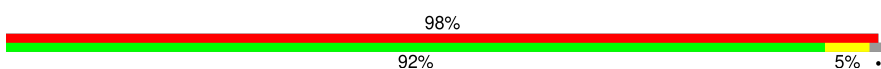
Chain F: 

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T61	I62	A63	M64	D65	G66	T67	E68	G69	L70	V71	R72	G73	E74	K75	V76	L77	D78	I79	G80	G81	P82	I83	S84	V85	P86	V87	R88	E89	E90	T91	L92	G93	R94	I95	I96	N97	V98	I99	G100	E101	G102	I103	D104	V105	R106	G107	P108	V109	A110	Q111	K112	L113	R114	K115	P116	I117	H118	A119	D120
P121	P122	S123	F124	I125	E126	Q127	S128	T129	S130	A131	E132	I133	L134	E135	T136	G137	I138	K139	V140	V141	D142	L143	L144	A145	P146	Y147	R148	G149	G150	G151	K152	I153	G154	L155	F156	G157	G158	A159	G160	V161	G162	K163	T164	V165	F166	I167	Q168	E169	L170	K171	I172	N173	L174	A175	K176	I177	H178	G179	G180
F181	S182	V183	F184	T185	G186	V187	G188	E189	R190	T191	R192	E193	G194	M195	D196	L197	Y198	R199	E200	M201	K202	E203	T204	G205	V206	I207	N208	L209	E210	G211	E212	S213	K214	V215	A216	L217	V218	F219	G220	Q221	G222	N223	E224	L285	P226	G227	A228	R229	A230	R231	V232	A233	L234	T235	Q236	L237	T238	I239	A240
E241	Y242	F243	R244	D245	E246	E247	G248	Q249	D250	V251	L252	L253	F254	L255	D256	N257	I258	F259	R260	F261	T262	Q263	A264	G265	S266	E267	V268	S269	A270	L271	L272	G273	R274	L275	P276	S277	A278	V279	G280	Y281	Q282	P283	T284	L285	A286	T287	D288	M289	Q290	L291	L292	Q293	E294	R295	I296	T297	T298	T299	K300

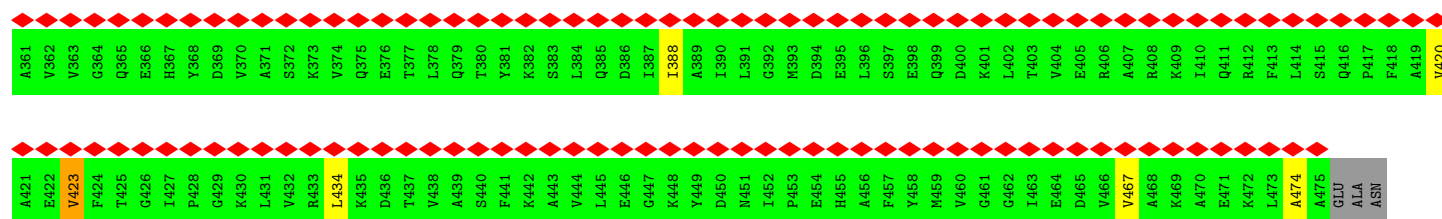


A421	A422	V423	F424	T425	G426	L427	P428	A429	K430	L431	V432	R433	L434	K435	D436	T437	V438	A439	S440	F441	K442	A443	V444	L445	E446	G447	K448	Y449	D450	M451	L452	P453	E454	H455	A456	F457	V458	M459	V460	G461	G462	L463	E464	D465	V466	V467	A468	K469	A470	E471	K472	L473	A474	A475	GLU	ALA	ASN		
A361	V362	V363	G364	Q365	E366	H367	V368	D369	G370	A371	S372	K373	V374	Q375	E376	T377	L378	Q379	T380	Y381	K382	S383	L384	Q385	D386	I387	L388	A389	I390	L391	G392	M393	D394	E395	L396	S397	E398	Q399	D400	K401	L402	T403	V404	E405	R406	A407	R408	K409	T410	Q411	R412	F413	L414	S415	Q416	F417	F418	A419	V420
K301	G302	S303	V304	T305	S306	V307	Q308	A309	V310	Y311	V312	P313	A314	D315	D316	L317	T318	D319	P320	A321	P322	A323	T324	T325	F326	I327	H328	L329	D330	A331	T332	T333	V334	L335	S336	R337	G338	I339	S340	E341	L342	G343	I344	Y345	P346	A347	V348	D349	P350	L351	D352	K353	K354	S355	R356	L357	L358	D359	A360
E241	Y242	F243	R244	D245	E246	E247	G248	Q249	D250	V251	L252	L253	F254	L255	D256	N257	I258	F259	R260	T261	K262	Q263	A264	G265	S266	E267	V268	S269	A270	L271	L272	G273	R274	L275	P276	S277	A278	V279	G280	Y281	Q282	P283	L284	L285	A286	T287	D288	M289	G290	L291	L292	Q293	E294	R295	I296	T297	T298	T299	K300
F181	S182	V183	F184	T185	G186	V187	G188	E189	R190	T191	R192	E193	G194	N195	D196	L197	Y198	R199	E200	M201	K202	E203	T204	G205	V206	I207	N208	L209	E210	G211	E212	S213	K214	V215	A216	L217	V218	F219	G220	Q221	M222	N223	E224	P225	P226	G227	A228	R229	A230	R231	V232	A233	L234	T235	G236	L237	T238	I239	A240
P121	P122	S123	F124	A125	E126	Q127	S128	T129	S130	A131	E132	I133	L134	E135	T136	G137	I138	K139	V140	V141	D142	L143	L144	A145	P146	Y147	A148	R149	G150	G151	K152	I153	G154	L155	F156	G157	G158	A159	G160	V161	G162	K163	T164	V165	F166	I167	Q168	E169	L170	I171	N172	M173	I174	A175	K176	A177	L178	G179	G180
T61	I62	A63	M64	D65	G66	T67	E68	G69	L70	V71	R72	G73	E74	K75	V76	L77	D78	T79	G80	G81	P82	I83	S84	V85	P86	V87	G88	R89	E90	T91	L92	G93	R94	I95	I96	N97	V98	I99	G100	E101	P102	I103	D104	E105	R106	G107	P108	I109	K110	S111	K112	R113	R114	K115	P116	H117	H118	A119	D120

• Molecule 12: ATP synthase subunit beta, mitochondrial

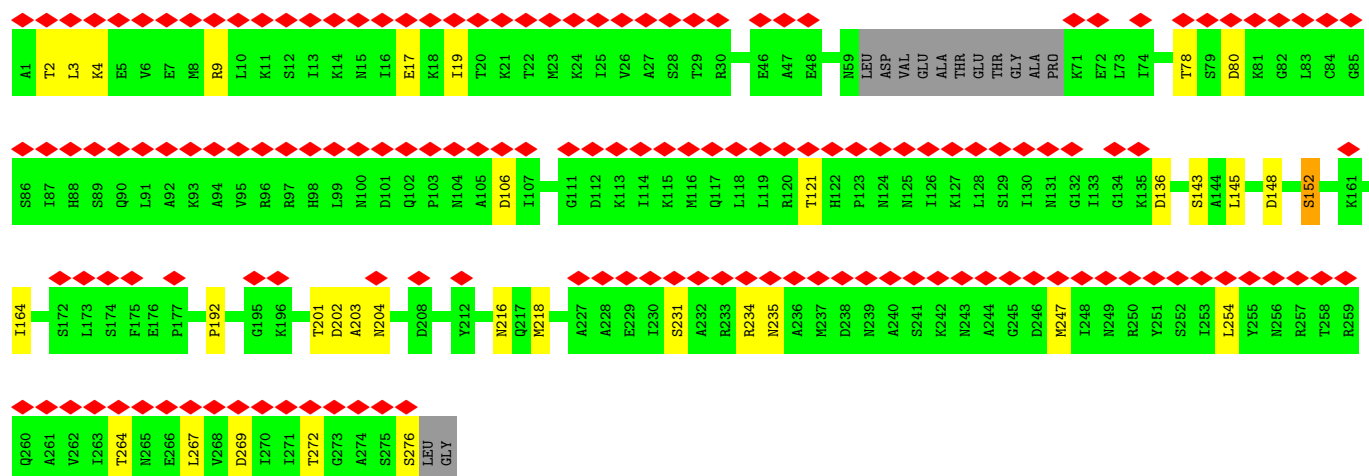
Chain c: 

ALA	SER	ALA	ALA	GLN	SER	T7	P8	I9	T10	G11	K12	V13	T14	A15	V16	I17	G18	A19	T20	D21	D22	V23	H24	F25	E26	Q27	S28	E29	L30	P31	A32	I33	L34	M35	A36	L37	E38	I39	K40	T41	P42	Q43	G44	K45	L46	V47	L48	E49	V50	A51	Q52	H53	L54	G55	E56	H57	T58	V59	R60																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															



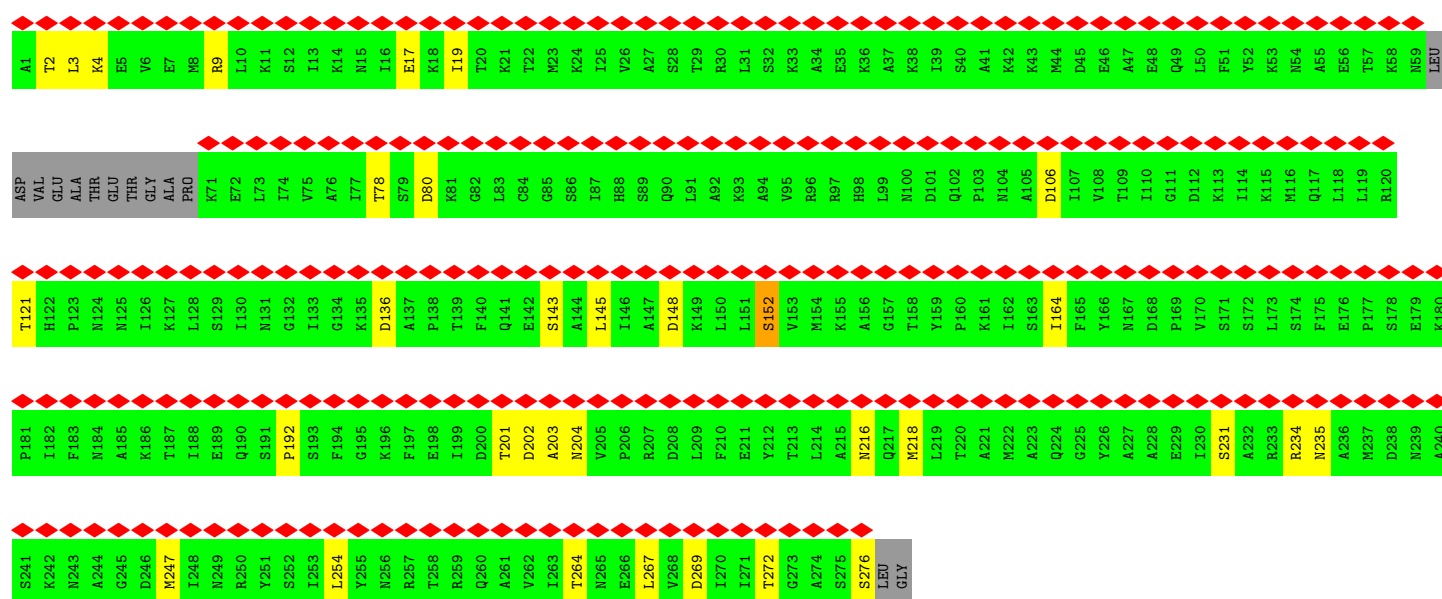
• Molecule 13: ATP synthase subunit gamma, mitochondrial

Chain G: 54%
83% 12% 5%

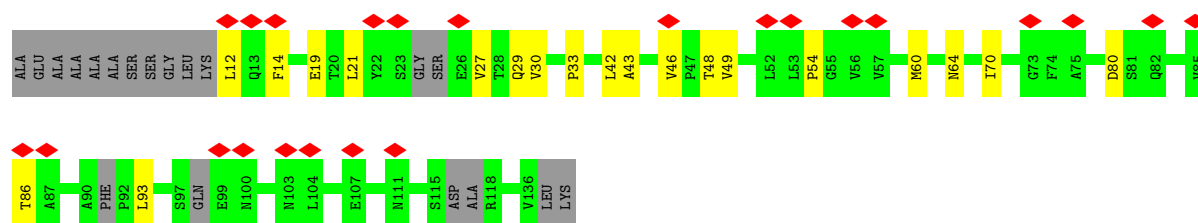
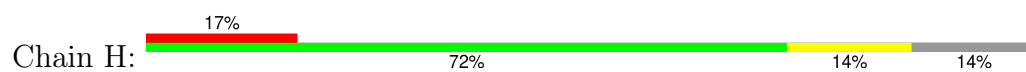


• Molecule 13: ATP synthase subunit gamma, mitochondrial

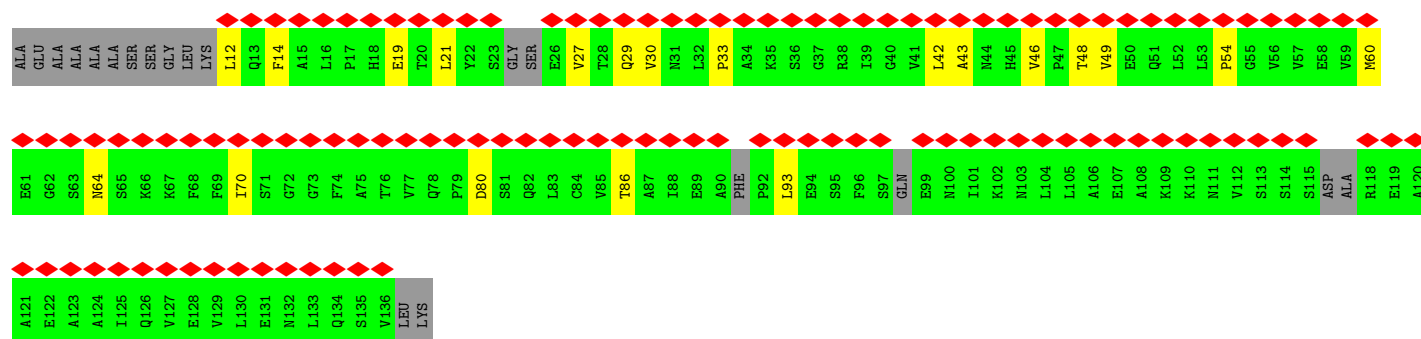
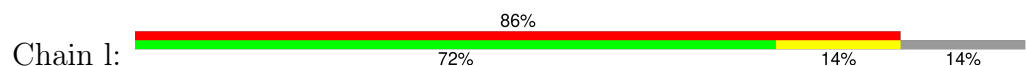
Chain j: 95%
83% 12% 5%



