



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 04:41 AM UTC

PDB ID : 6B8H / pdb_00006b8h
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:

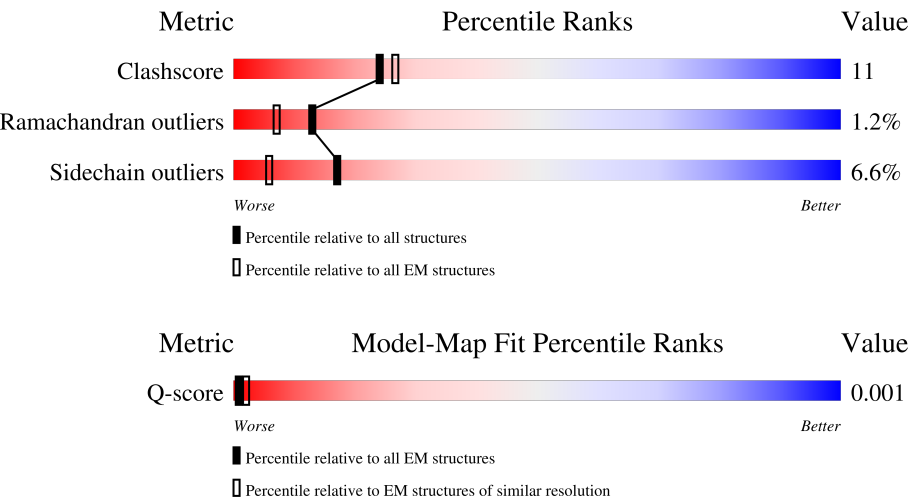
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	412 (6.90 - 7.90)

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	
1	1	76	
1	2	76	
1	3	76	

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Mol	Chain	Length	Quality of chain
1	4	76	28% 92% 5% ..
1	5	76	29% 87% 11% ..
1	6	76	37% 88% 9% .
1	7	76	66% 87% 9% .
1	8	76	51% 93% 5% .
1	9	76	47% 92% 5% .
1	J	76	99% 93% 5% .
1	L	76	99% 92% 7% .
1	M	76	99% 86% 13% .
1	N	76	97% 91% 7% .
1	P	76	99% 91% 7% ..
1	Q	76	99% 87% 11% ..
1	R	76	97% 88% 9% .
1	S	76	96% 87% 9% .
1	T	76	99% 93% 5% .
1	U	76	97% 92% 5% .
2	A	48	100% 83% 17%
2	V	48	100% 83% 17%
3	a	249	60% 86% 14%
3	p	249	100% 87% 13%
4	b	209	96% 92% ...
4	q	209	96% 92% ...
5	d	173	87% 82% 8% . 9%
5	r	173	91% 82% 8% . 9%
6	e	49	100% 100%

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Mol	Chain	Length	Quality of chain
6	s	49	100% 100%
7	f	95	88% 76% 12% 12%
7	t	95	88% 76% 12% 12%
8	g	106	100% 99%
8	u	106	100% 99%
9	i	59	100% 97%
9	w	59	100% 97%
10	k	68	16% 32% 65%
10	x	68	35% 32% 65%
11	B	510	96% 60% 32% 5%
11	C	510	98% 67% 29%
11	K	510	98% 68% 28%
11	W	510	96% 61% 31% 5%
11	X	510	98% 67% 28%
11	n	510	98% 68% 27%
12	D	478	98% 69% 27%
12	E	478	98% 65% 31%
12	F	478	98% 62% 33%
12	Y	478	98% 70% 26%
12	Z	478	98% 64% 32%
12	c	478	98% 64% 31%
13	G	278	54% 59% 29% 6% 5%
13	j	278	95% 59% 29% 6% 5%
14	H	138	17% 55% 23% 8% 14%
14	l	138	86% 55% 23% 8% 14%

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Mol	Chain	Length	Quality of chain
15	I	61	28%39%28%10%•21%
15	m	61	79%39%28%10%•21%
16	O	195	83%76%5%•17%
16	o	195	83%76%5%•17%
17	h	21	100%76%24%
17	v	21	100%76%24%

2 Entry composition

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		

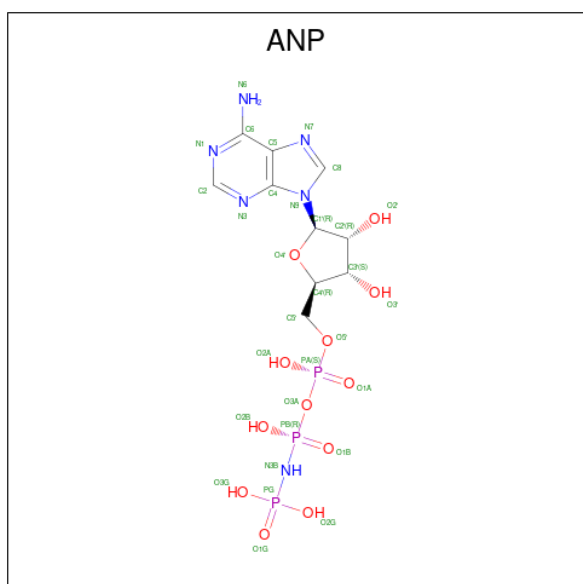
- Molecule 16 is a protein called ATP synthase subunit 5, mitochondrial.

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 (CCD ID: 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	

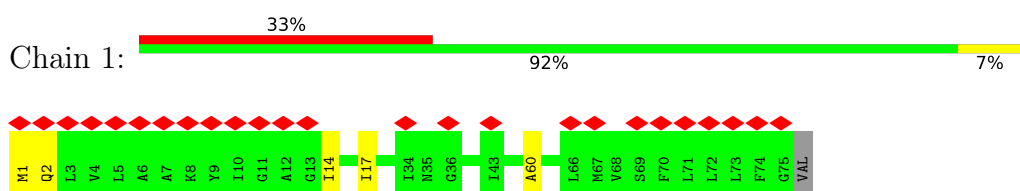
- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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	

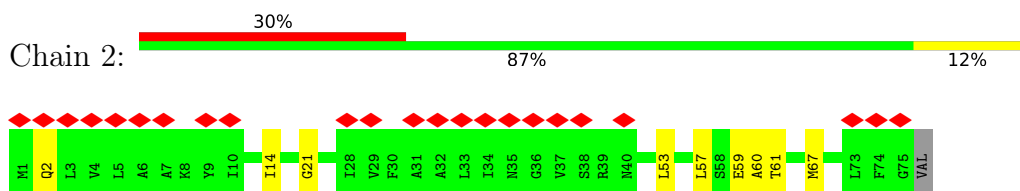
3 Residue-property plots

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.

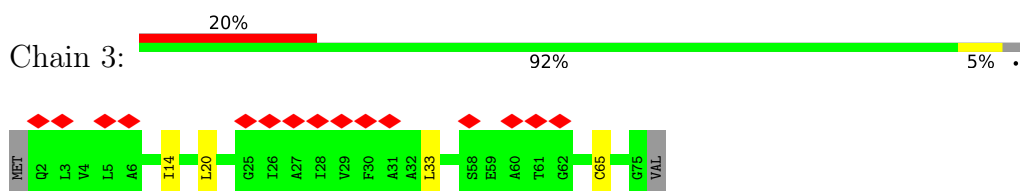
- Molecule 1: ATP synthase subunit 9, mitochondrial



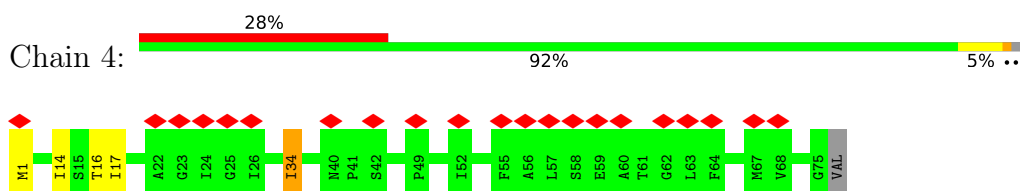
- Molecule 1: ATP synthase subunit 9, mitochondrial



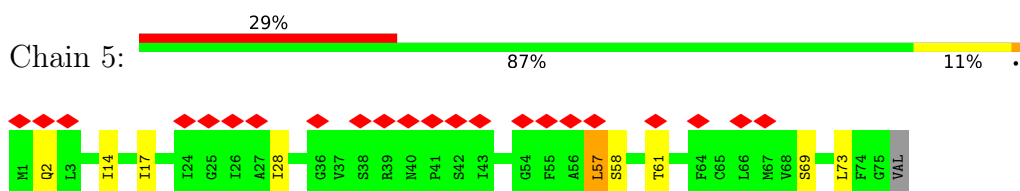
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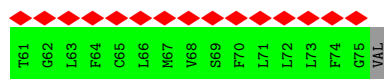
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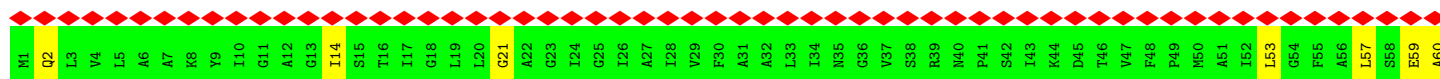
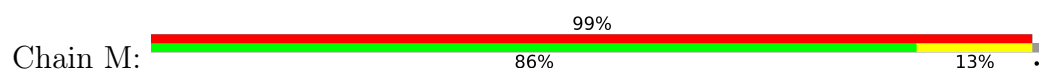
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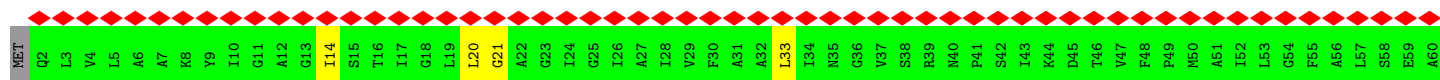
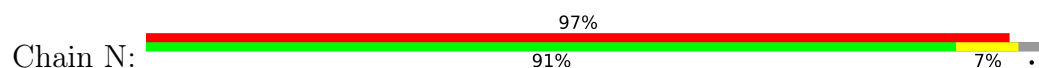
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|----|----|----|----|----|----|----|----|----|-----|
| M1 | Q2 | L3 | V4 | L5 | A6 | A7 | K8 | Y9 | I10 | G11 | A12 | G13 | I14 | S15 | T16 | I17 | G18 | L19 | L20 | G21 | A22 | G23 | T24 | G25 | T26 | A27 | T28 | V29 | F30 | A31 | A32 | L33 | L34 | N35 | G36 | V37 | S38 | R39 | M40 | P41 | S42 | I43 | K44 | D45 | T46 | V47 | F48 | P49 | M50 | A51 | I52 | L53 | G54 | F55 | A56 | L57 | S58 | E59 | L60 |
|----|----|----|----|----|----|----|----|----|-----|



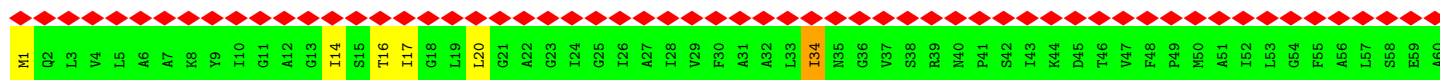
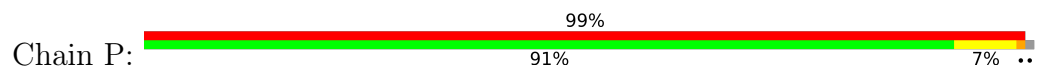
- Molecule 1: ATP synthase subunit 9, mitochondrial



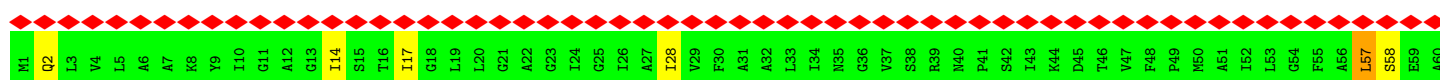
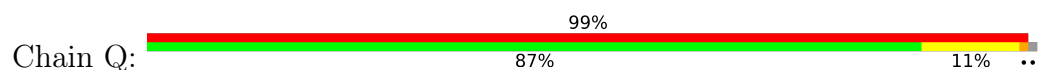
- Molecule 1: ATP synthase subunit 9, mitochondrial



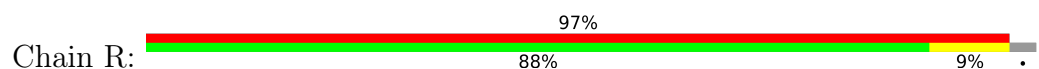
- Molecule 1: ATP synthase subunit 9, mitochondrial

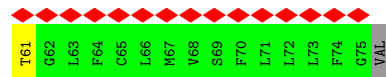


- Molecule 1: ATP synthase subunit 9, mitochondrial

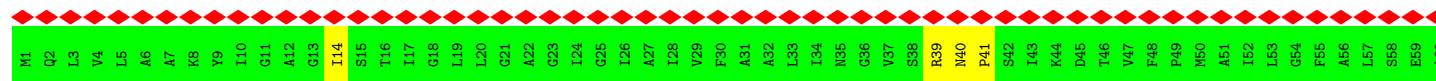
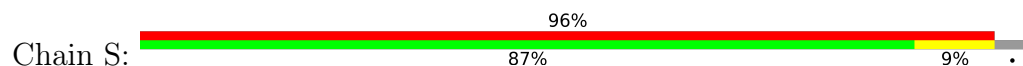


- Molecule 1: ATP synthase subunit 9, mitochondrial

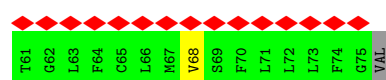
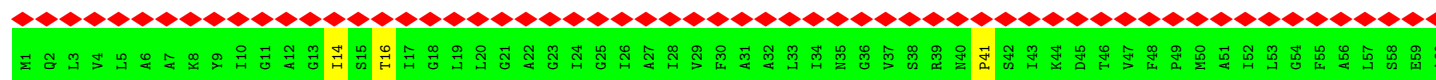




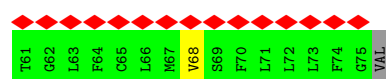
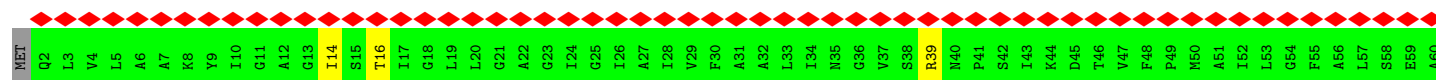
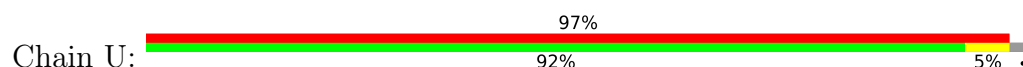
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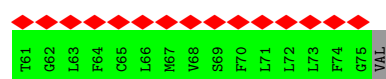
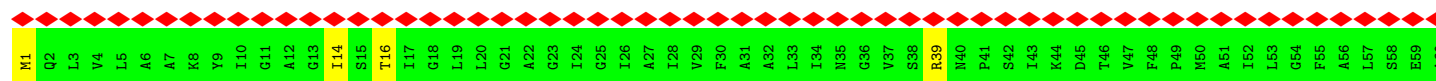
- Molecule 1: ATP synthase subunit 9, mitochondrial



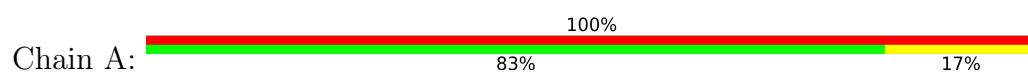
- Molecule 1: ATP synthase subunit 9, mitochondrial



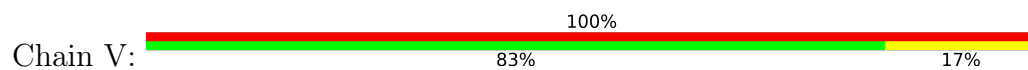
- Molecule 1: ATP synthase subunit 9, mitochondrial



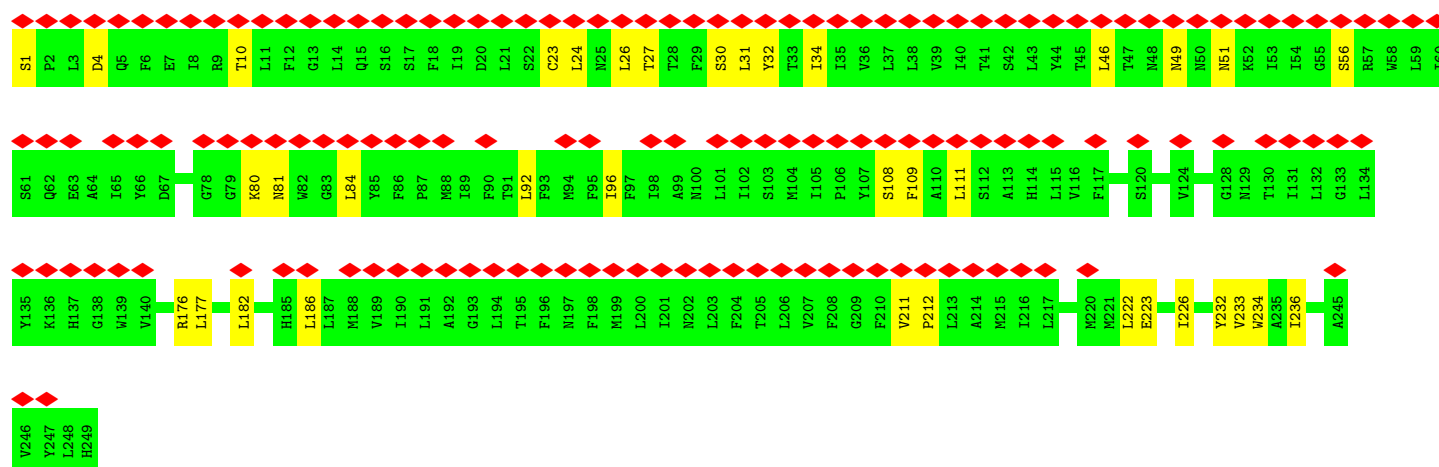
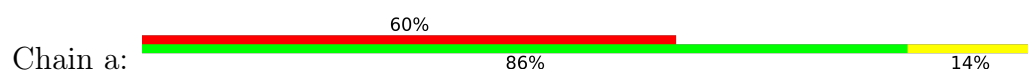
- Molecule 2: ATP synthase protein 8



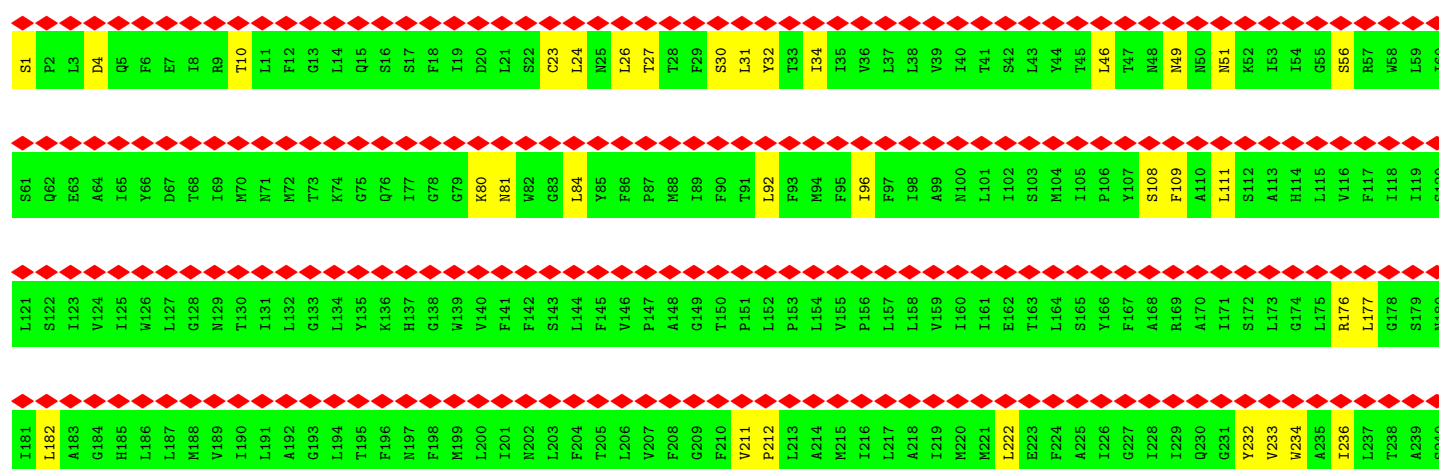
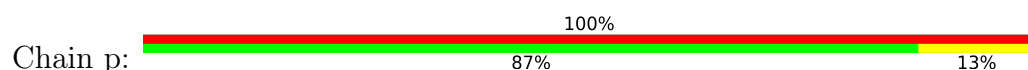
- Molecule 2: ATP synthase protein 8



- Molecule 3: ATP synthase subunit a

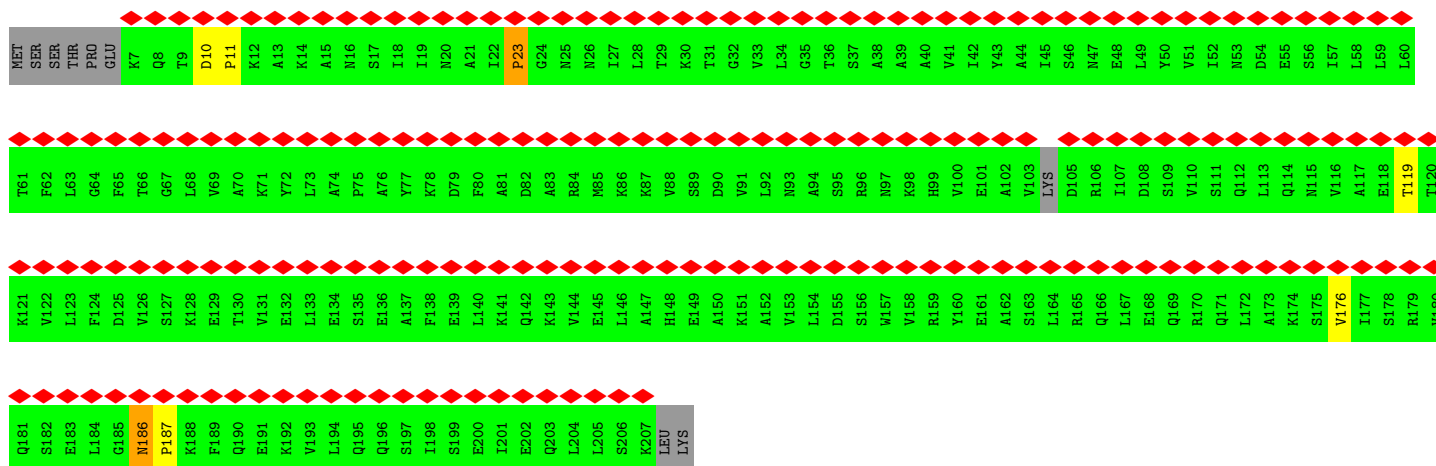
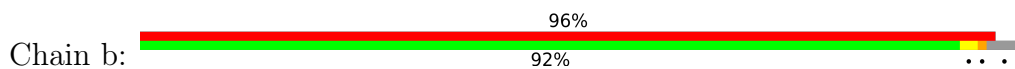