• Molecule 14: ATP synthase subunit delta, mitochondrial



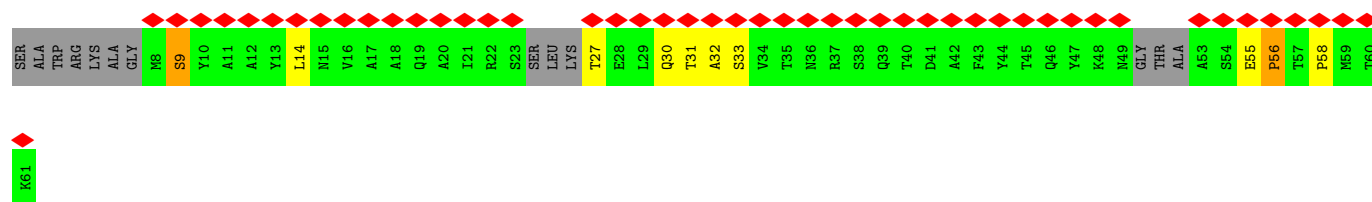
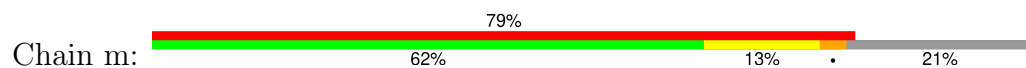
- Molecule 14: ATP synthase subunit delta, mitochondrial



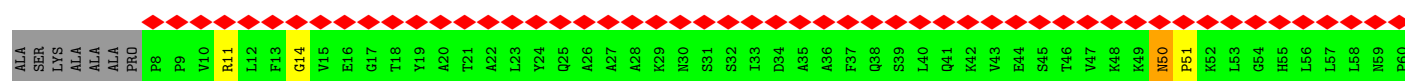
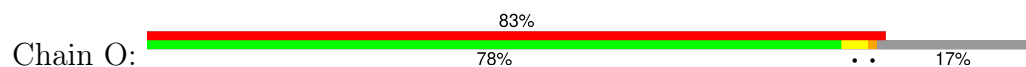
- Molecule 15: ATP synthase catalytic sector F1 epsilon subunit

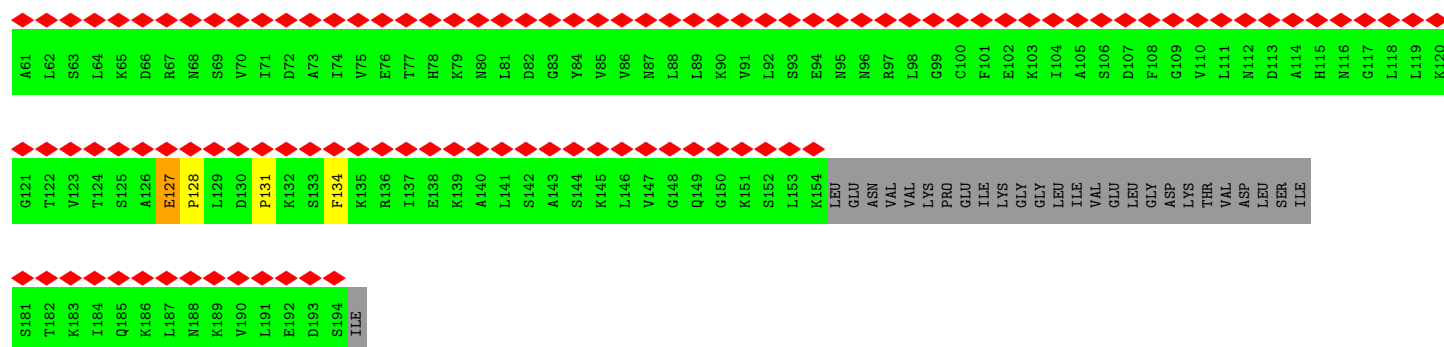


- Molecule 15: ATP synthase catalytic sector F1 epsilon subunit

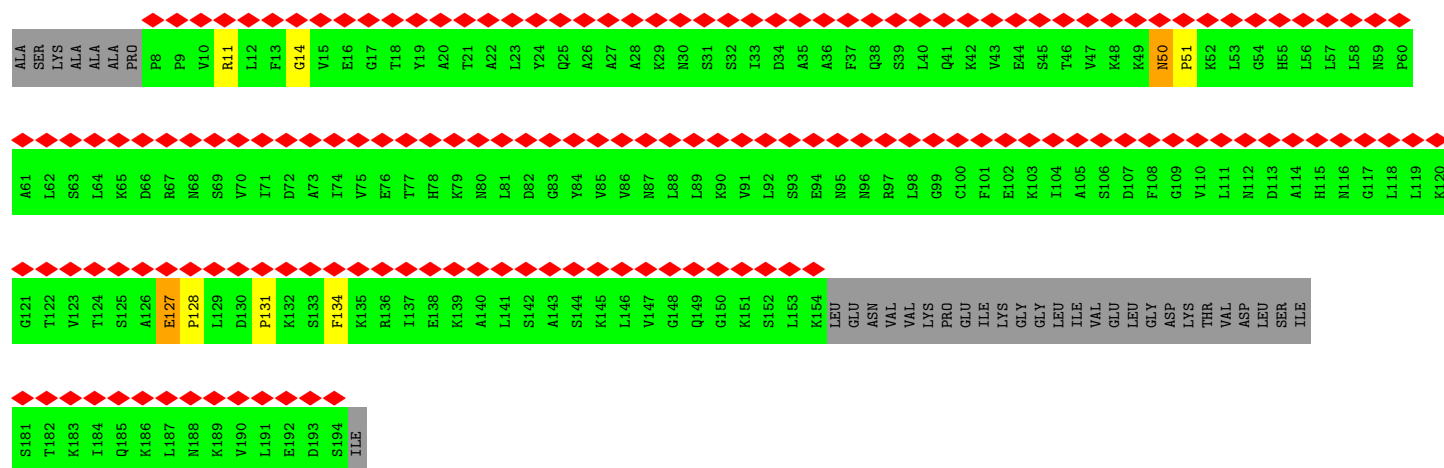
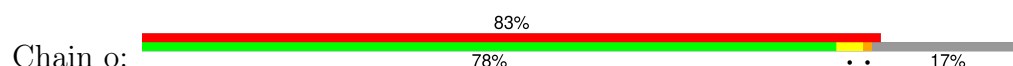


- Molecule 16: ATP synthase subunit 5, mitochondrial

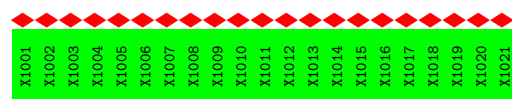




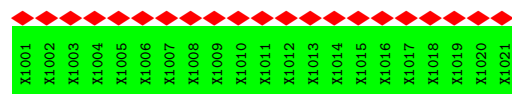
• Molecule 16: ATP synthase subunit 5, mitochondrial



• Molecule 17: ATP synthase subunit h



• Molecule 17: ATP synthase subunit h



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	238848	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 ($e^-/\text{\AA}^2$)	71	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.103	Depositor
Minimum map value	-0.374	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.156	Depositor
Map size (Å)	464.0, 464.0, 464.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45, 1.45, 1.45	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0	0.34	0/545	0.60	0/737
1	1	0.35	0/545	0.55	0/737
1	2	0.38	0/545	0.67	1/737 (0.1%)
1	3	0.37	0/537	0.61	1/727 (0.1%)
1	4	0.34	0/545	0.61	0/737
1	5	0.32	0/545	0.58	0/737
1	6	0.33	0/537	0.60	0/727
1	7	0.31	0/529	0.56	0/716
1	8	0.32	0/545	0.56	0/737
1	9	0.32	0/537	0.57	0/727
1	J	0.34	0/545	0.61	0/737
1	L	0.35	0/545	0.55	0/737
1	M	0.38	0/545	0.67	1/737 (0.1%)
1	N	0.37	0/537	0.61	1/727 (0.1%)
1	P	0.34	0/545	0.60	0/737
1	Q	0.32	0/545	0.58	0/737
1	R	0.34	0/537	0.59	0/727
1	S	0.31	0/529	0.56	0/716
1	T	0.32	0/545	0.56	0/737
1	U	0.32	0/537	0.57	0/727
2	A	0.50	0/422	0.77	1/570 (0.2%)
2	V	0.50	0/422	0.77	1/570 (0.2%)
3	a	0.45	0/2023	0.70	0/2758
3	p	0.45	0/2023	0.70	0/2758
4	b	0.46	0/1159	0.72	2/1599 (0.1%)
4	q	0.46	0/1159	0.72	2/1599 (0.1%)
5	d	0.56	0/936	0.81	1/1286 (0.1%)
5	r	0.56	0/936	0.81	1/1286 (0.1%)
7	f	0.40	0/624	0.64	2/845 (0.2%)
7	t	0.41	0/624	0.64	2/845 (0.2%)
9	i	0.42	0/488	0.60	0/659
9	w	0.42	0/488	0.60	0/659

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
10	k	0.28	0/185	0.68	0/250
10	x	0.28	0/185	0.68	0/250
11	B	0.46	0/3753	0.62	0/5080
11	C	0.56	0/3793	0.71	2/5137 (0.0%)
11	K	0.50	0/3798	0.65	0/5143
11	W	0.46	0/3753	0.62	0/5080
11	X	0.56	0/3793	0.71	2/5137 (0.0%)
11	n	0.50	0/3798	0.65	0/5143
12	D	0.55	0/3605	0.67	0/4889
12	E	0.44	0/3592	0.59	1/4870 (0.0%)
12	F	0.52	0/3599	0.69	0/4881
12	Y	0.55	0/3605	0.67	0/4889
12	Z	0.44	0/3592	0.59	1/4870 (0.0%)
12	c	0.52	0/3599	0.69	0/4881
13	G	0.44	0/2055	0.58	0/2766
13	j	0.44	0/2055	0.58	0/2766
14	H	0.46	0/759	0.59	0/1040
14	l	0.46	0/759	0.59	0/1040
15	I	0.48	0/326	0.80	2/445 (0.4%)
15	m	0.48	0/326	0.79	2/445 (0.4%)
16	O	0.61	0/793	0.99	2/1101 (0.2%)
16	o	0.62	0/793	0.99	2/1101 (0.2%)
All	All	0.48	0/74640	0.66	30/101276 (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
4	b	0	1
4	q	0	1
8	g	0	2
8	u	0	2
15	I	0	1
15	m	0	1
16	O	0	1
16	o	0	1
All	All	0	10

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	r	170	LEU	CA-CB-CG	7.82	133.28	115.30
5	d	170	LEU	CA-CB-CG	7.81	133.25	115.30
2	V	26	LEU	CA-CB-CG	7.74	133.09	115.30
2	A	26	LEU	CA-CB-CG	7.73	133.08	115.30
15	m	56	PRO	N-CA-CB	6.38	110.96	103.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	I	9	SER	Peptide
16	O	50	ASN	Peptide
4	b	186	ASN	Peptide
8	g	80	UNK	Peptide,Mainchain
4	q	186	ASN	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	73/76 (96%)	73 (100%)	0	0	100	100
1	1	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	3	72/76 (95%)	72 (100%)	0	0	100	100
1	4	73/76 (96%)	73 (100%)	0	0	100	100
1	5	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
1	6	72/76 (95%)	72 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7	71/76 (93%)	71 (100%)	0	0	100	100
1	8	73/76 (96%)	73 (100%)	0	0	100	100
1	9	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
1	J	73/76 (96%)	73 (100%)	0	0	100	100
1	L	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	M	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	N	72/76 (95%)	72 (100%)	0	0	100	100
1	P	73/76 (96%)	73 (100%)	0	0	100	100
1	Q	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
1	R	72/76 (95%)	72 (100%)	0	0	100	100
1	S	71/76 (93%)	71 (100%)	0	0	100	100
1	T	73/76 (96%)	73 (100%)	0	0	100	100
1	U	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
2	A	46/48 (96%)	43 (94%)	2 (4%)	1 (2%)	5	32
2	V	46/48 (96%)	43 (94%)	2 (4%)	1 (2%)	5	32
3	a	247/249 (99%)	228 (92%)	19 (8%)	0	100	100
3	p	247/249 (99%)	228 (92%)	19 (8%)	0	100	100
4	b	196/209 (94%)	186 (95%)	6 (3%)	4 (2%)	6	34
4	q	196/209 (94%)	186 (95%)	6 (3%)	4 (2%)	6	34
5	d	153/173 (88%)	145 (95%)	7 (5%)	1 (1%)	19	53
5	r	153/173 (88%)	145 (95%)	7 (5%)	1 (1%)	19	53
7	f	80/95 (84%)	70 (88%)	9 (11%)	1 (1%)	10	41
7	t	80/95 (84%)	70 (88%)	9 (11%)	1 (1%)	10	41
9	i	57/59 (97%)	50 (88%)	7 (12%)	0	100	100
9	w	57/59 (97%)	50 (88%)	7 (12%)	0	100	100
10	k	22/68 (32%)	19 (86%)	3 (14%)	0	100	100
10	x	22/68 (32%)	19 (86%)	3 (14%)	0	100	100
11	B	486/510 (95%)	439 (90%)	45 (9%)	2 (0%)	30	63
11	C	496/510 (97%)	449 (90%)	44 (9%)	3 (1%)	22	55
11	K	495/510 (97%)	434 (88%)	56 (11%)	5 (1%)	13	46
11	W	486/510 (95%)	439 (90%)	45 (9%)	2 (0%)	30	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	X	496/510 (97%)	449 (90%)	44 (9%)	3 (1%)	22	55
11	n	495/510 (97%)	434 (88%)	56 (11%)	5 (1%)	13	46
12	D	468/478 (98%)	429 (92%)	37 (8%)	2 (0%)	30	63
12	E	466/478 (98%)	424 (91%)	36 (8%)	6 (1%)	10	41
12	F	467/478 (98%)	417 (89%)	42 (9%)	8 (2%)	7	37
12	Y	468/478 (98%)	429 (92%)	37 (8%)	2 (0%)	30	63
12	Z	466/478 (98%)	424 (91%)	36 (8%)	6 (1%)	10	41
12	c	467/478 (98%)	417 (89%)	42 (9%)	8 (2%)	7	37
13	G	261/278 (94%)	229 (88%)	25 (10%)	7 (3%)	4	28
13	j	261/278 (94%)	230 (88%)	24 (9%)	7 (3%)	4	28
14	H	109/138 (79%)	89 (82%)	15 (14%)	5 (5%)	2	18
14	l	109/138 (79%)	89 (82%)	15 (14%)	5 (5%)	2	18
15	I	42/61 (69%)	27 (64%)	9 (21%)	6 (14%)	0	3
15	m	42/61 (69%)	27 (64%)	9 (21%)	6 (14%)	0	3
16	O	157/195 (80%)	126 (80%)	24 (15%)	7 (4%)	2	18
16	o	157/195 (80%)	126 (80%)	24 (15%)	7 (4%)	2	18
All	All	9946/10594 (94%)	9045 (91%)	785 (8%)	116 (1%)	14	43

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	b	187	PRO
7	f	14	ASN
12	D	29	GLU
12	F	28	SER
13	G	152	SER