- Molecule 3: ATP synthase subunit a

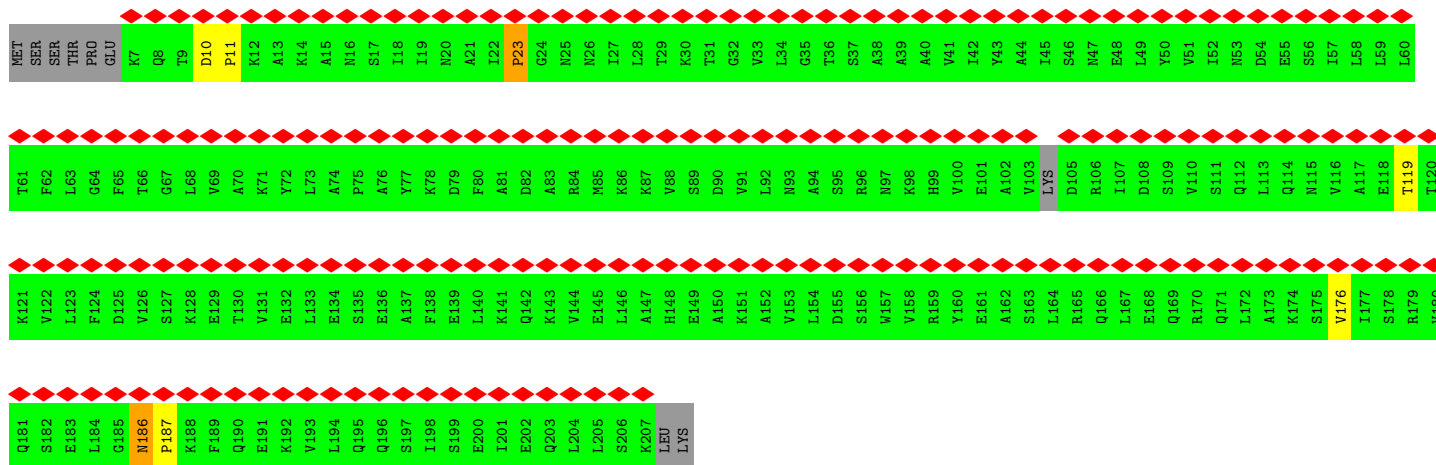
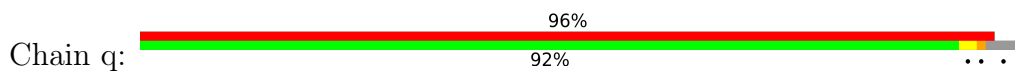




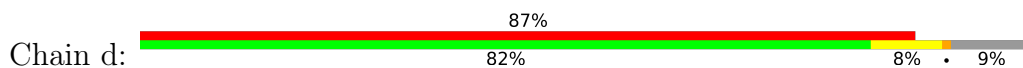
• Molecule 4: ATP synthase subunit 4, mitochondrial

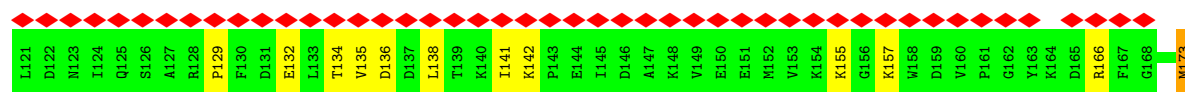


• Molecule 4: ATP synthase subunit 4, mitochondrial

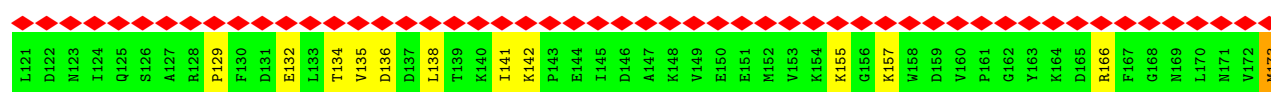
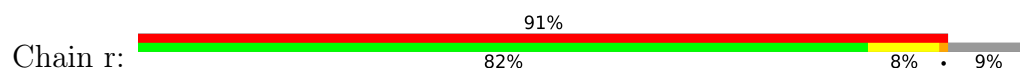


• Molecule 5: ATP synthase subunit d, mitochondrial

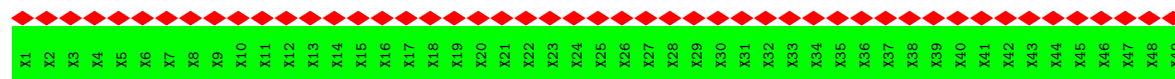




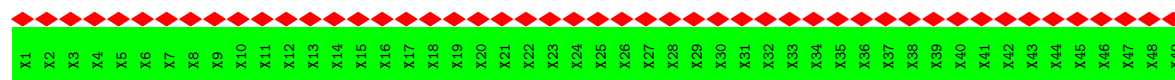
- Molecule 5: ATP synthase subunit d, mitochondrial



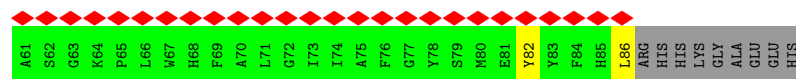
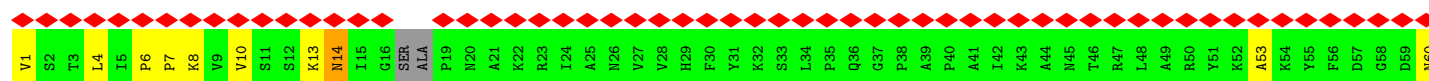
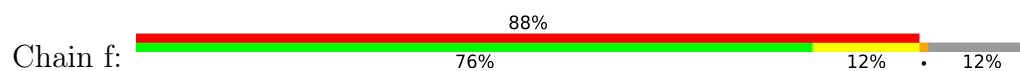
- Molecule 6: ATP synthase subunit e, mitochondrial



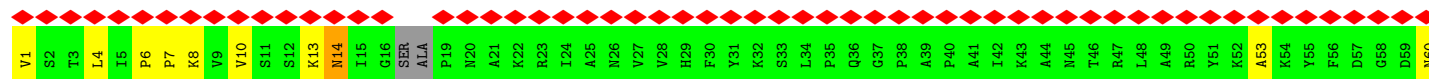
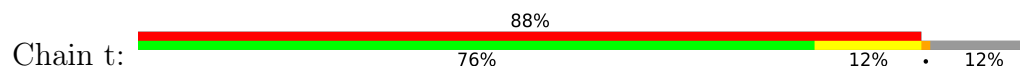
- Molecule 6: ATP synthase subunit e, mitochondrial

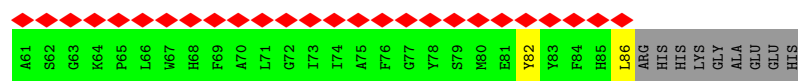


- Molecule 7: ATP synthase subunit f, mitochondrial

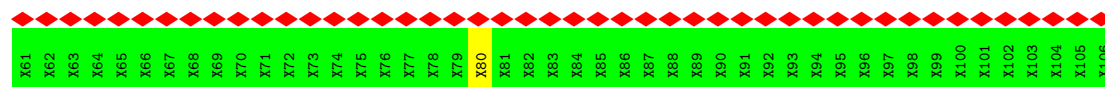
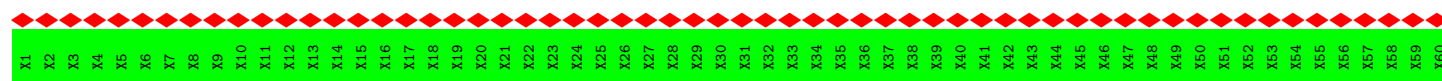


- Molecule 7: ATP synthase subunit f, mitochondrial

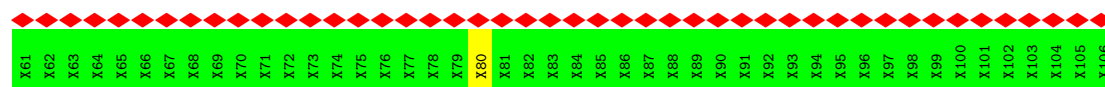
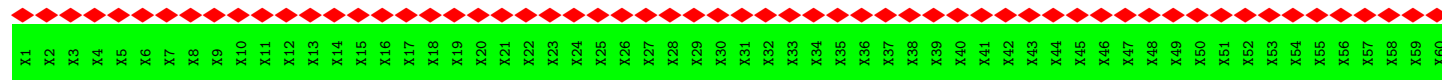




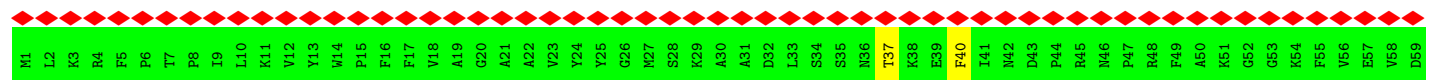
- Molecule 8: AATP synthase subunit g



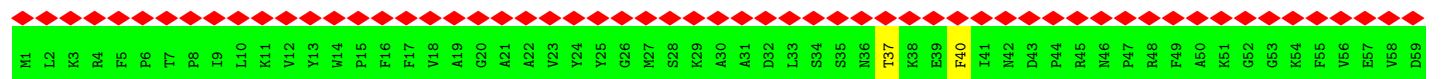
- Molecule 8: AATP synthase subunit g



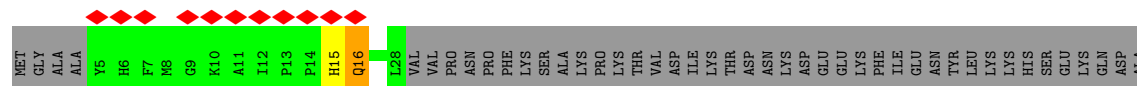
- Molecule 9: ATP synthase subunit J, mitochondrial



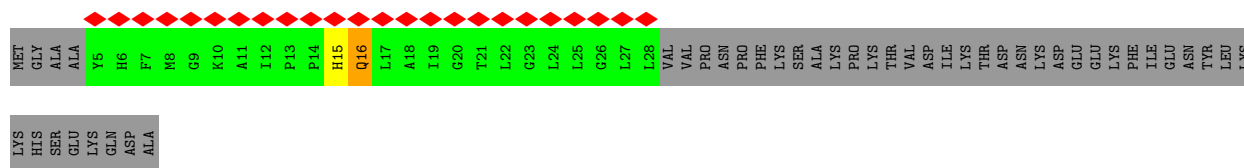
- Molecule 9: ATP synthase subunit J, mitochondrial