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	0	55/56 (98%)	55 (100%)	0	100	100
1	1	55/56 (98%)	55 (100%)	0	100	100
1	2	55/56 (98%)	55 (100%)	0	100	100
1	3	54/56 (96%)	54 (100%)	0	100	100
1	4	55/56 (98%)	55 (100%)	0	100	100
1	5	55/56 (98%)	54 (98%)	1 (2%)	54	74
1	6	54/56 (96%)	54 (100%)	0	100	100
1	7	54/56 (96%)	54 (100%)	0	100	100
1	8	55/56 (98%)	55 (100%)	0	100	100
1	9	54/56 (96%)	54 (100%)	0	100	100
1	J	55/56 (98%)	55 (100%)	0	100	100
1	L	55/56 (98%)	55 (100%)	0	100	100
1	M	55/56 (98%)	55 (100%)	0	100	100
1	N	54/56 (96%)	54 (100%)	0	100	100
1	P	55/56 (98%)	55 (100%)	0	100	100
1	Q	55/56 (98%)	54 (98%)	1 (2%)	54	74
1	R	54/56 (96%)	54 (100%)	0	100	100
1	S	54/56 (96%)	54 (100%)	0	100	100
1	T	55/56 (98%)	55 (100%)	0	100	100
1	U	54/56 (96%)	54 (100%)	0	100	100
2	A	47/47 (100%)	47 (100%)	0	100	100
2	V	47/47 (100%)	47 (100%)	0	100	100
3	a	217/217 (100%)	216 (100%)	1 (0%)	86	93
3	p	217/217 (100%)	216 (100%)	1 (0%)	86	93
4	b	48/182 (26%)	48 (100%)	0	100	100
4	q	48/182 (26%)	48 (100%)	0	100	100
5	d	42/158 (27%)	40 (95%)	2 (5%)	21	51
5	r	42/158 (27%)	40 (95%)	2 (5%)	21	51
7	f	46/76 (60%)	46 (100%)	0	100	100
7	t	46/76 (60%)	46 (100%)	0	100	100
9	i	49/49 (100%)	49 (100%)	0	100	100
9	w	49/49 (100%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	k	18/57 (32%)	18 (100%)	0	100	100
10	x	18/57 (32%)	18 (100%)	0	100	100
11	B	384/412 (93%)	348 (91%)	36 (9%)	7	30
11	C	384/412 (93%)	356 (93%)	28 (7%)	11	38
11	K	384/412 (93%)	365 (95%)	19 (5%)	21	50
11	W	384/412 (93%)	348 (91%)	36 (9%)	7	30
11	X	384/412 (93%)	356 (93%)	28 (7%)	11	38
11	n	384/412 (93%)	365 (95%)	19 (5%)	21	50
12	D	380/384 (99%)	360 (95%)	20 (5%)	19	48
12	E	378/384 (98%)	357 (94%)	21 (6%)	17	47
12	F	379/384 (99%)	359 (95%)	20 (5%)	19	48
12	Y	380/384 (99%)	360 (95%)	20 (5%)	19	48
12	Z	378/384 (98%)	357 (94%)	21 (6%)	17	47
12	c	379/384 (99%)	359 (95%)	20 (5%)	19	48
13	G	218/236 (92%)	191 (88%)	27 (12%)	4	20
13	j	218/236 (92%)	191 (88%)	27 (12%)	4	20
14	H	54/112 (48%)	39 (72%)	15 (28%)	0	2
14	l	54/112 (48%)	39 (72%)	15 (28%)	0	2
15	I	23/48 (48%)	20 (87%)	3 (13%)	3	19
15	m	23/48 (48%)	20 (87%)	3 (13%)	3	19
All	All	7194/8260 (87%)	6808 (95%)	386 (5%)	21	48

5 of 386 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	W	221	THR
12	Y	204	THR
11	W	318	GLU
11	X	210	GLN
12	Z	89	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
14	H	44	ASN
13	j	90	GLN
11	n	407	GLN
13	j	54	ASN
15	m	30	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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	$\# Z > 2$
18	ANP	D	501	19	29,33,33	3.05	8 (27%)	31,52,52	1.81	7 (22%)
18	ANP	F	501	19	29,33,33	3.04	8 (27%)	31,52,52	2.04	8 (25%)
18	ANP	W	601	19	29,33,33	3.01	8 (27%)	31,52,52	1.56	6 (19%)
18	ANP	C	601	19	29,33,33	2.87	8 (27%)	31,52,52	2.45	8 (25%)
18	ANP	B	601	19	29,33,33	3.01	7 (24%)	31,52,52	1.56	6 (19%)
18	ANP	X	601	19	29,33,33	2.87	8 (27%)	31,52,52	2.45	8 (25%)
18	ANP	Y	501	19	29,33,33	3.06	8 (27%)	31,52,52	1.81	7 (22%)
18	ANP	n	601	19	29,33,33	2.96	8 (27%)	31,52,52	1.65	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	ANP	K	601	19	29,33,33	2.95	8 (27%)	31,52,52	1.65	8 (25%)
18	ANP	c	501	19	29,33,33	3.04	8 (27%)	31,52,52	2.04	8 (25%)

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
18	ANP	D	501	19	-	3/14/38/38	0/3/3/3
18	ANP	F	501	19	-	1/14/38/38	0/3/3/3
18	ANP	W	601	19	-	3/14/38/38	0/3/3/3
18	ANP	C	601	19	-	3/14/38/38	0/3/3/3
18	ANP	B	601	19	-	3/14/38/38	0/3/3/3
18	ANP	X	601	19	-	3/14/38/38	0/3/3/3
18	ANP	Y	501	19	-	3/14/38/38	0/3/3/3
18	ANP	n	601	19	-	1/14/38/38	0/3/3/3
18	ANP	K	601	19	-	1/14/38/38	0/3/3/3
18	ANP	c	501	19	-	1/14/38/38	0/3/3/3

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	n	601	ANP	PG-O1G	9.91	1.61	1.46
18	K	601	ANP	PG-O1G	9.86	1.61	1.46
18	Y	501	ANP	PG-O1G	9.25	1.60	1.46
18	D	501	ANP	PG-O1G	9.22	1.60	1.46
18	X	601	ANP	PG-O1G	9.18	1.60	1.46

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	X	601	ANP	O4'-C1'-N9	9.16	120.89	108.75
18	C	601	ANP	O4'-C1'-N9	9.12	120.83	108.75
18	c	501	ANP	O1B-PB-N3B	-5.49	103.68	111.77
18	F	501	ANP	O1B-PB-N3B	-5.47	103.71	111.77
18	C	601	ANP	O1G-PG-N3B	-5.20	104.11	111.77

There are no chirality outliers.

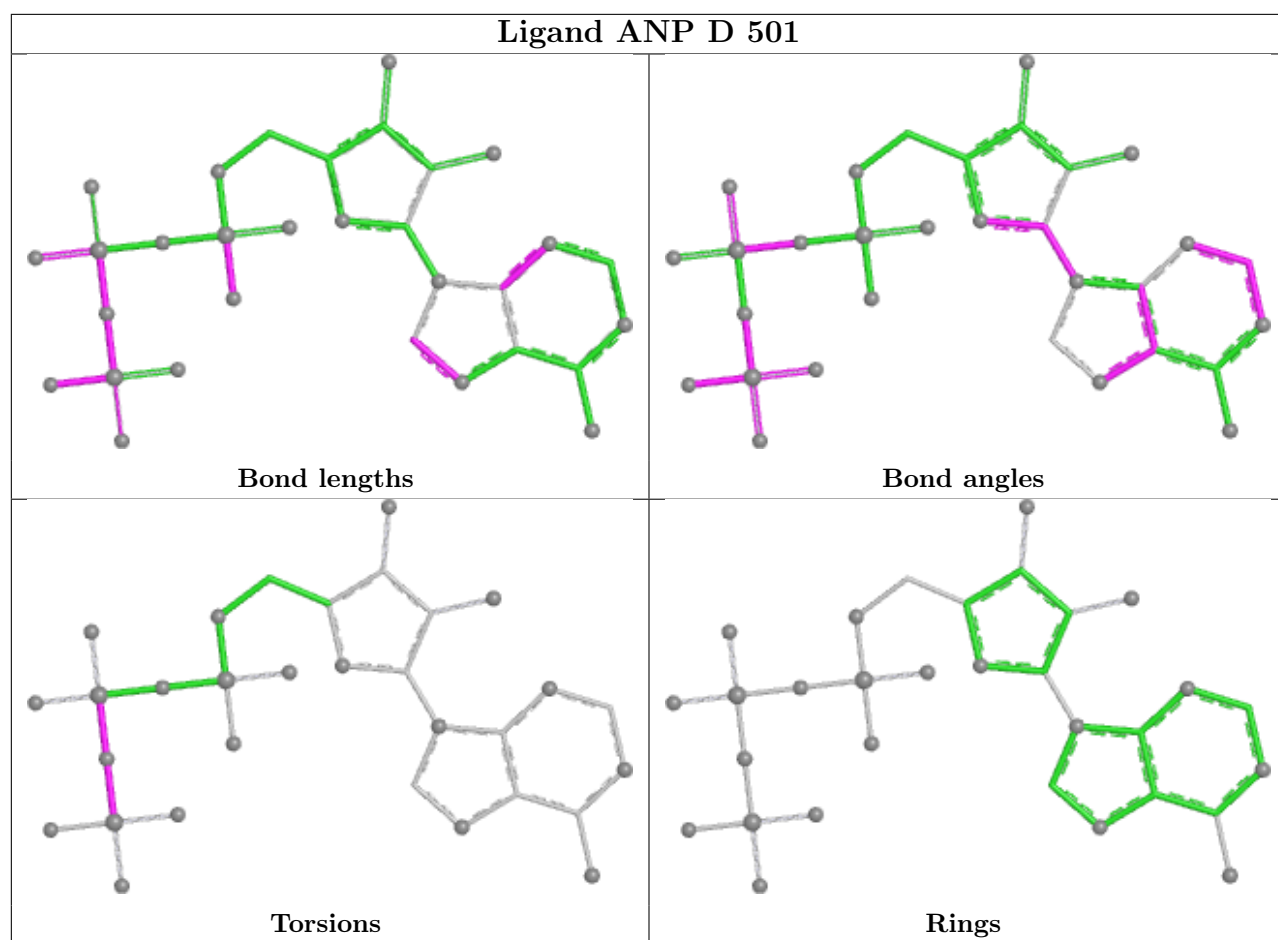
5 of 22 torsion outliers are listed below:

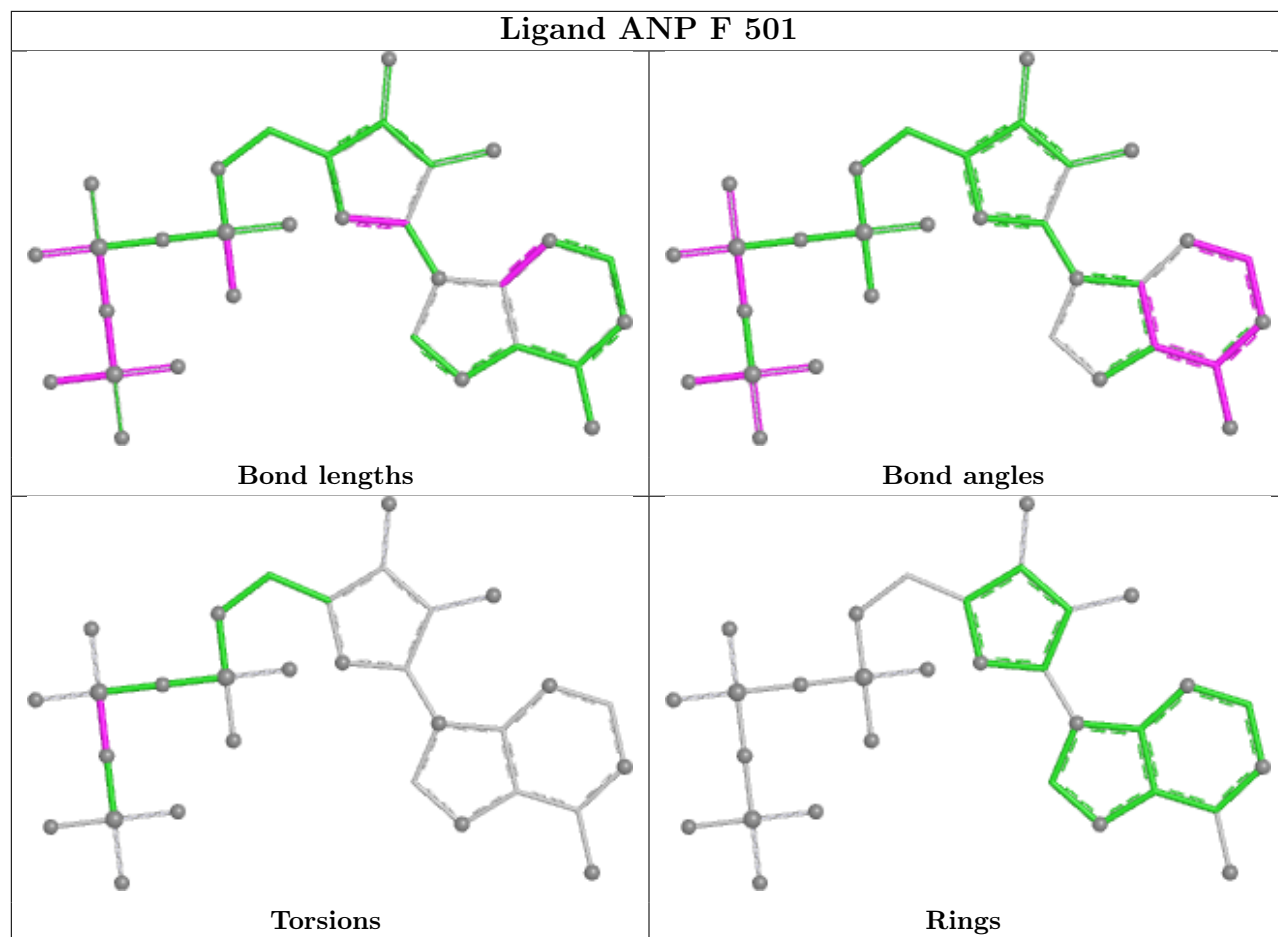
Mol	Chain	Res	Type	Atoms
18	K	601	ANP	PG-N3B-PB-O1B
18	B	601	ANP	PG-N3B-PB-O1B
18	C	601	ANP	PB-N3B-PG-O1G
18	C	601	ANP	PG-N3B-PB-O1B
18	D	501	ANP	PB-N3B-PG-O1G