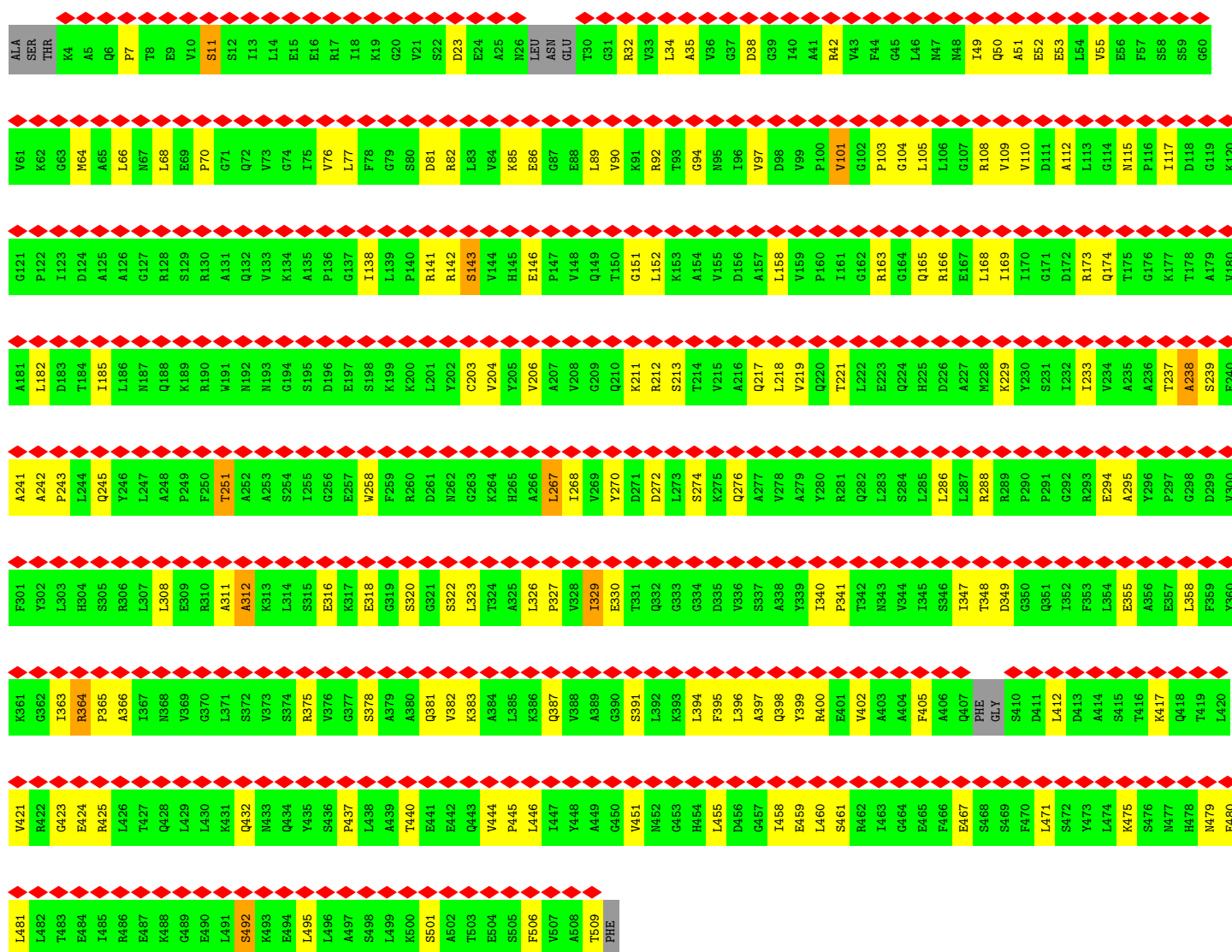
- Molecule 10: ATP synthase subunit K, mitochondrial



- Molecule 10: ATP synthase subunit K, mitochondrial



• Molecule 11: ATP synthase subunit alpha, mitochondrial



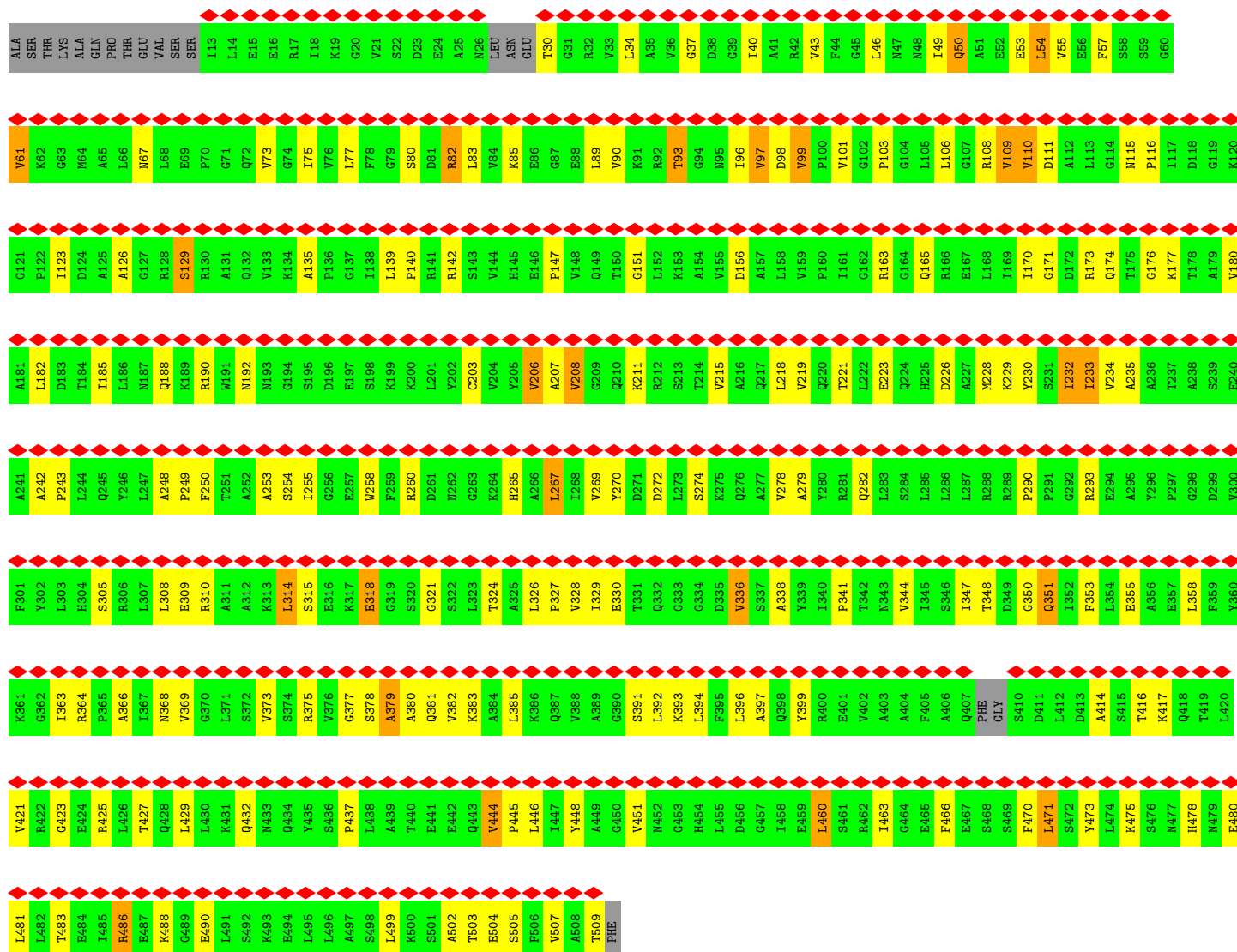
• Molecule 11: ATP synthase subunit alpha, mitochondrial



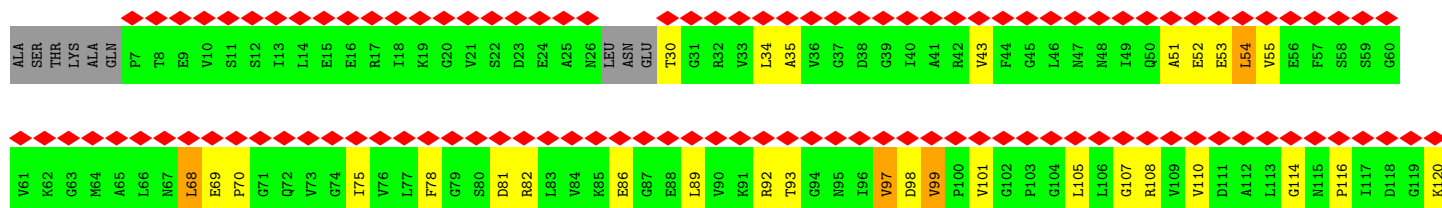




- Molecule 11: ATP synthase subunit alpha, mitochondrial



- Molecule 11: ATP synthase subunit alpha, mitochondrial



G121	A181	A241	F301	K361	V421	L481
P122	L182	A242	Y302	G362	R422	L482
I123	D183	P243	L303	I363	G423	T483
D124	T184	L244	H304	R364	E424	E484
A125	I185	Q245	S305	P365	R425	L485
A126	L186	Q246	R306	A366	L426	R486
G127	N187	L247	L307	I367	T427	E487
R128	Q188	A248	L308	N368	Q428	K488
S129	K189	P249	E309	V369	L429	G489
R130	R190	F250	R310	G370	L430	E490
A131	W191	T251	A311	L371	K431	L491
Q132	N192	A252	A312	S372	Q432	S492
V133	N193	A253	K313	V373	M433	K493
K134	G194	S254	L314	S374	Q434	E494
A135	S195	I255	S315	R375	Y435	L495
P136	D196	G256	E316	V376	S436	L496
G137	E197	G257	K317	G377	P437	A497
I138	E198	W258	E318	S378	L438	S498
L139	K199	F259	G319	A379	A439	L499
P140	K200	R260	S320	A380	T440	K500
R141	L201	D261	G321	Q381	E441	S501
R142	Y202	N262	S322	V382	E442	A502
S143	C203	G263	L323	K383	Q443	T503
V144	V204	K264	T324	A384	V444	E504
H145	Y205	H265	A325	L385	P445	S505
E146	Y206	A266	L326	K386	L446	F506
P147	A207	L267	F327	Q387	I447	V507
V148	V208	I268	V328	V388	Y448	A508
Q149	G209	V269	I329	A389	A449	T509
T150	Q210	Y270	E330	G390	G450	PHE
G151	K211	D271	T331	S391	V451	
K152	R212	D272	Q332	L392	M452	
K153	S213	L273	G333	K393	G453	
A154	T214	S274	G334	L394	H454	
V155	V215	K275	D335	F395	L455	
D156	A216	Q276	V336	L396	D456	
A157	Q217	A277	S337	A397	G457	
L158	L218	V278	A338	Q398	I458	
V159	V219	A279	Y339	Y399	E459	
P160	Q220	Y280	I340	R400	L460	
I161	T221	R281	F341	E401	S461	
G162	L222	Q282	T342	V402	M462	
R163	E223	L283	N343	A403	I463	
G164	Q224	S284	V344	A404	G464	
Q165	H225	L285	I345	F405	E465	
R166	D226	L286	S346	A406	F466	
E167	A227	L287	I347	Q407	E467	
L168	M228	R288	T348	F408	S468	
I169	K229	R289	D349	G409	S469	
I170	I230	P290	G350	S410	F470	
G171	S231	P291	Q351	D411	L471	
D172	I232	G292	I352	L412	S472	
R173	I233	R293	F353	D413	Y473	
Q174	V234	E294	L354	A414	L474	
T175	A235	A295	E355	S415	K475	
G176	A236	Y296	A356	T416	S476	
K177	T237	P297	E357	K417	M477	
T178	A238	D298	L358	Q418	H478	
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V180	E240	V300	Y360	L420	E480	