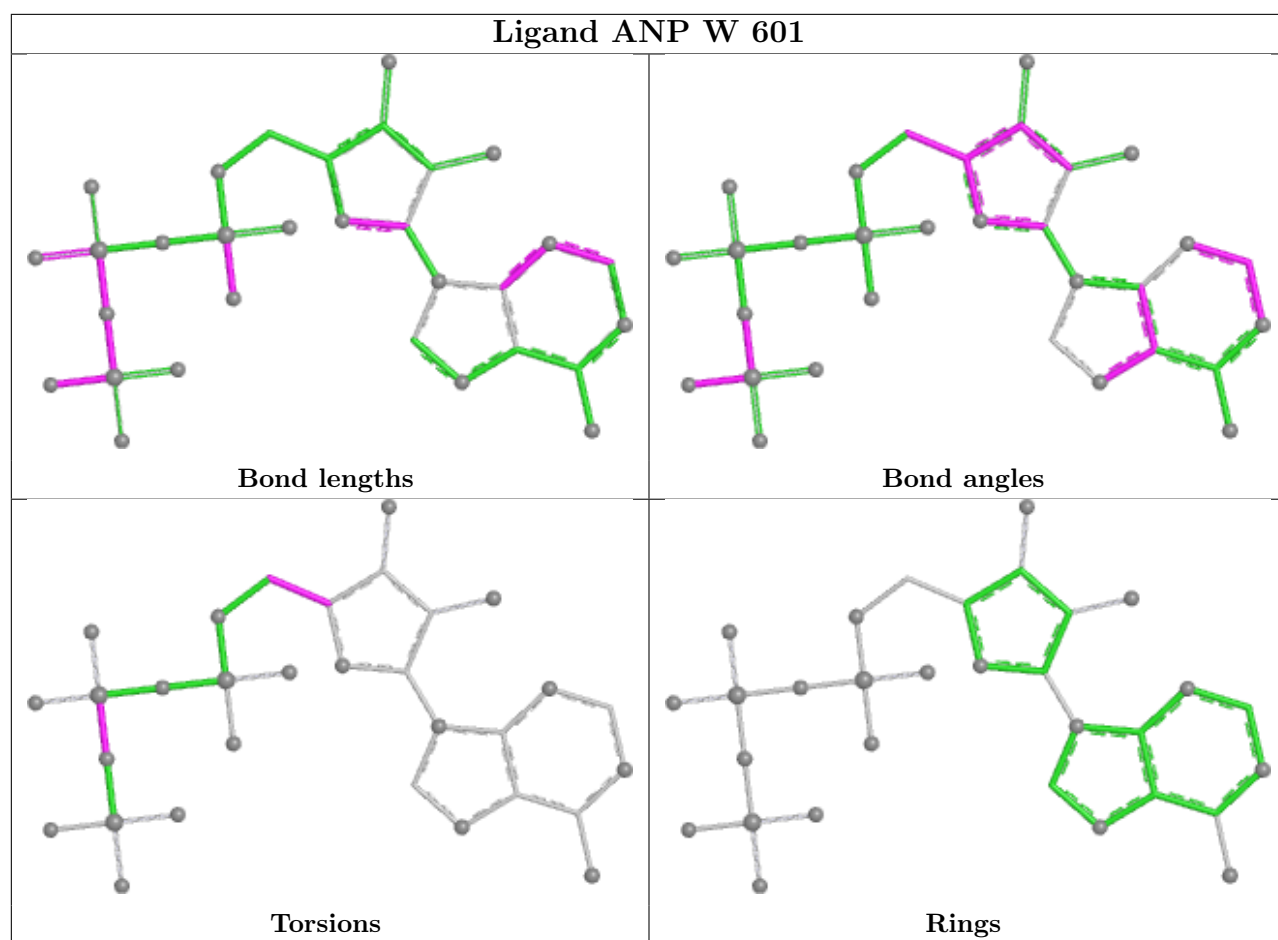
There are no ring outliers.

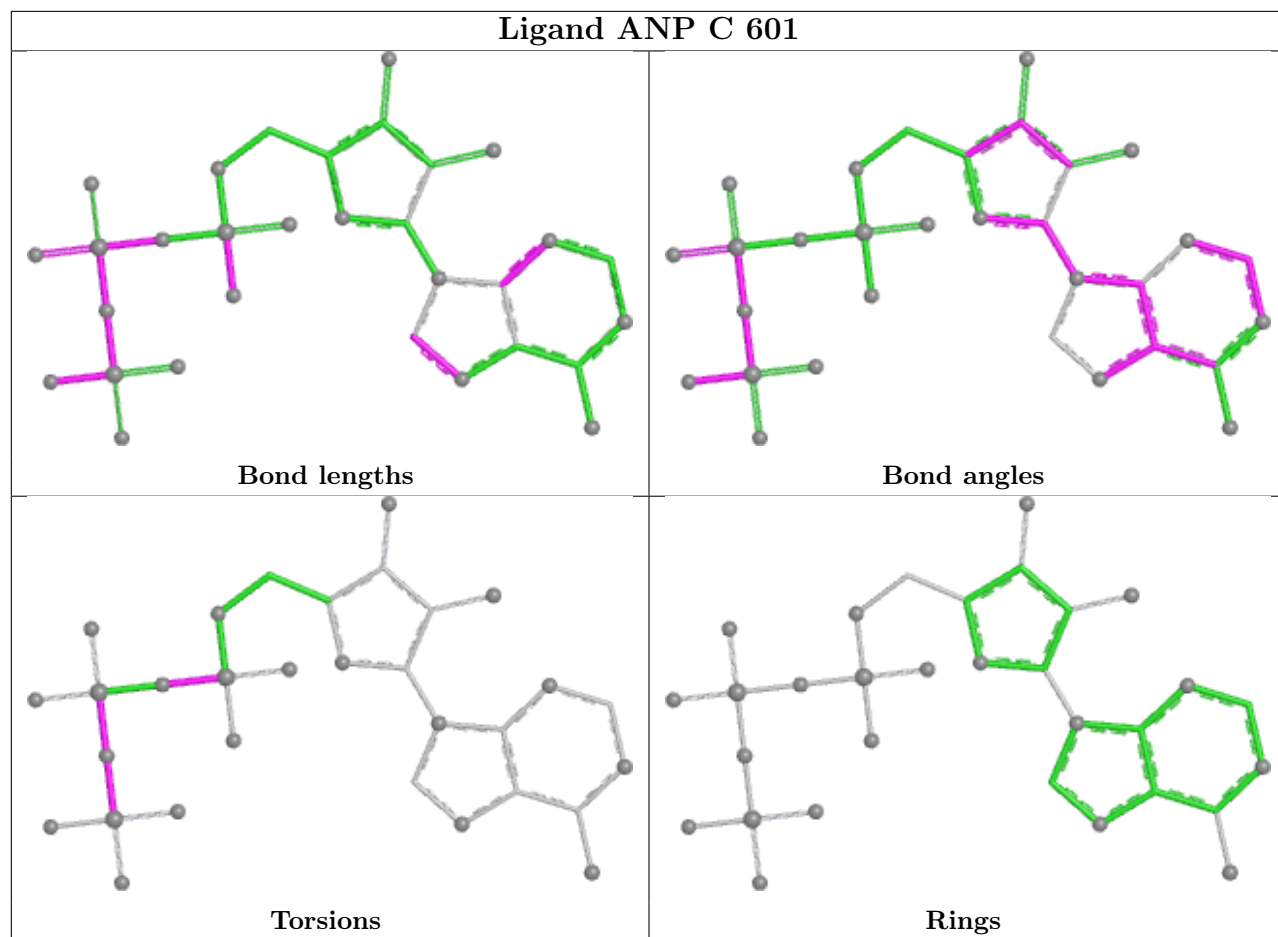
No monomer is involved in short contacts.

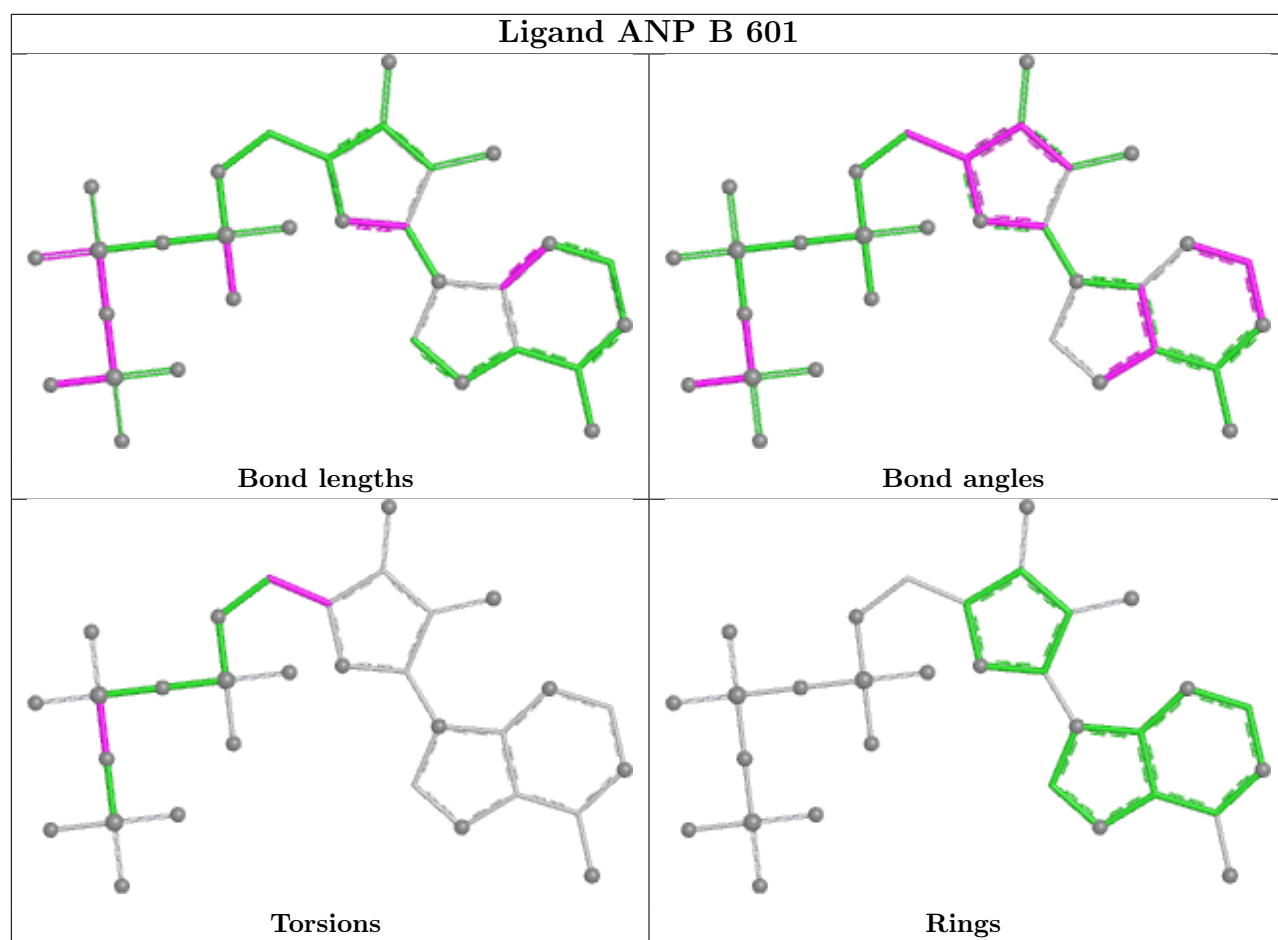
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