• Molecule 12: ATP synthase subunit beta, mitochondrial

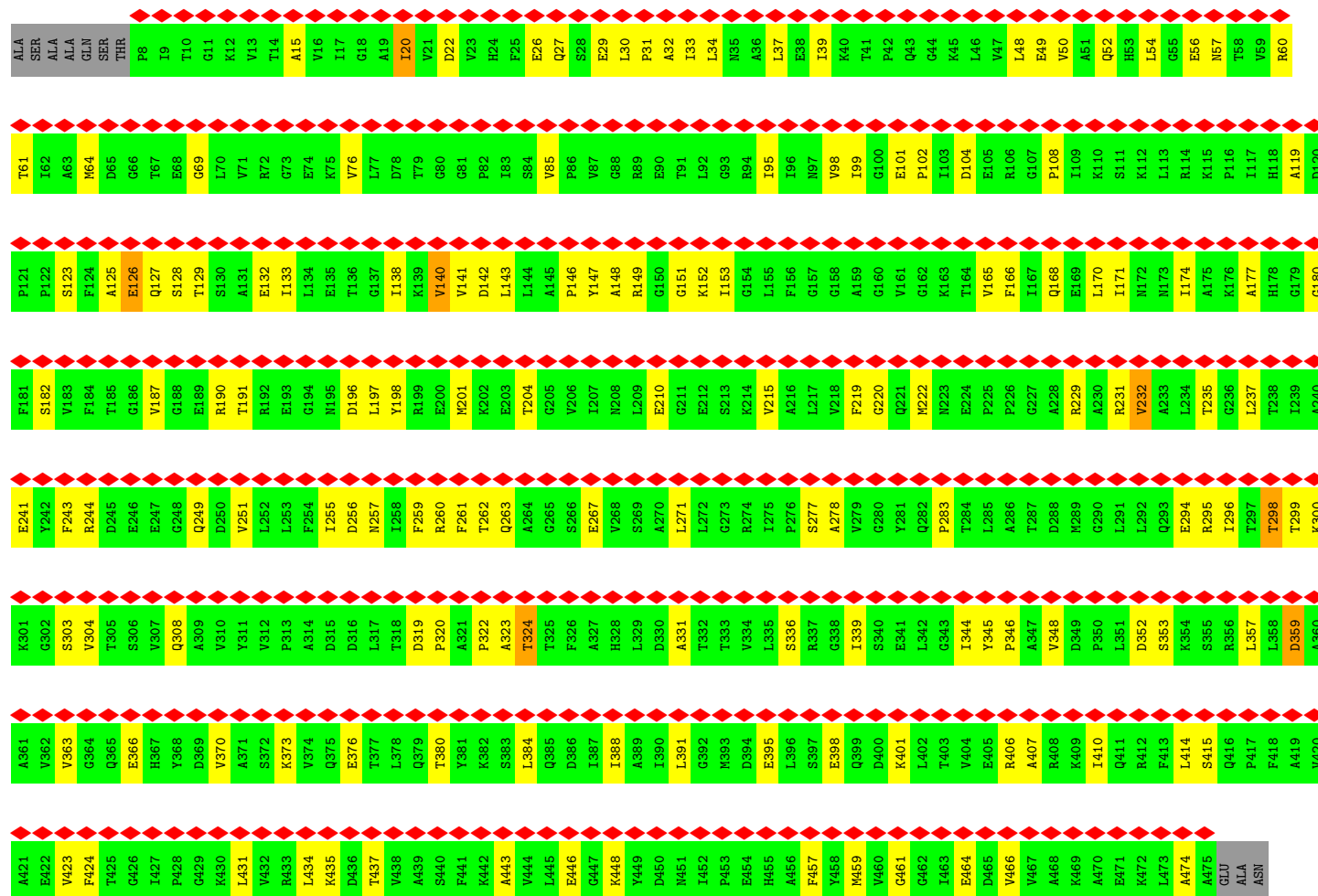


ALA	P121	F181	E241	K301
SER	P122	S182	Y242	G302
ALA	S123	V183	F243	S303
ALA	F124	F184	R244	V304
GLN	A125	T185	D245	T305
S6	E126	G186	E246	S306
T7	Q127	V187	E247	V307
P8	S128	G188	G248	Q308
I9	T129	E189	Q249	A309
T10	L70	R190	D250	V310
G11	V71	T191	V251	Y311
K12	R72	R192	L252	V312
V13	G73	E193	L253	P313
T14	E74	G194	F254	A314
A15	K75	M195	I255	D315
V16	Y76	D196	D256	D316
I17	L77	L197	N257	L317
G18	D78	Y198	I258	T318
A19	T79	R199	F259	D319
I20	G80	E200	R260	P320
V21	G81	M201	F261	A321
D22	P82	K202	T262	P322
V23	I83	E203	Q263	A323
H24	S84	T204	A264	T324
F25	V85	G205	G265	T325
E26	P86	V206	S266	F326
S27	Y87	I207	E267	A327
S28	G88	M208	V268	H328
E29	R89	L209	S269	L329
L30	E90	E210	A270	D330
P31	T91	G211	L271	A331
A32	L92	E212	L272	T332
I33	G93	S213	G273	T333
L34	R94	K214	R274	V334
N35	I95	V215	I275	L335
A36	I96	A216	P276	S336
F37	Y97	G157	T277	R337
E38	V98	L158	A278	G338
I39	I99	A159	V279	I339
K40	T41	G160	G280	S340
T41	P42	V161	Y281	E341
Q43	P102	G162	Q282	L342
G44	I103	K163	P283	G343
K45	D104	T164	T284	I344
L46	E105	V165	P225	Y345
V47	R106	F166	A286	P346
L48	G107	I167	T287	A347
E49	P108	Q168	D288	V348
V50	I109	E169	R229	D349
A51	K110	L170	A230	P350
Q52	S111	I171	L291	L351
H53	K112	M172	Q292	D352
L54	L113	M173	Q293	S353
G55	R114	I174	E294	K354
E56	K115	A175	R295	S355
N57	P116	K176	I296	R356
T58	I117	A177	T297	L357
V59	H118	H178	T298	L358
R60	A119	G179	T299	D359
	D120	G180	K300	A360



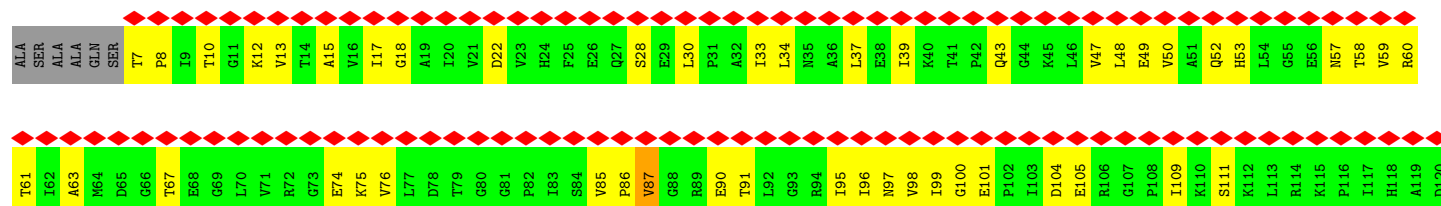
• Molecule 12: ATP synthase subunit beta, mitochondrial

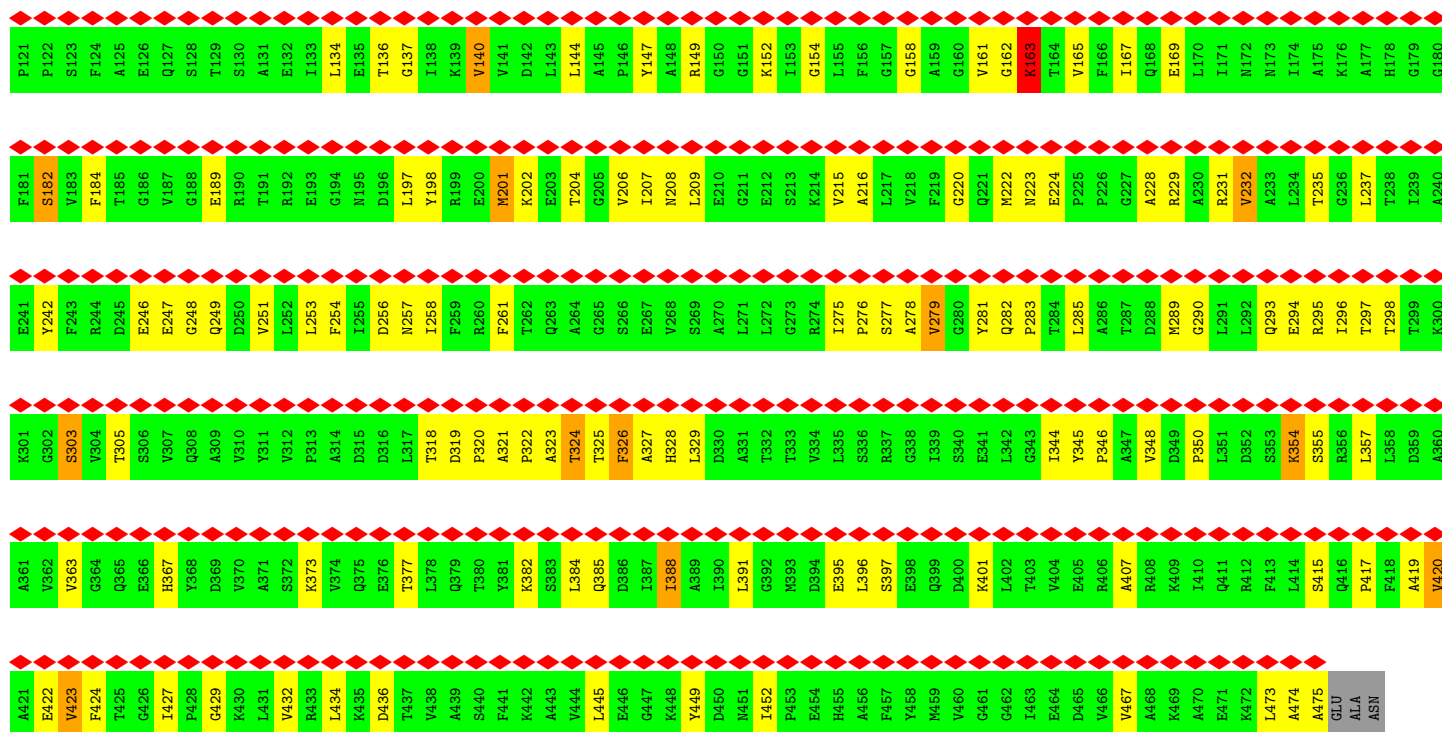
Chain E: 98% 65% 31%



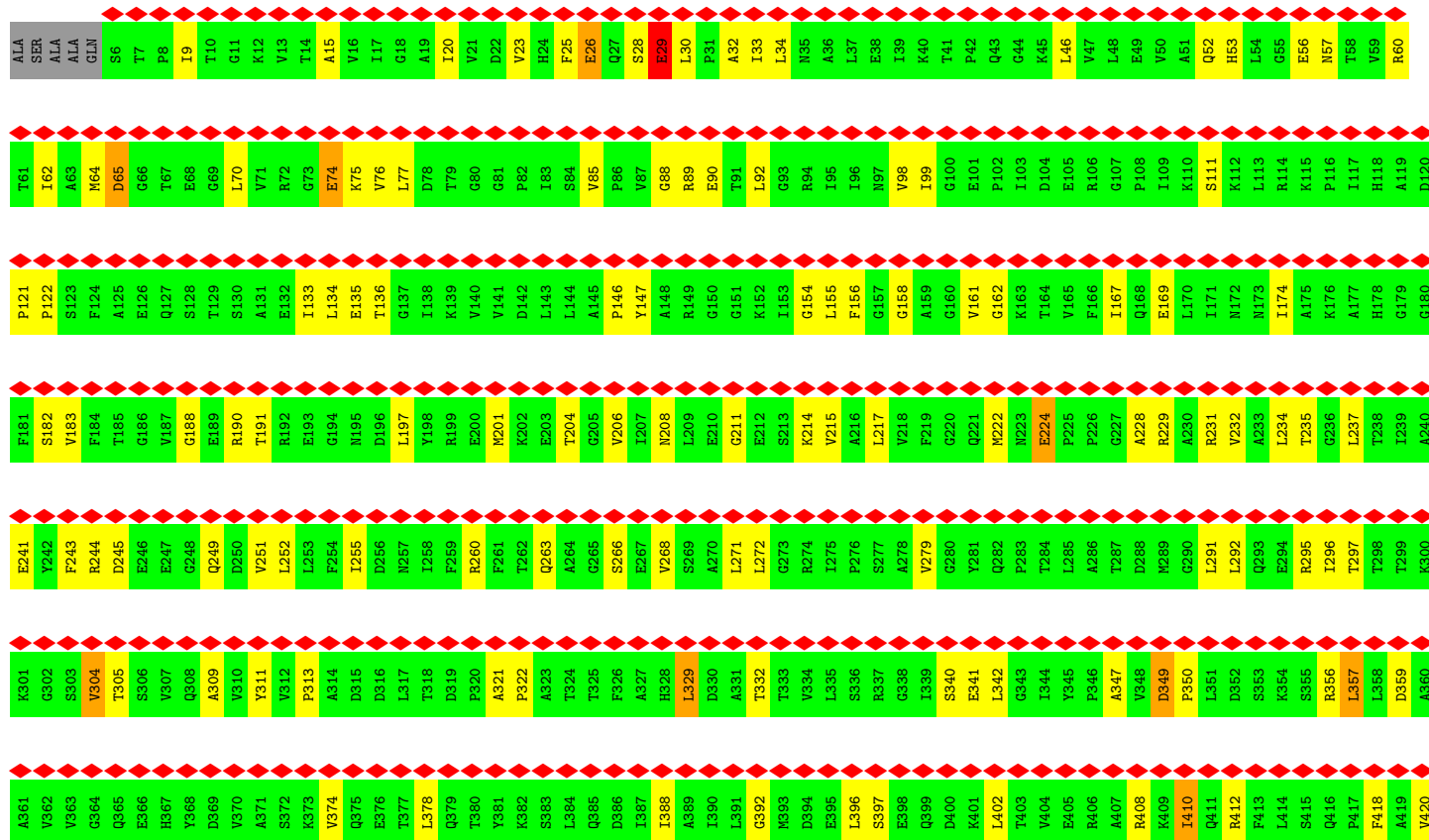
• Molecule 12: ATP synthase subunit beta, mitochondrial