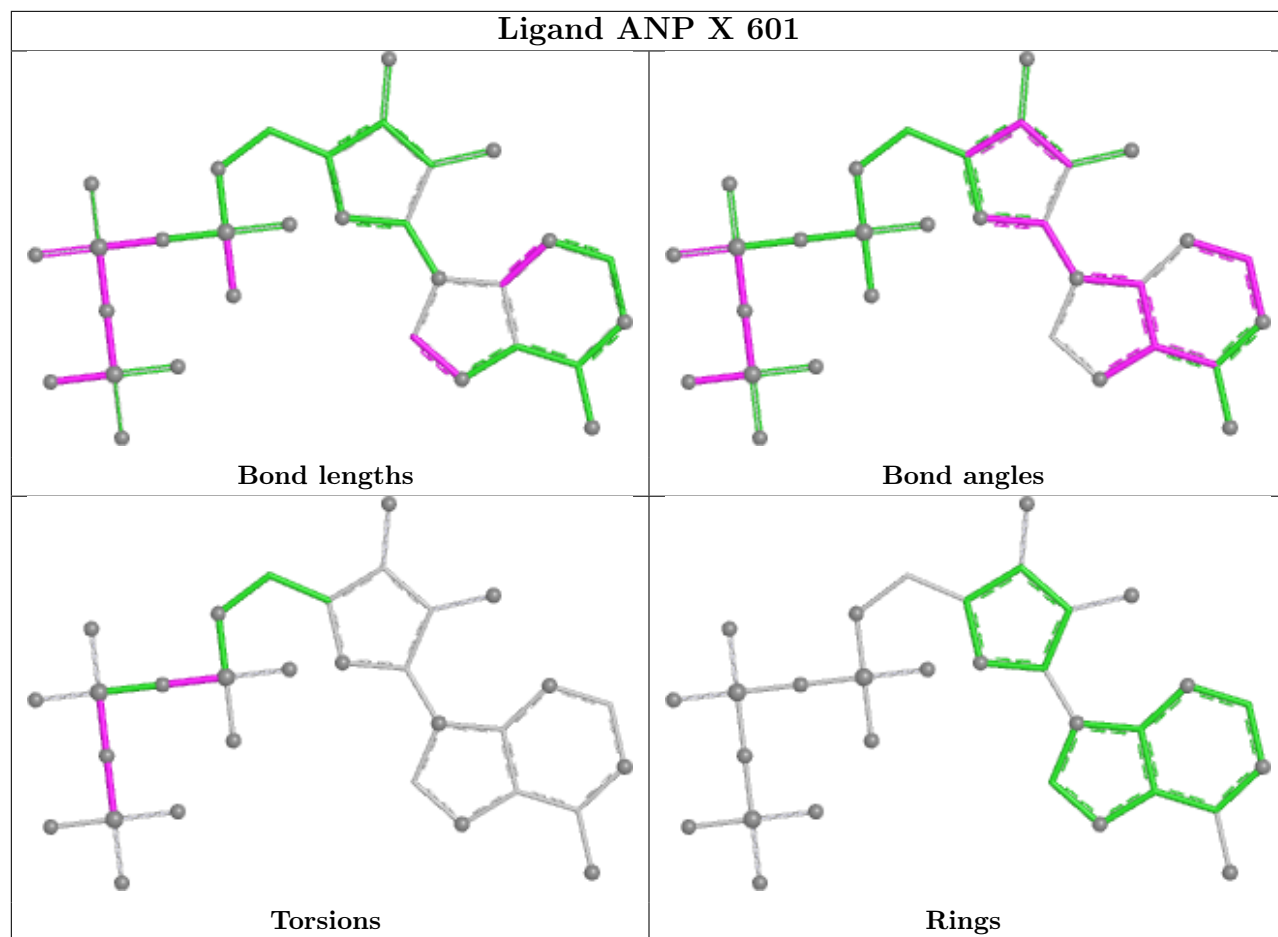


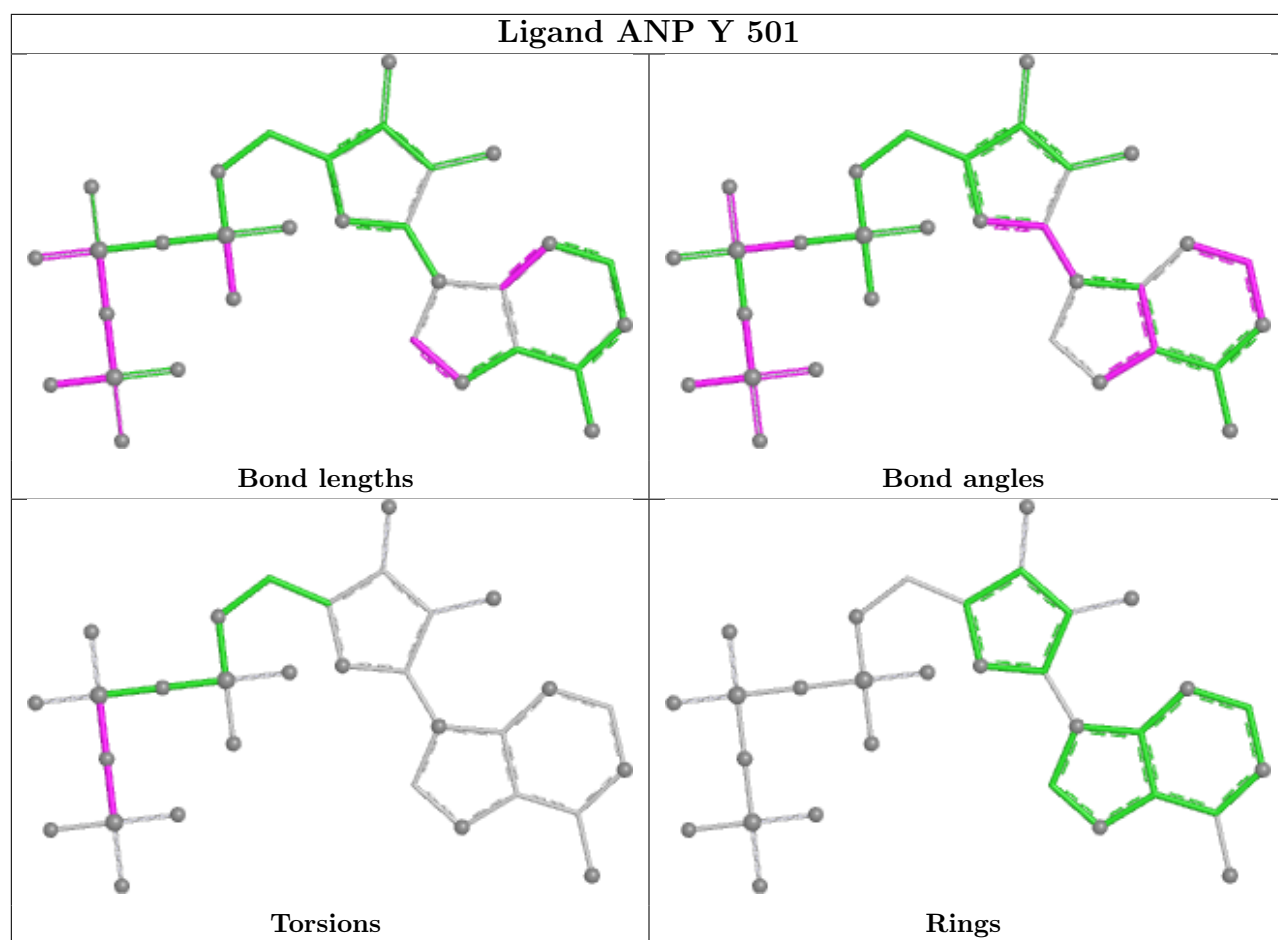


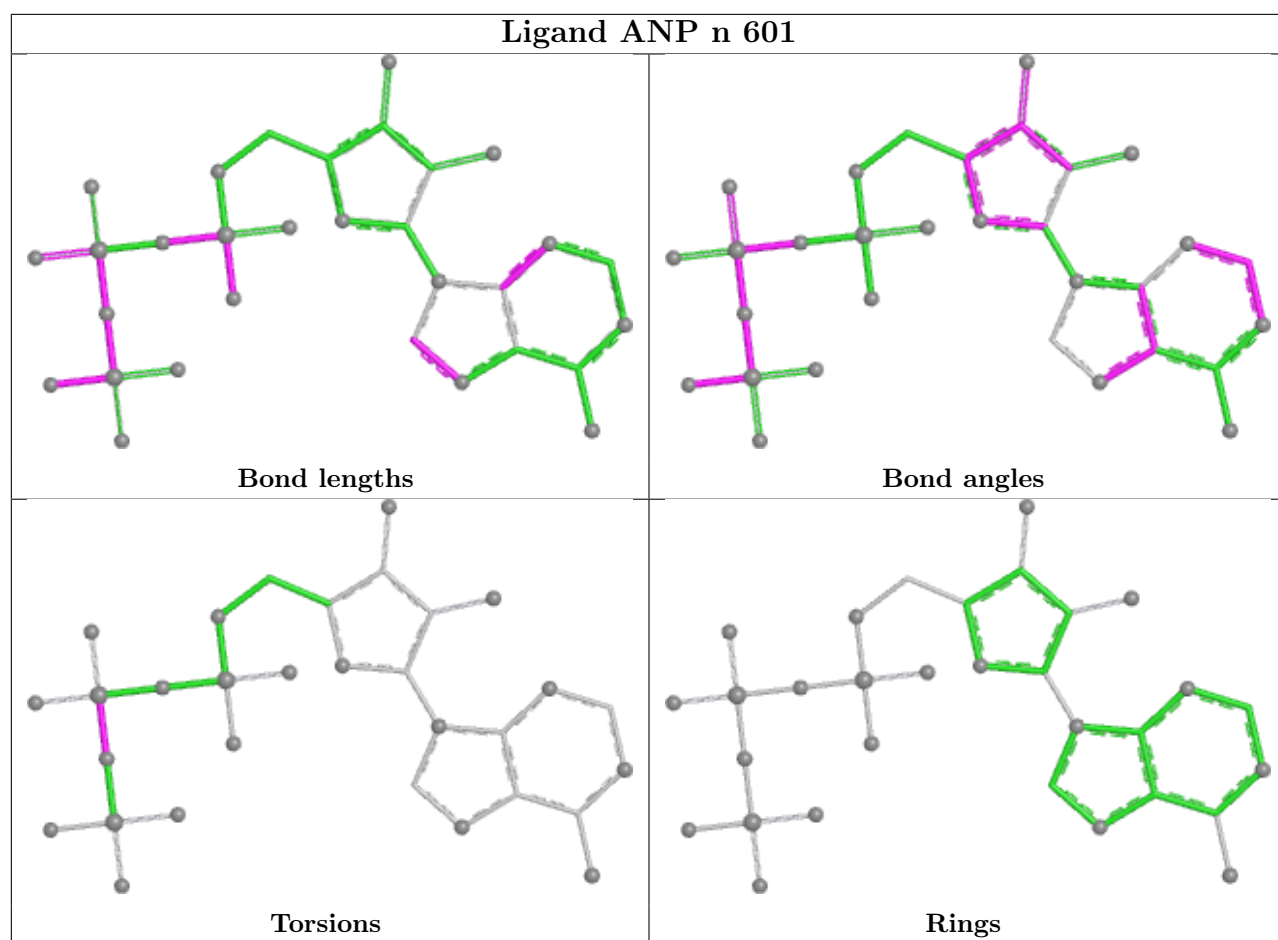


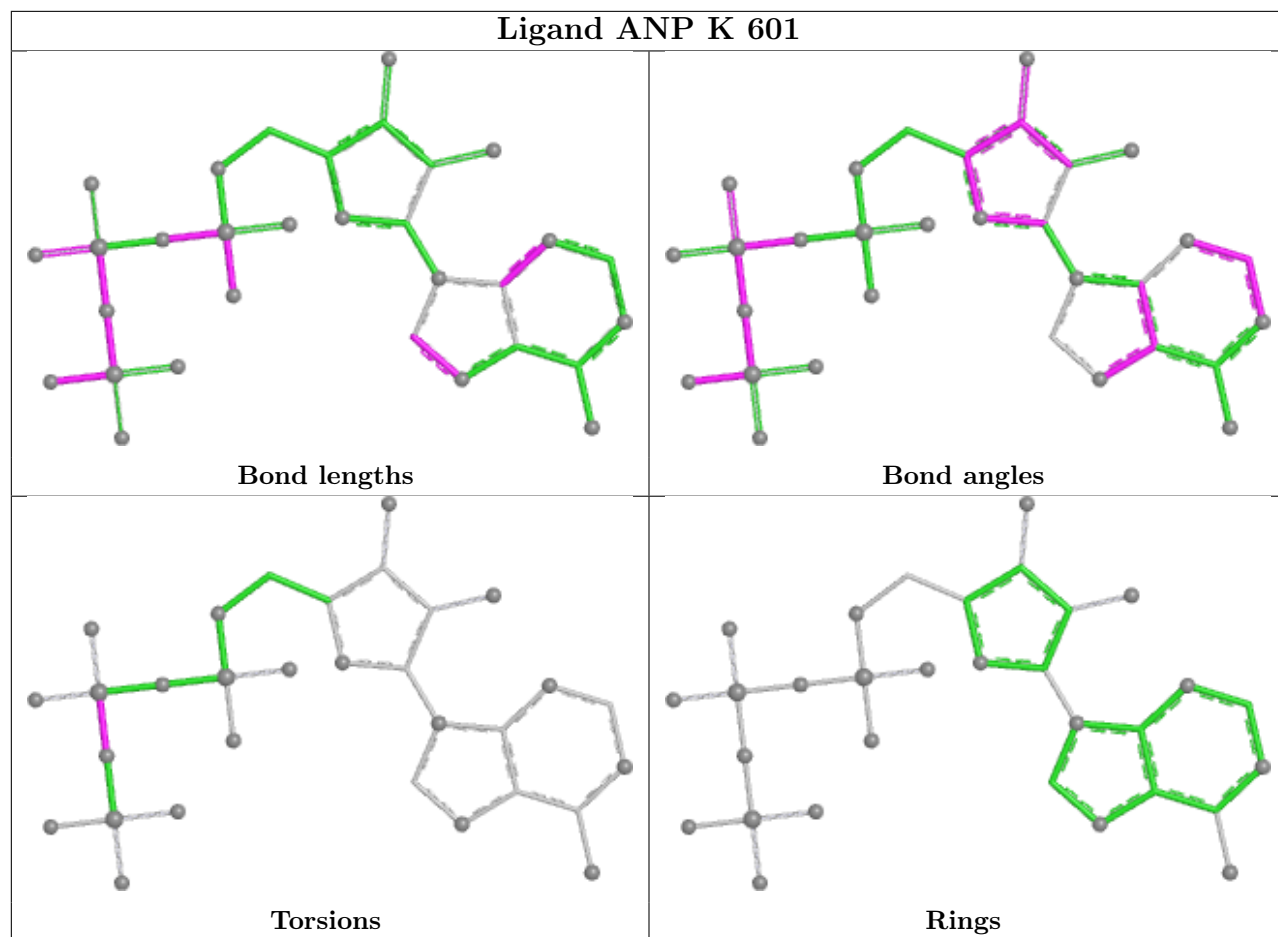


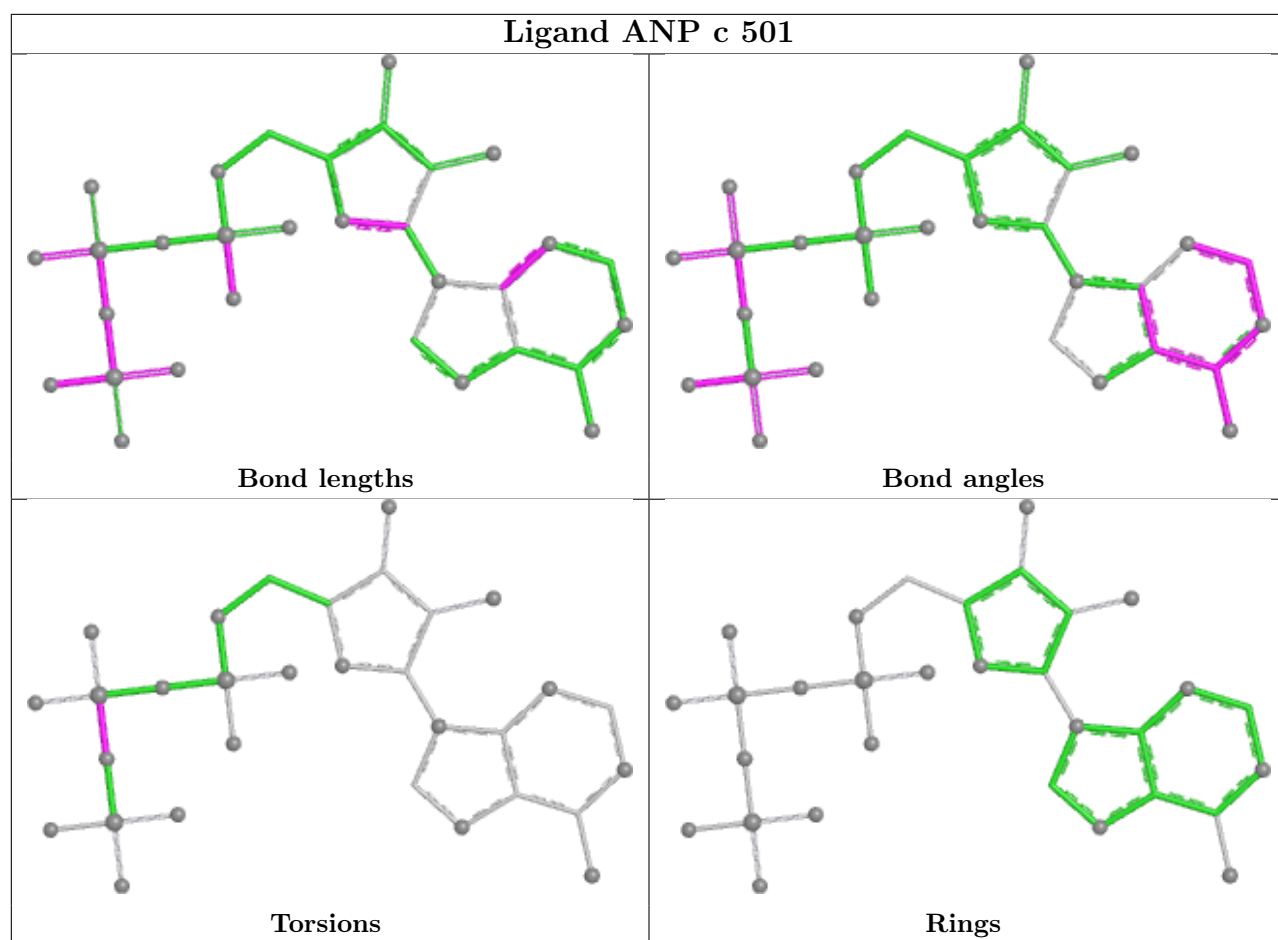












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

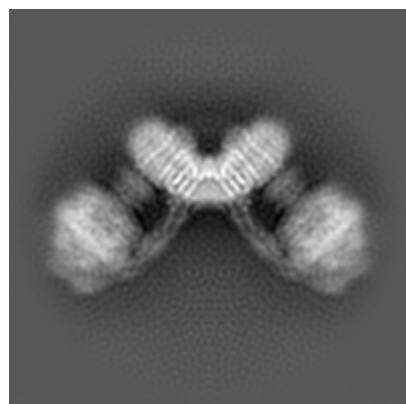
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7067. These allow visual inspection of the internal detail of the map and identification of artifacts.