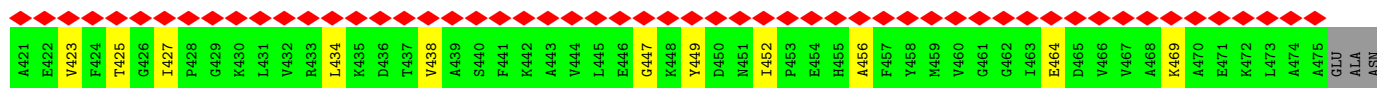
Chain F: 98% 62% 33%



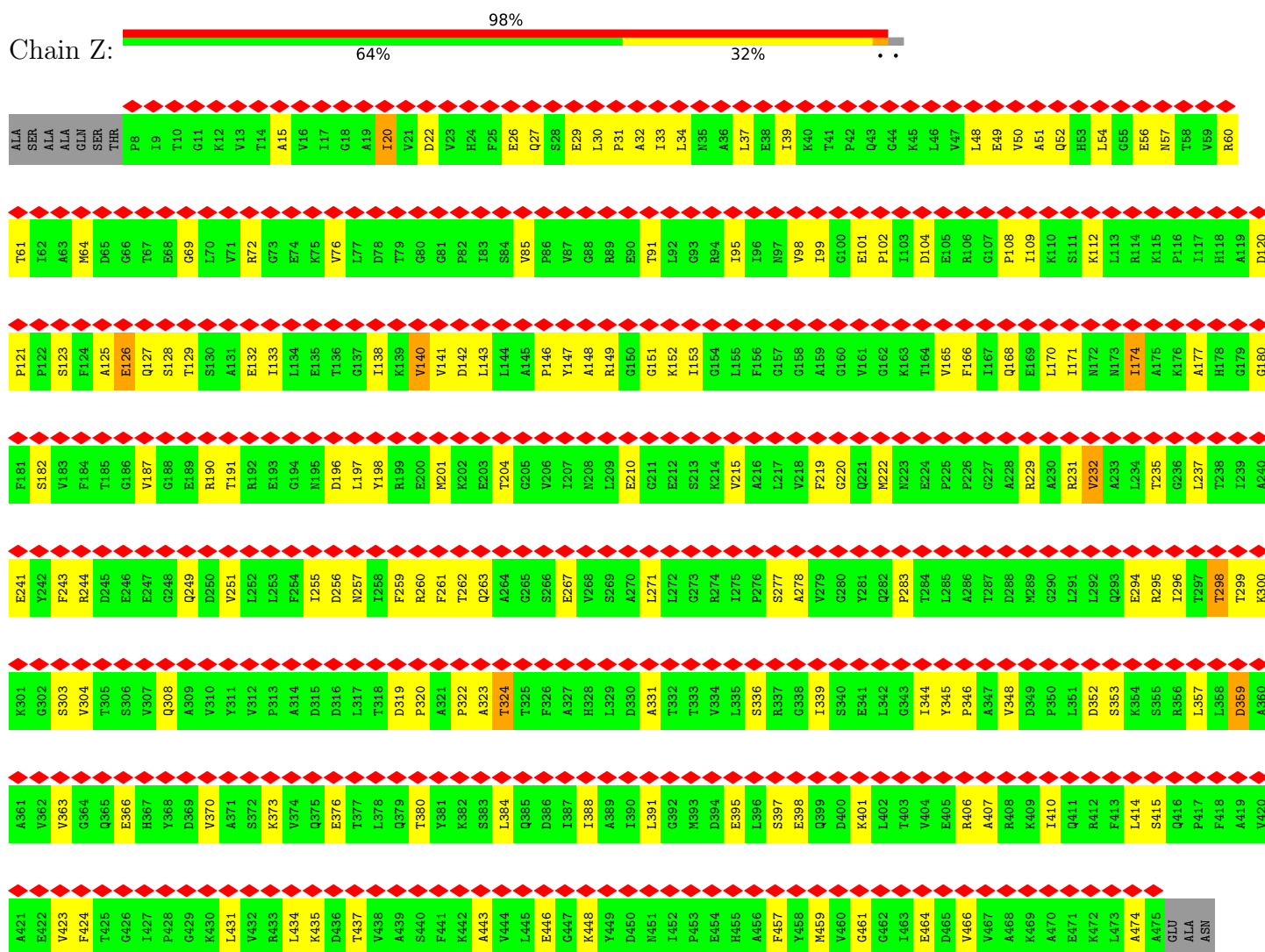


● Molecule 12: ATP synthase subunit beta, mitochondrial

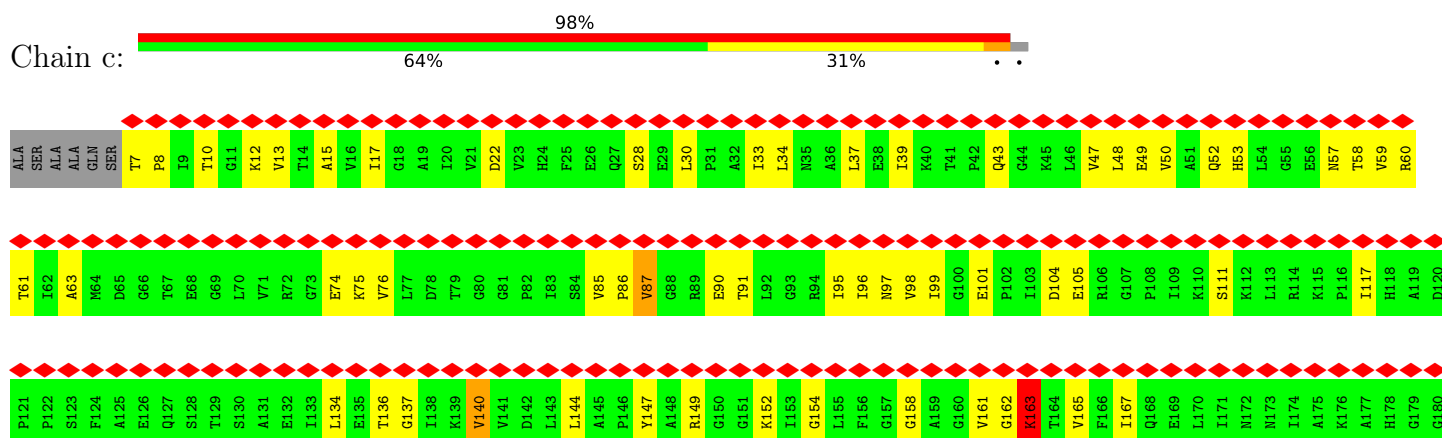


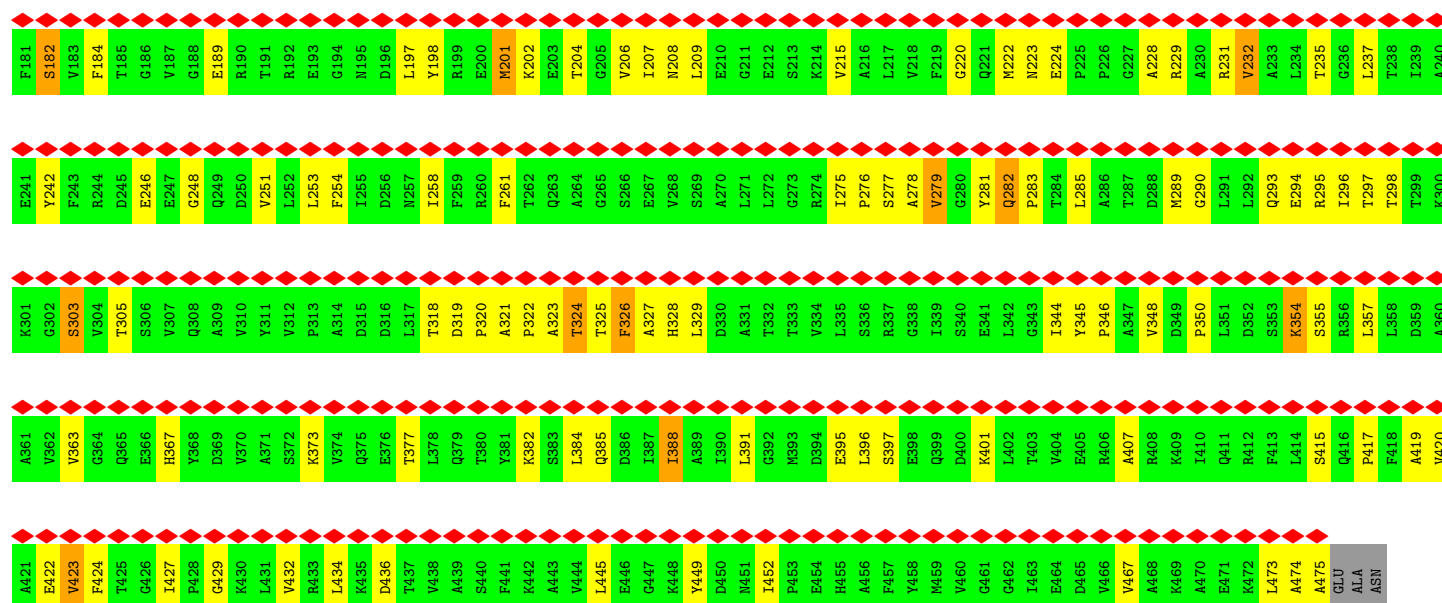


• Molecule 12: ATP synthase subunit beta, mitochondrial



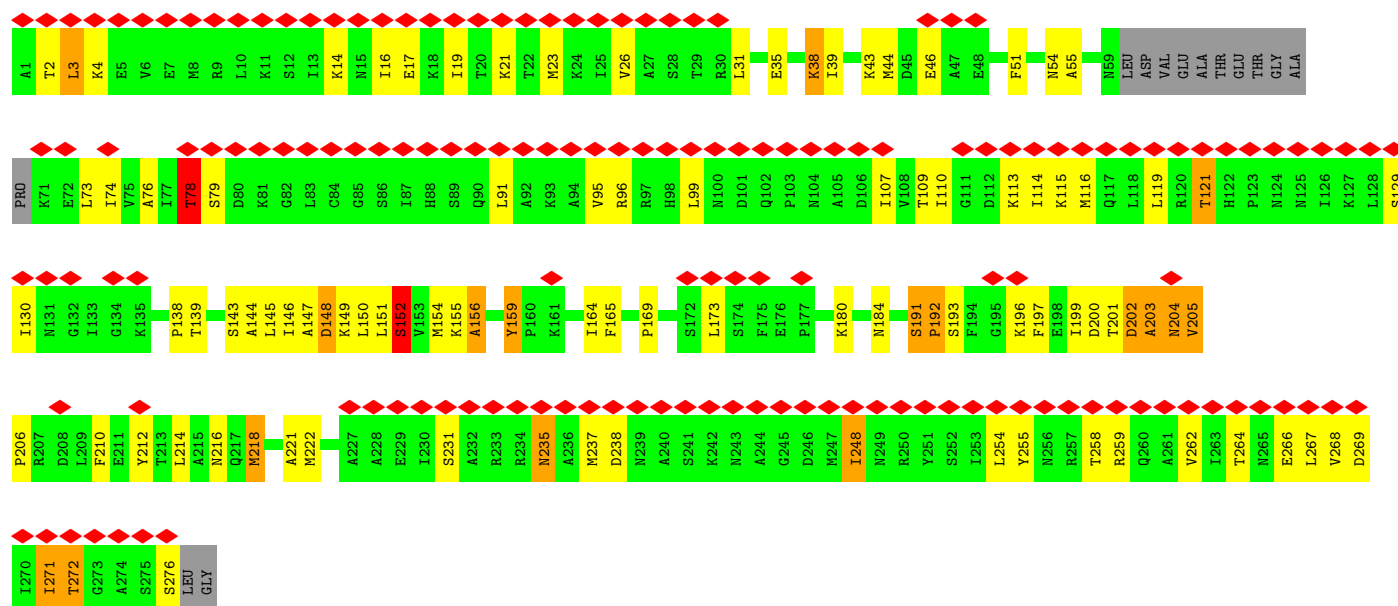
• Molecule 12: ATP synthase subunit beta, mitochondrial





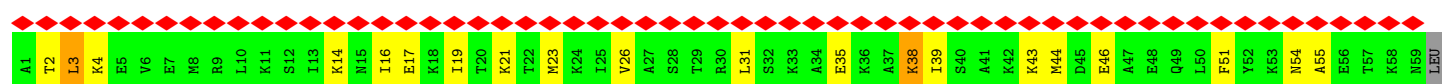
• Molecule 13: ATP synthase subunit gamma, mitochondrial

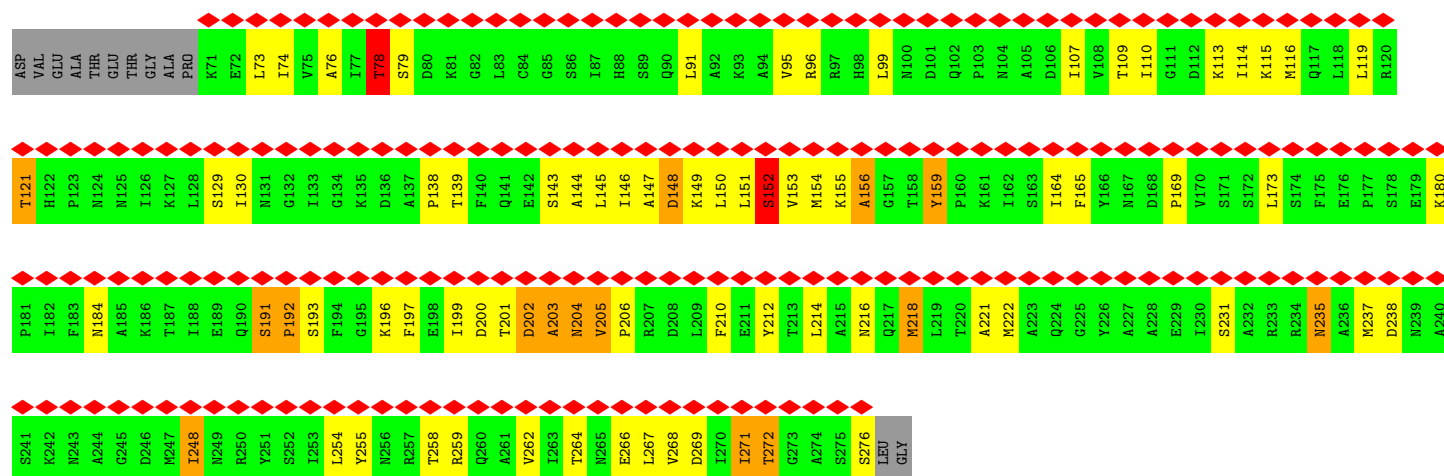
Chain G: 54% 59% 29% 6% • 5%



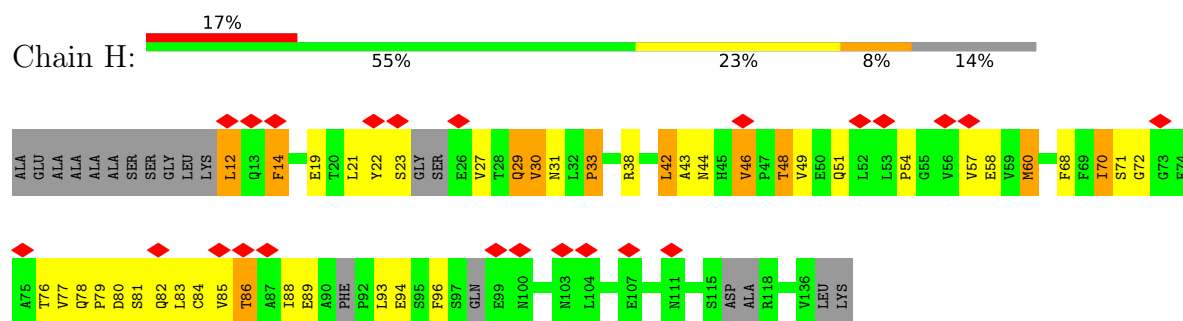
• Molecule 13: ATP synthase subunit gamma, mitochondrial

Chain j: 95% 59% 29% 6% • 5%

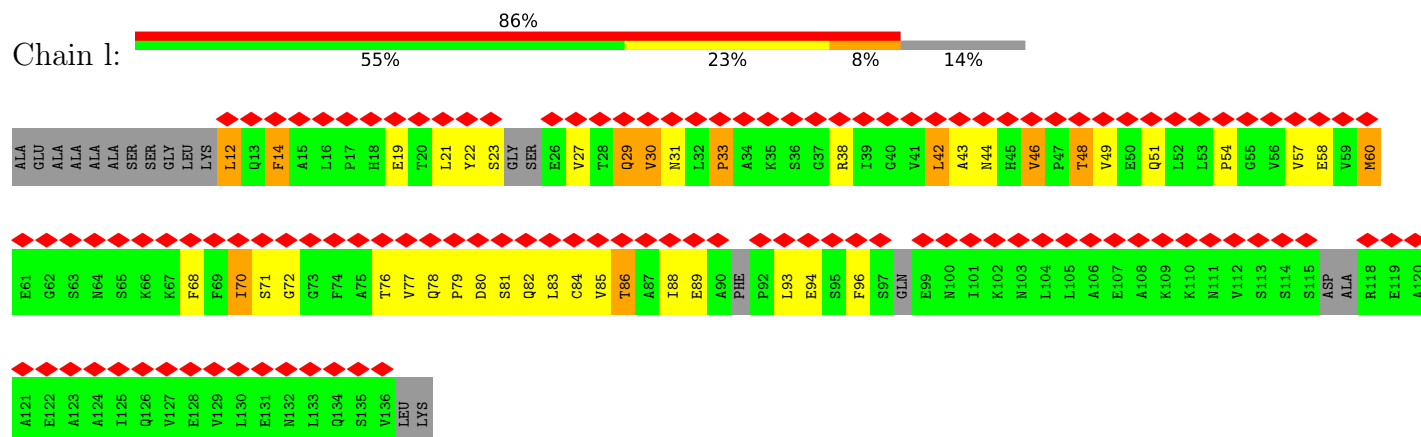




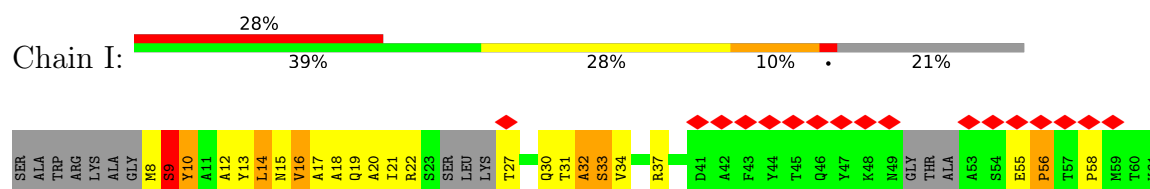
• Molecule 14: ATP synthase subunit delta, mitochondrial



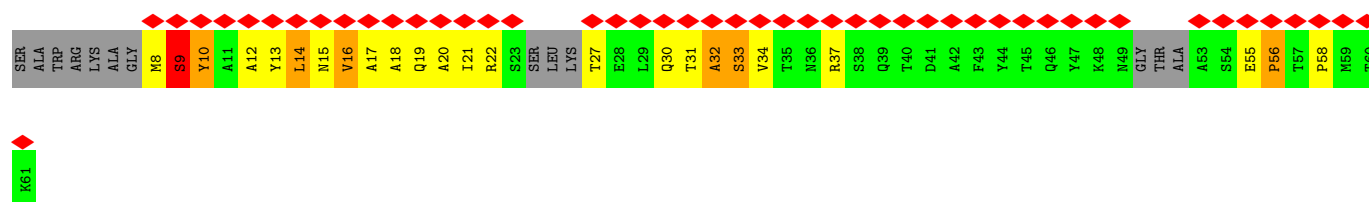
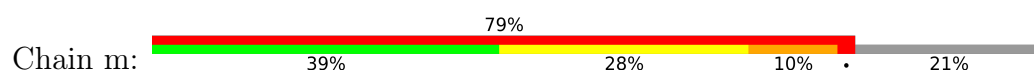
• Molecule 14: ATP synthase subunit delta, mitochondrial



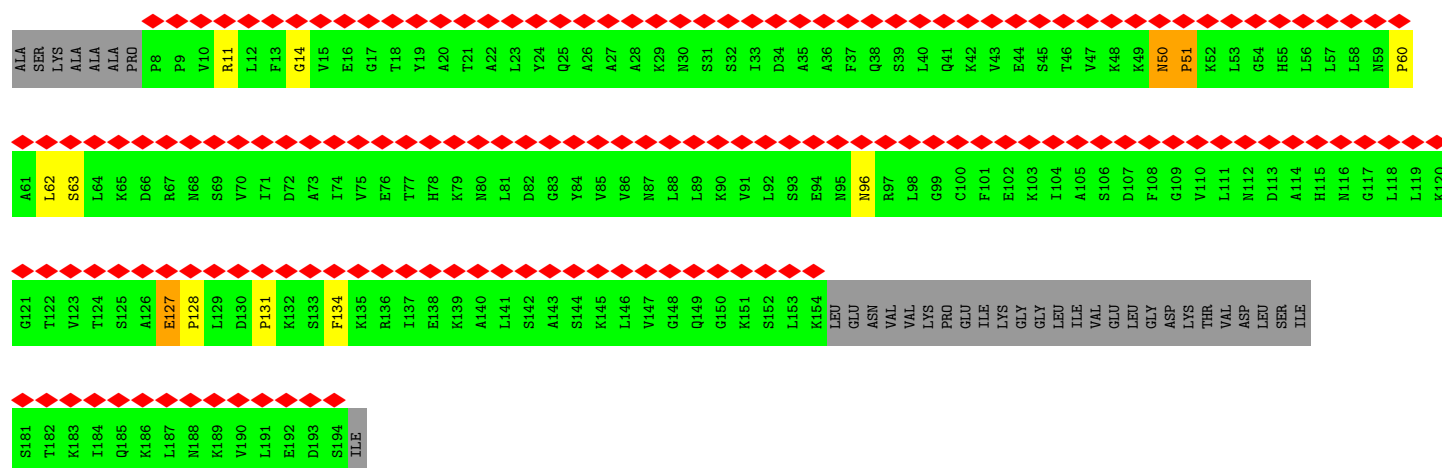
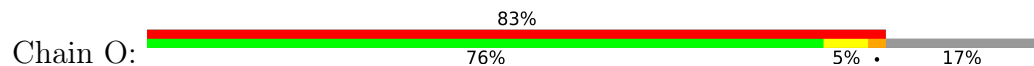
• Molecule 15: ATP synthase catalytic sector F1 epsilon subunit