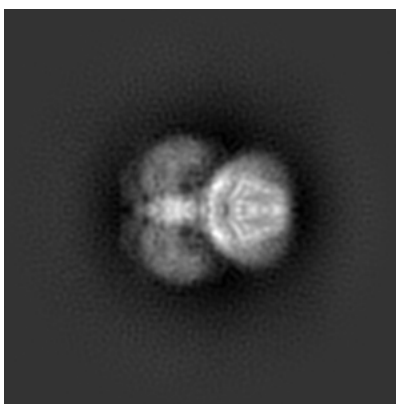
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

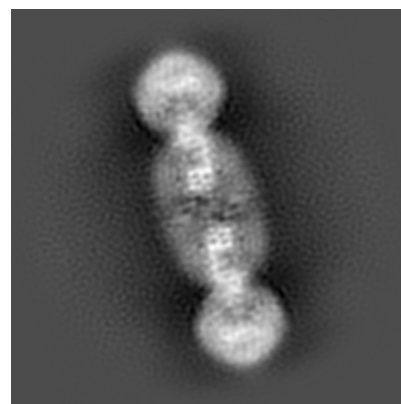
6.1.1 Primary map



X

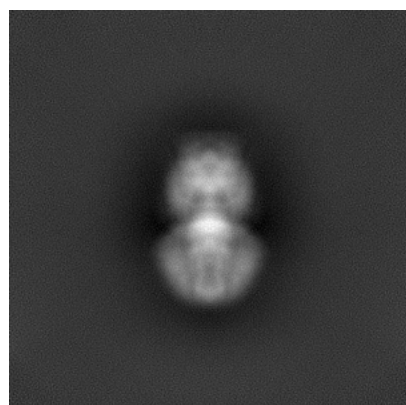


Y

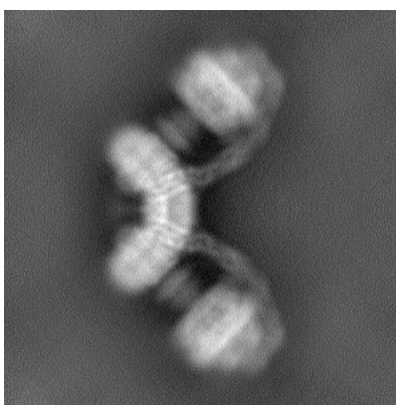


Z

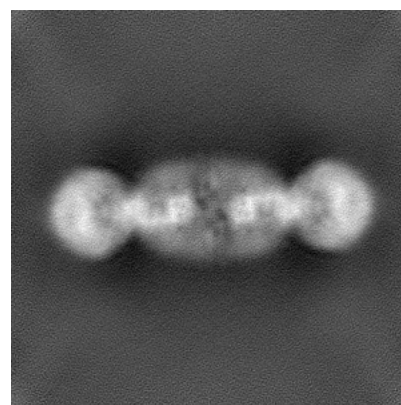
6.1.2 Raw map



X



Y

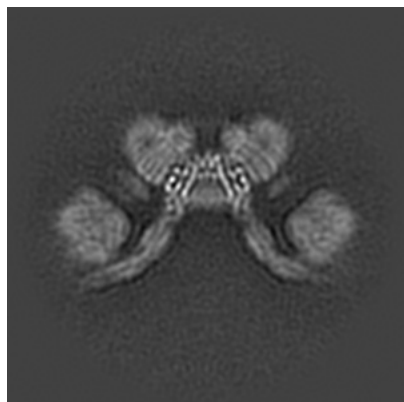


Z

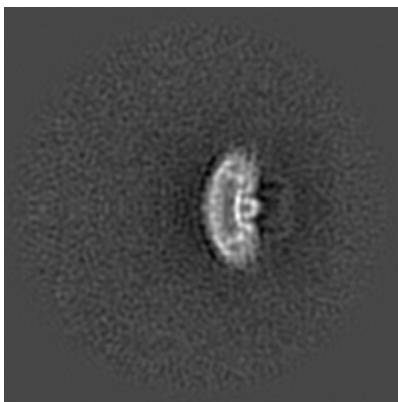
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

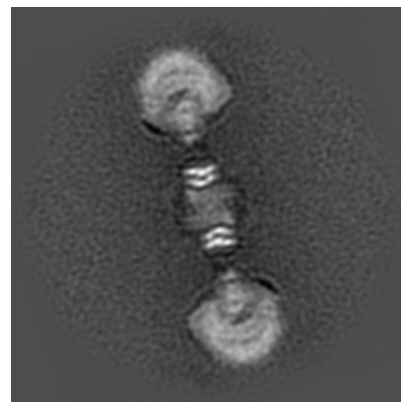
6.2.1 Primary map



X Index: 160

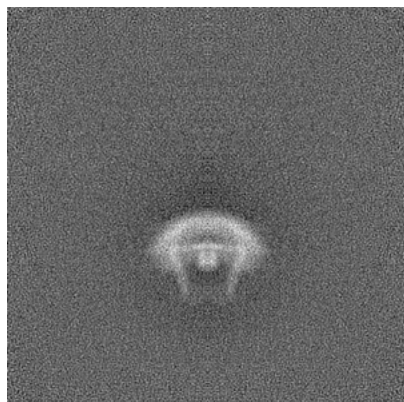


Y Index: 160

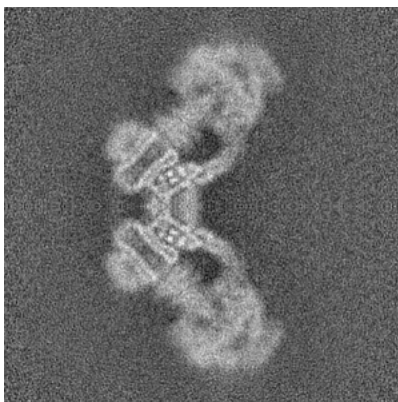


Z Index: 160

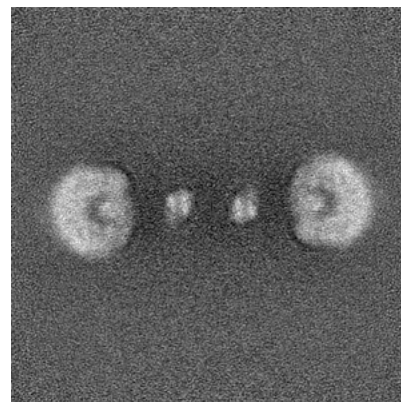
6.2.2 Raw map



X Index: 160



Y Index: 160

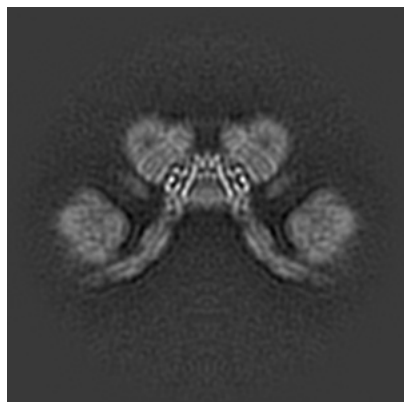


Z Index: 160

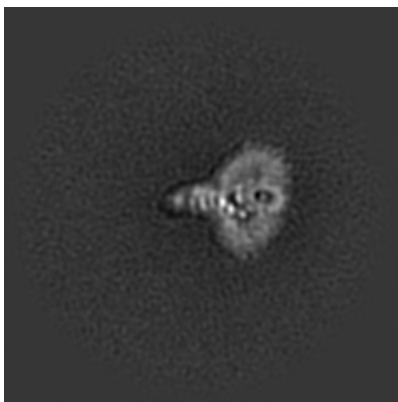
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

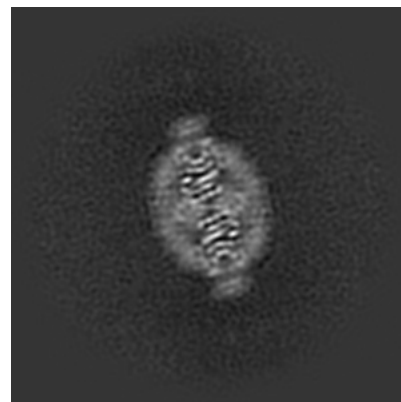
6.3.1 Primary map



X Index: 159

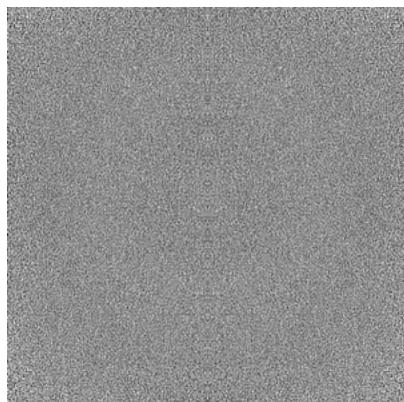


Y Index: 130

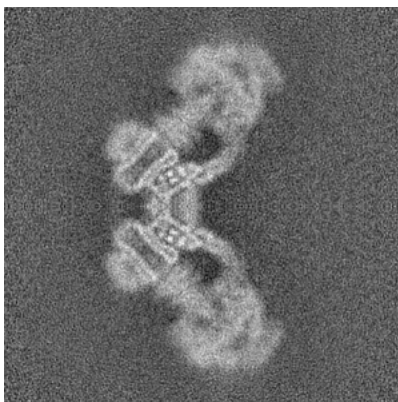


Z Index: 188

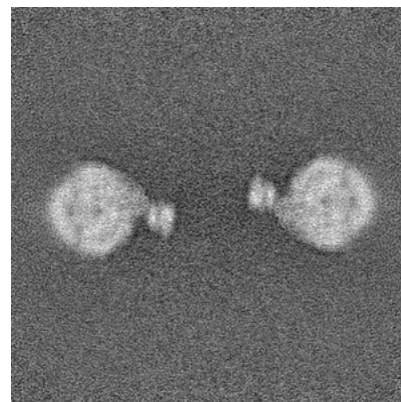
6.3.2 Raw map



X Index: 0



Y Index: 160

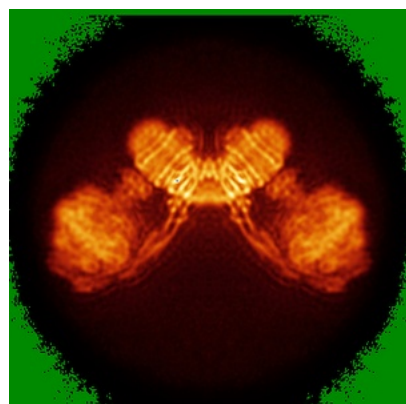


Z Index: 181

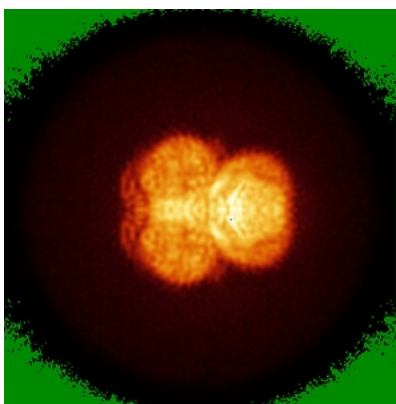
The images above show the largest variance slices of the map in three orthogonal directions.

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

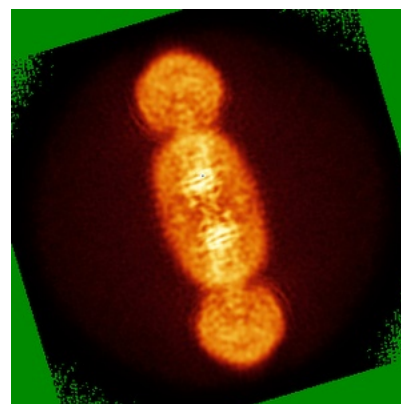
6.4.1 Primary map



X

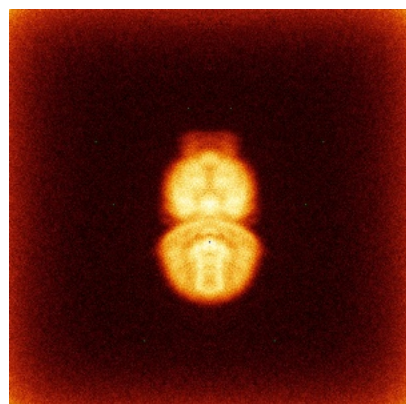


Y

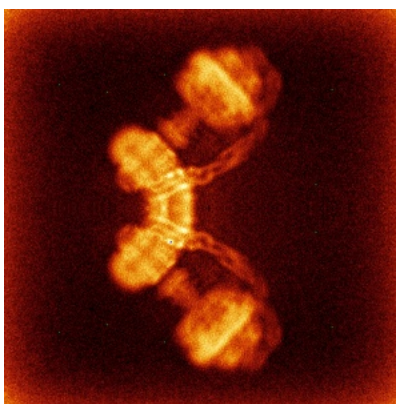


Z

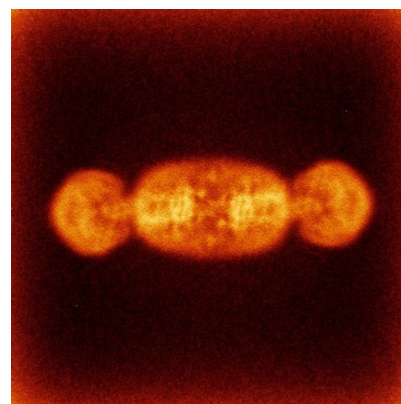
6.4.2 Raw map



X



Y

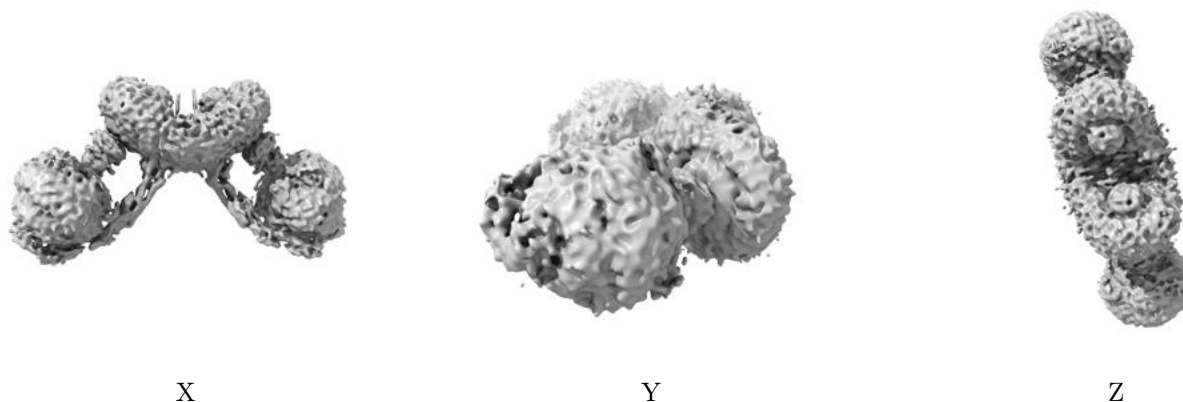


Z

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

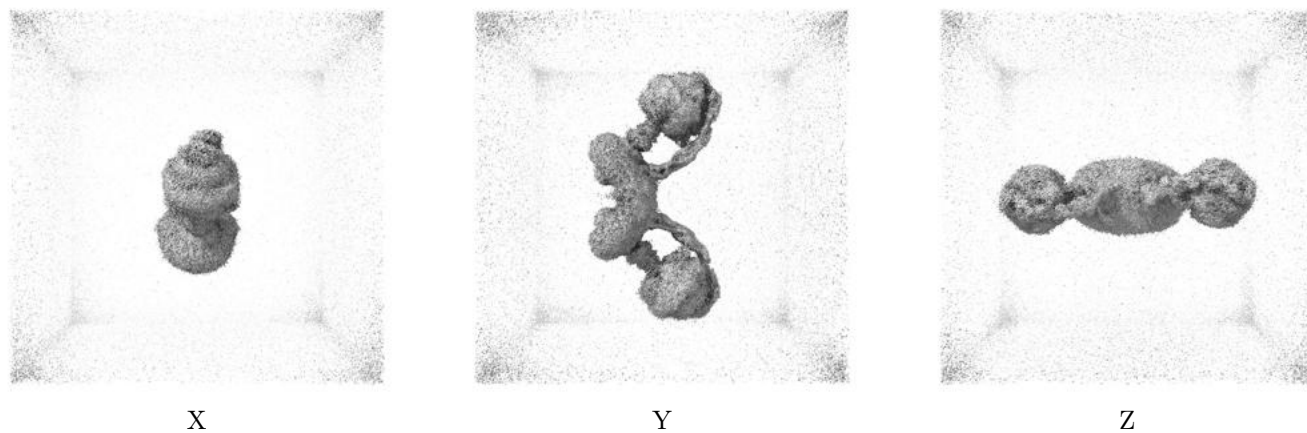
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.156. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

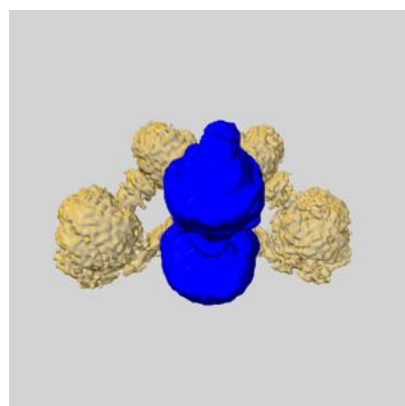
6.6 Mask visualisation [i](#)

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

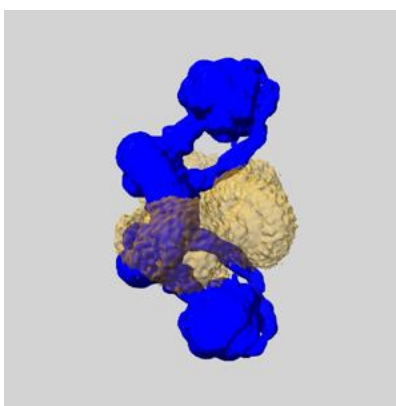
A mask typically either:

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

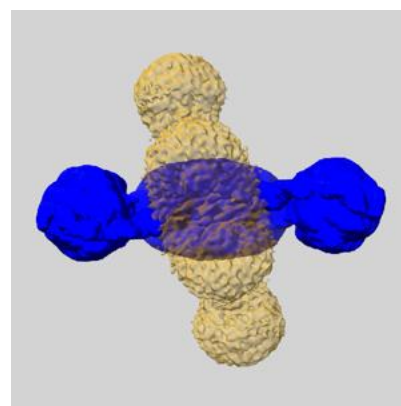
6.6.1 emd_7067_msk_1.map [i](#)



X



Y

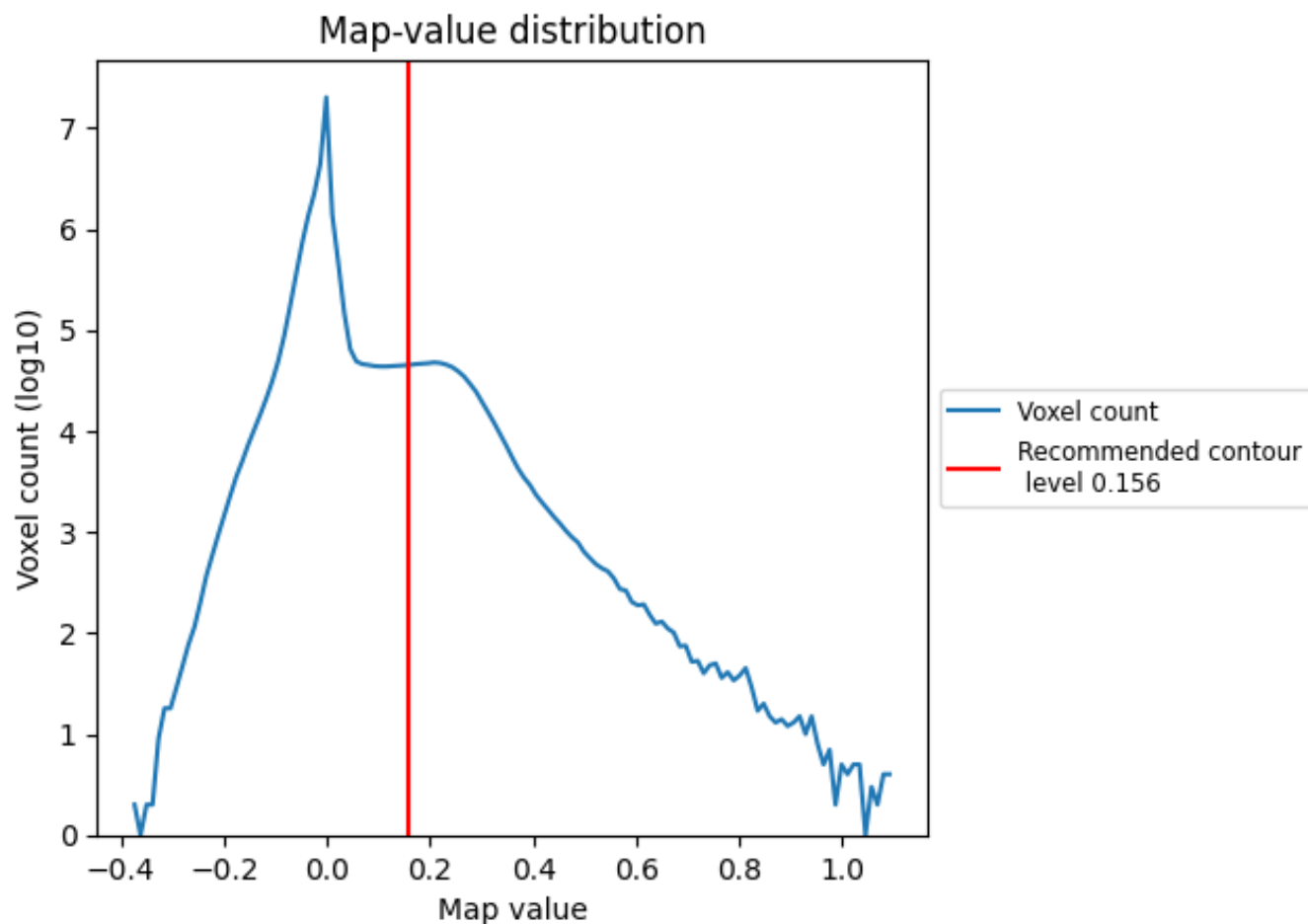


Z

7 Map analysis [i](#)

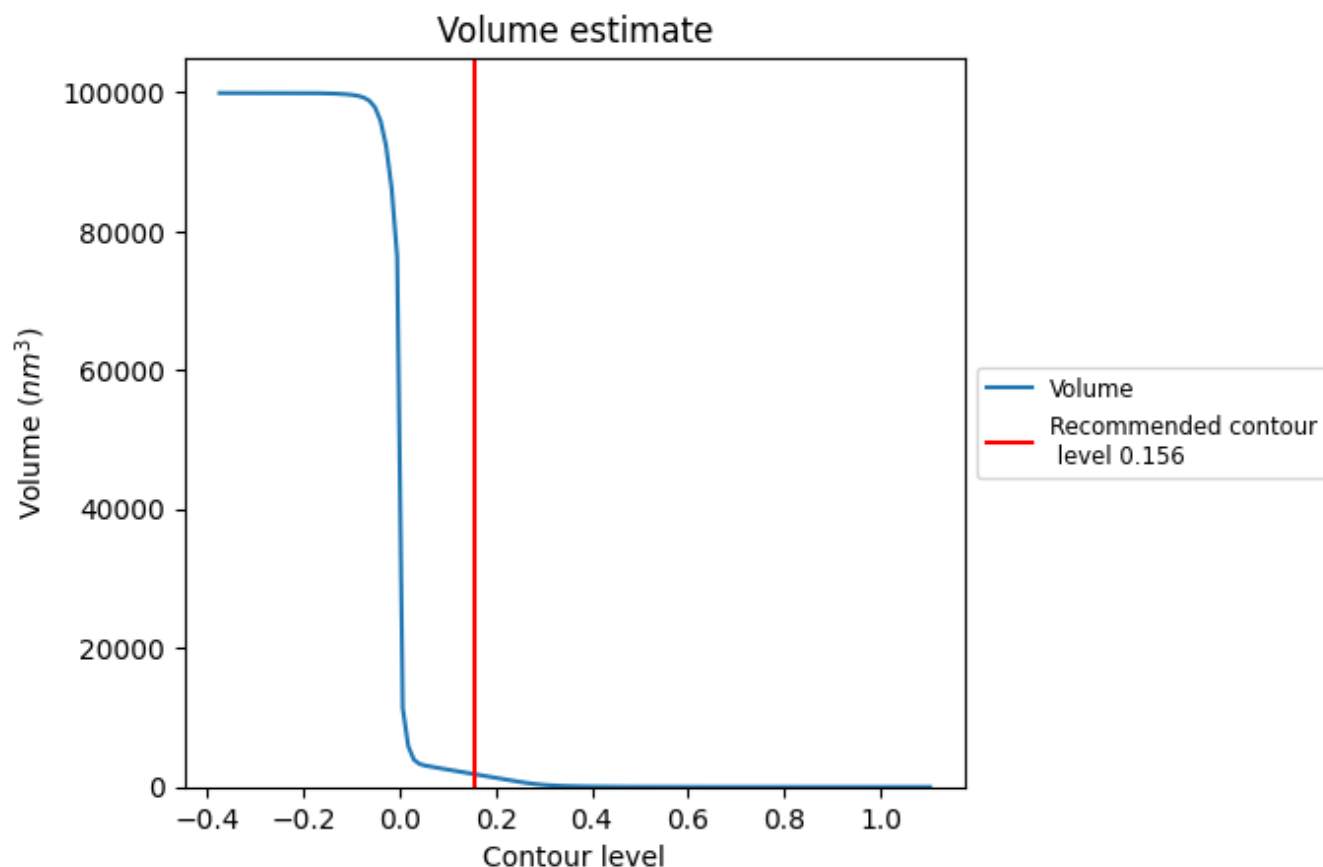
This section contains the results of statistical analysis of the map.

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.

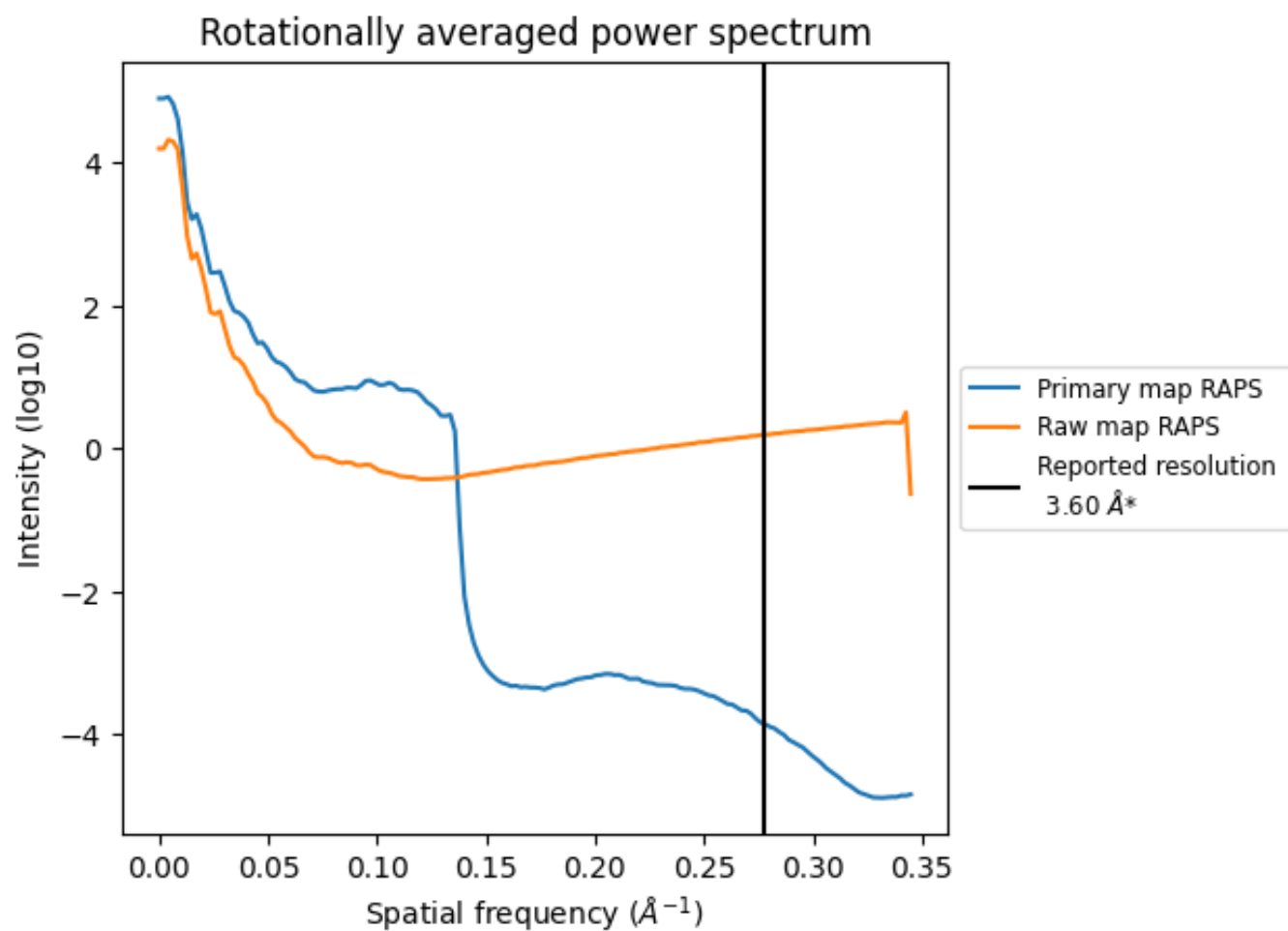
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1866 nm³; this corresponds to an approximate mass of 1686 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 ⓘ

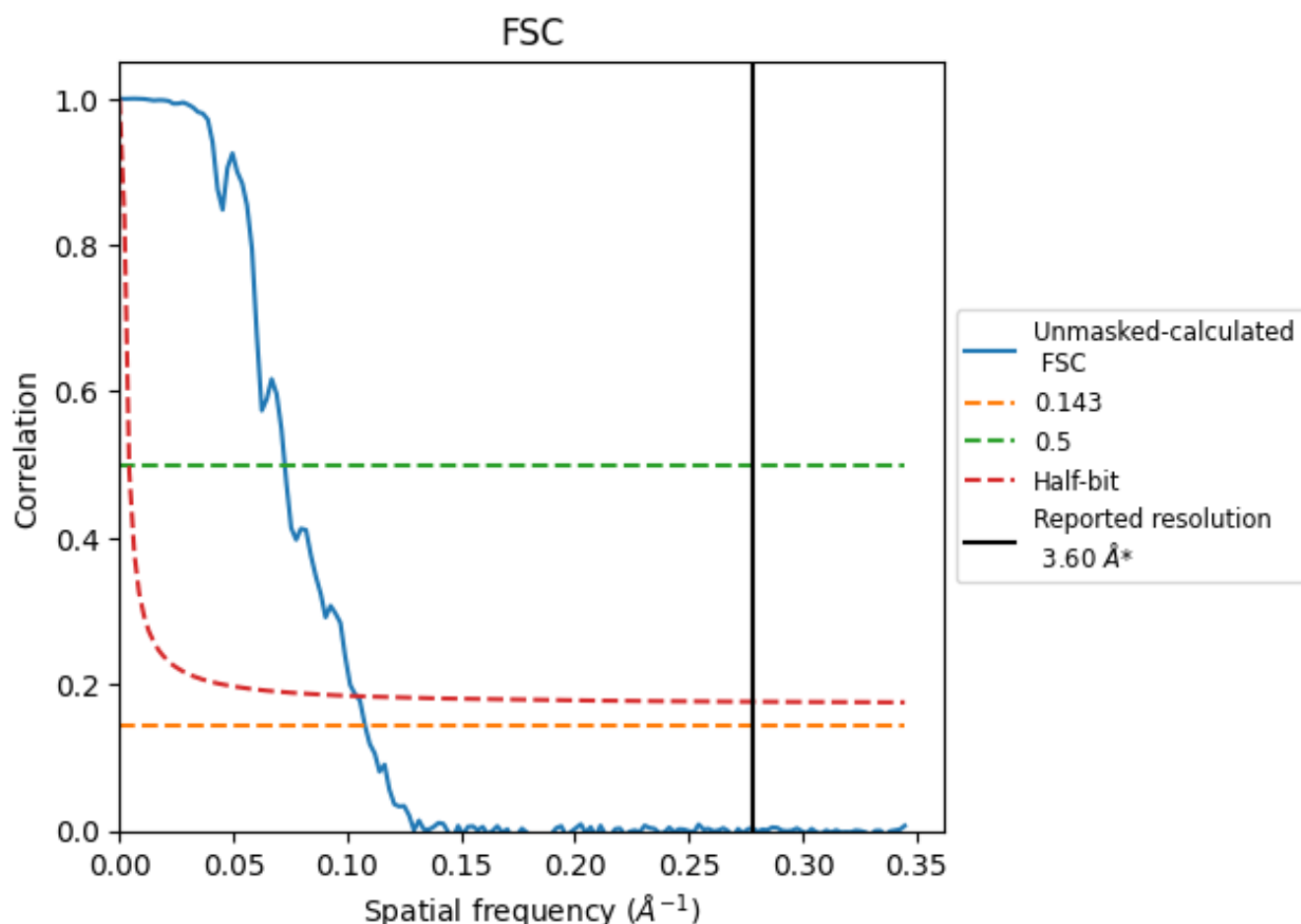


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

8.2 Resolution estimates [i](#)

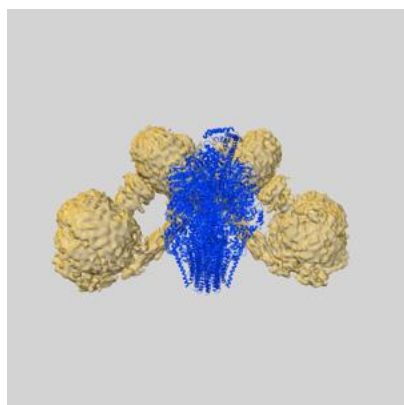
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.28	13.77	9.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.28 differs from the reported value 3.6 by more than 10 %

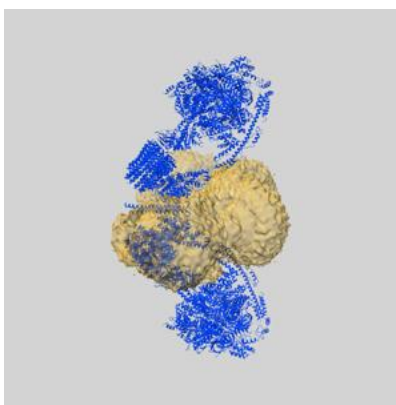
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7067 and PDB model 6B8H. Per-residue inclusion information can be found in section [3](#) on page [12](#).

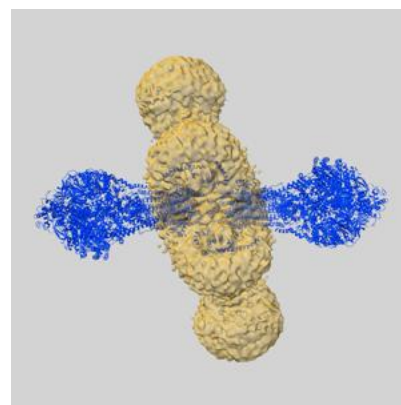
9.1 Map-model overlay [i](#)



X



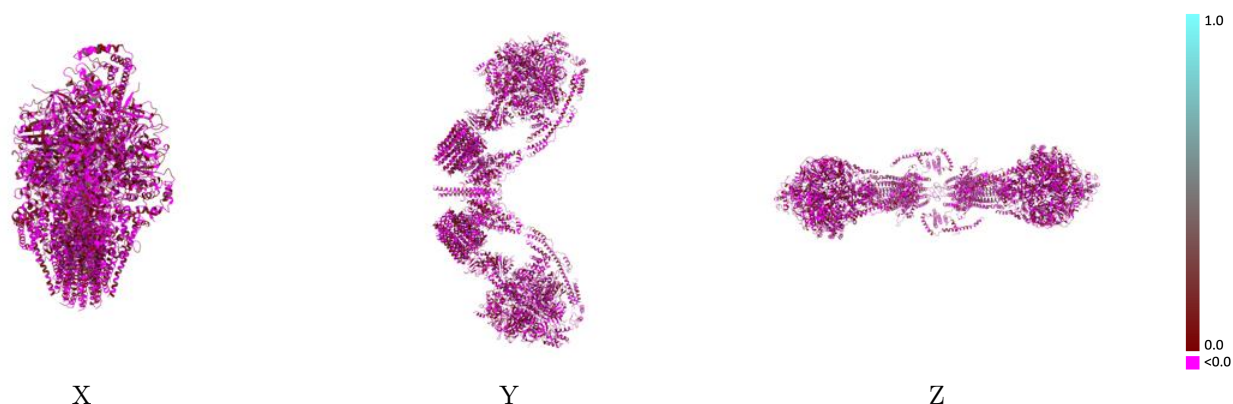
Y



Z

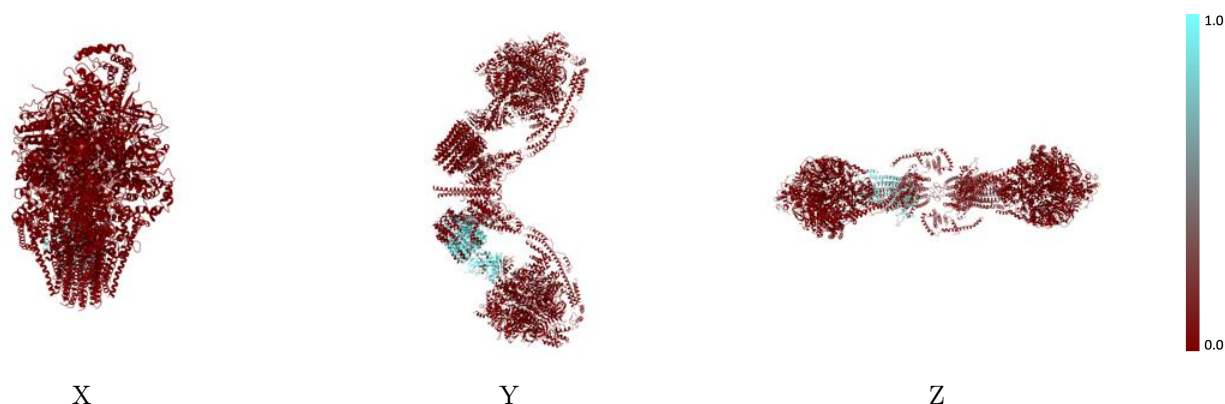
The images above show the 3D surface view of the map at the recommended contour level 0.156 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



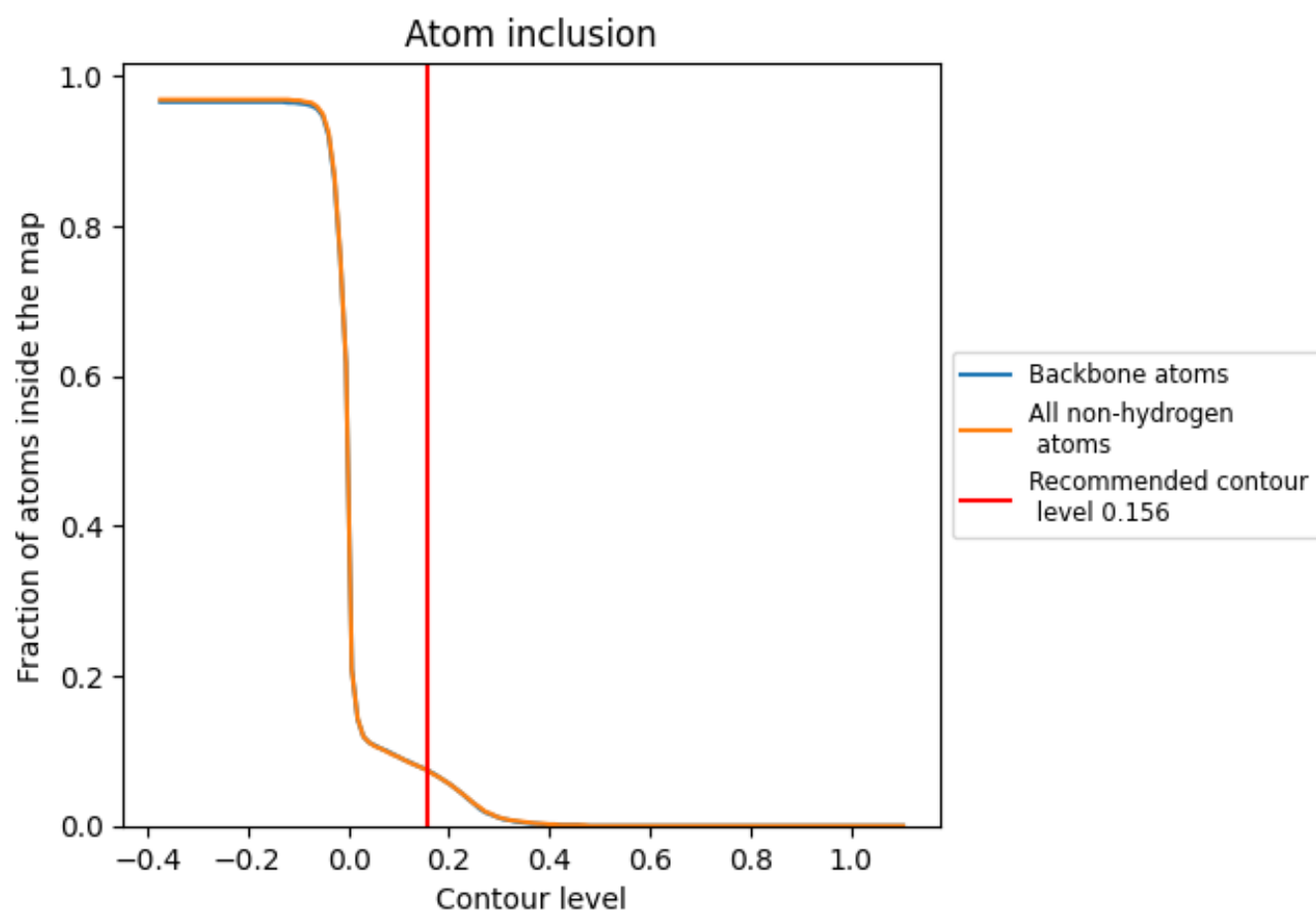
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.156).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 8% of all backbone atoms, 7% 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 (0.156) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0740	 0.0010
0	 0.5750	 -0.0100
1	 0.6350	 0.0120
2	 0.6700	 0.0120
3	 0.7660	 -0.0290
4	 0.6780	 -0.0130
5	 0.6540	 -0.0530
6	 0.5630	 0.0120
7	 0.3080	 -0.0080
8	 0.4190	 0.0180
9	 0.4900	 -0.0090
A	 0.0100	 0.0150
B	 0.0000	 0.0050
C	 0.0000	 -0.0040
D	 0.0000	 -0.0040
E	 0.0010	 0.0140
F	 0.0000	 0.0020
G	 0.4170	 0.0020
H	 0.7950	 0.0290
I	 0.5910	 0.0070
J	 0.0000	 -0.0160
K	 0.0000	 -0.0030
L	 0.0000	 0.0190
M	 0.0000	 0.0340
N	 0.0000	 -0.0280
O	 0.0000	 0.0050
P	 0.0000	 0.0020
Q	 0.0000	 0.0060
R	 0.0000	 -0.0160
S	 0.0000	 0.0000
T	 0.0000	 0.0250
U	 0.0000	 -0.0190
V	 0.0000	 0.0110
W	 0.0000	 -0.0040
X	 0.0000	 -0.0050



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Chain	Atom inclusion	Q-score
Y	 0.0000	 0.0060
Z	 0.0000	 0.0020
a	 0.3590	 -0.0080
b	 0.0050	 0.0120
c	 0.0000	 0.0050
d	 0.0440	 0.0250
e	 0.0000	 0.0130
f	 0.0000	 0.0010
g	 0.0000	 -0.0100
h	 0.0000	 0.0980
i	 0.0000	 -0.0340
j	 0.0000	 0.0040
k	 0.4860	 0.0580
l	 0.0000	 0.0020
m	 0.0000	 -0.0070
n	 0.0000	 -0.0040
o	 0.0000	 0.0180
p	 0.0000	 -0.0150
q	 0.0000	 0.0040
r	 0.0000	 -0.0180
s	 0.0040	 0.0420
t	 0.0000	 -0.0100
u	 0.0000	 -0.0330
v	 0.0000	 0.0890
w	 0.0000	 0.0140
x	 0.0000	 -0.0200