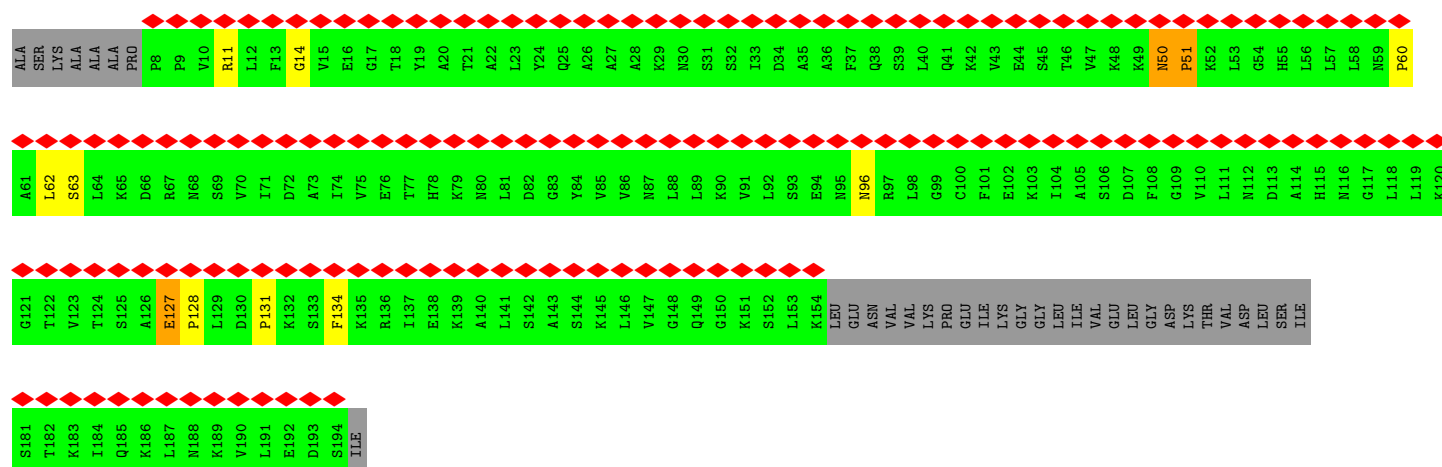
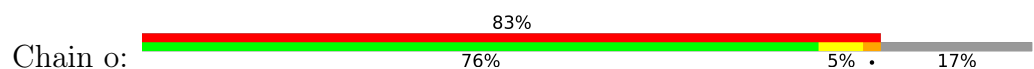
• Molecule 15: ATP synthase catalytic sector F1 epsilon subunit



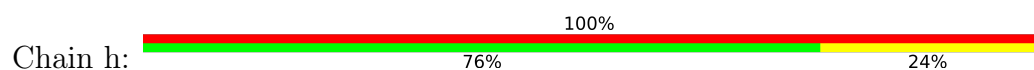
• Molecule 16: ATP synthase subunit 5, mitochondrial

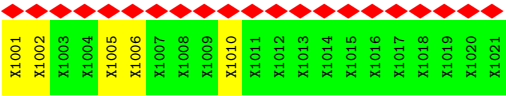


• Molecule 16: ATP synthase subunit 5, mitochondrial

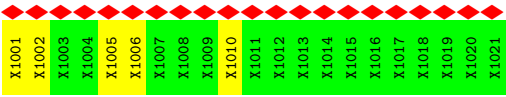
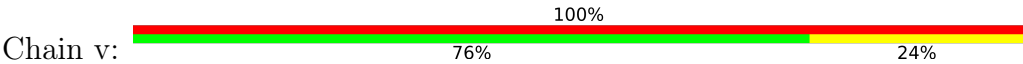


• Molecule 17: ATP synthase subunit h





● 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: ANP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.29	0/545	0.63	0/737
1	1	0.32	0/545	0.61	0/737
1	2	0.37	0/545	0.67	0/737
1	3	0.35	0/537	0.64	0/727
1	4	0.28	0/545	0.57	0/737
1	5	0.27	0/545	0.58	0/737
1	6	0.27	0/537	0.58	0/727
1	7	0.25	0/529	0.55	0/716
1	8	0.27	0/545	0.55	0/737
1	9	0.28	0/537	0.52	0/727
1	J	0.29	0/545	0.63	0/737
1	L	0.32	0/545	0.61	0/737
1	M	0.37	0/545	0.66	0/737
1	N	0.35	0/537	0.64	0/727
1	P	0.28	0/545	0.57	0/737
1	Q	0.28	0/545	0.58	0/737
1	R	0.27	0/537	0.57	0/727
1	S	0.25	0/529	0.56	0/716
1	T	0.27	0/545	0.55	0/737
1	U	0.28	0/537	0.52	0/727
2	A	0.46	0/422	0.78	0/570
2	V	0.46	0/422	0.78	0/570
3	a	0.41	0/2023	0.76	0/2758
3	p	0.41	0/2023	0.76	0/2758
4	b	0.63	0/1159	1.13	3/1599 (0.2%)
4	q	0.63	0/1159	1.13	3/1599 (0.2%)
5	d	0.85	0/936	1.20	3/1286 (0.2%)
5	r	0.85	0/936	1.20	3/1286 (0.2%)
7	f	0.44	0/624	0.82	2/845 (0.2%)
7	t	0.44	0/624	0.82	2/845 (0.2%)
9	i	0.33	0/488	0.61	0/659
9	w	0.33	0/488	0.61	0/659

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
10	k	0.23	0/185	0.73	2/250 (0.8%)
10	x	0.23	0/185	0.73	2/250 (0.8%)
11	B	0.60	0/3753	0.93	5/5080 (0.1%)
11	C	0.71	0/3793	1.03	7/5137 (0.1%)
11	K	0.66	0/3798	0.95	3/5143 (0.1%)
11	W	0.60	0/3753	0.93	5/5080 (0.1%)
11	X	0.71	0/3793	1.03	7/5137 (0.1%)
11	n	0.66	0/3798	0.95	3/5143 (0.1%)
12	D	0.70	0/3605	1.03	9/4889 (0.2%)
12	E	0.57	0/3592	0.89	0/4870
12	F	0.67	1/3599 (0.0%)	1.00	4/4881 (0.1%)
12	Y	0.70	0/3605	1.03	9/4889 (0.2%)
12	Z	0.57	0/3592	0.89	0/4870
12	c	0.67	1/3599 (0.0%)	1.00	4/4881 (0.1%)
13	G	0.57	0/2055	0.96	5/2766 (0.2%)
13	j	0.56	0/2055	0.96	5/2766 (0.2%)
14	H	0.63	0/759	1.05	0/1040
14	l	0.63	0/759	1.04	0/1040
15	I	0.63	0/326	1.19	5/445 (1.1%)
15	m	0.63	0/326	1.19	5/445 (1.1%)
16	O	0.94	1/793 (0.1%)	1.45	6/1101 (0.5%)
16	o	0.95	1/793 (0.1%)	1.45	6/1101 (0.5%)
All	All	0.60	4/74640 (0.0%)	0.94	108/101276 (0.1%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	c	297	THR	CA-CB	5.85	1.63	1.53
12	F	297	THR	CA-CB	5.82	1.63	1.53
16	o	127	GLU	CA-C	5.46	1.59	1.52
16	O	127	GLU	CA-C	5.45	1.59	1.52

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Y	224	GLU	CA-C-N	10.45	127.29	119.66
12	Y	224	GLU	C-N-CA	10.45	127.29	119.66
12	D	224	GLU	CA-C-N	10.38	127.24	119.66
12	D	224	GLU	C-N-CA	10.38	127.24	119.66
15	I	16	VAL	N-CA-C	-7.61	105.73	112.12

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	Mainchain,Peptide
4	q	186	ASN	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	0	537	0	582	5	0
1	1	537	0	582	5	0
1	2	537	0	582	8	0
1	3	529	0	570	4	0
1	4	537	0	582	5	0
1	5	537	0	582	6	0
1	6	529	0	570	7	0
1	7	522	0	570	20	0
1	8	537	0	582	10	0
1	9	529	0	570	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	537	0	582	5	0
1	L	537	0	582	5	0
1	M	537	0	582	9	0
1	N	529	0	570	5	0
1	P	537	0	582	6	0
1	Q	537	0	582	6	0
1	R	529	0	570	7	0
1	S	522	0	570	20	0
1	T	537	0	582	10	0
1	U	529	0	570	5	0
2	A	410	0	444	5	0
2	V	410	0	444	5	0
3	a	1971	0	2071	39	0
3	p	1971	0	2071	37	0
4	b	1153	0	781	2	0
4	q	1153	0	781	2	0
5	d	930	0	618	15	0
5	r	930	0	618	16	0
6	e	245	0	51	0	0
6	s	245	0	51	0	0
7	f	607	0	527	30	0
7	t	607	0	527	30	0
8	g	530	0	108	0	0
8	u	530	0	108	0	0
9	i	473	0	476	1	0
9	w	473	0	476	1	0
10	k	180	0	192	1	0
10	x	180	0	192	1	0
11	B	3700	0	3749	125	0
11	C	3739	0	3767	94	0
11	K	3745	0	3769	95	0
11	W	3700	0	3749	124	0
11	X	3739	0	3767	93	0
11	n	3745	0	3769	99	0
12	D	3549	0	3620	81	0
12	E	3536	0	3610	101	0
12	F	3543	0	3615	112	0
12	Y	3549	0	3620	79	0
12	Z	3536	0	3610	108	0
12	c	3543	0	3615	109	0
13	G	2030	0	2081	57	0
13	j	2030	0	2081	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	H	751	0	598	58	0
14	l	751	0	598	56	0
15	I	324	0	249	23	0
15	m	324	0	249	21	0
16	O	795	0	367	12	0
16	o	795	0	367	12	0
17	h	105	0	23	4	0
17	v	105	0	23	4	0
18	B	31	0	13	1	0
18	C	31	0	13	3	0
18	D	31	0	13	3	0
18	F	31	0	13	7	0
18	K	31	0	13	1	0
18	W	31	0	13	1	0
18	X	31	0	13	3	0
18	Y	31	0	13	3	0
18	c	31	0	13	7	0
18	n	31	0	13	1	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	D	1	0	0	0	0
19	F	1	0	0	0	0
19	K	1	0	0	0	0
19	W	1	0	0	0	0
19	X	1	0	0	0	0
19	Y	1	0	0	0	0
19	c	1	0	0	0	0
19	n	1	0	0	0	0
All	All	75614	0	73106	1599	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 11.

The worst 5 of 1599 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)
3:p:80:LYS:CG	7:t:1:VAL:CB	1.82	1.56
3:a:80:LYS:CG	7:f:1:VAL:CB	1.82	1.53
1:T:41:PRO:CG	14:l:42:LEU:HD11	1.46	1.45
3:p:80:LYS:HG3	7:t:1:VAL:CB	0.96	1.44
1:8:41:PRO:CG	14:H:42:LEU:HD11	1.46	1.42

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	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
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	30
2	V	46/48 (96%)	43 (94%)	2 (4%)	1 (2%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	32
4	q	196/209 (94%)	186 (95%)	6 (3%)	4 (2%)	6	32
5	d	153/173 (88%)	145 (95%)	7 (5%)	1 (1%)	18	51
5	r	153/173 (88%)	145 (95%)	7 (5%)	1 (1%)	18	51
7	f	80/95 (84%)	70 (88%)	9 (11%)	1 (1%)	9	39
7	t	80/95 (84%)	70 (88%)	9 (11%)	1 (1%)	9	39
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	61
11	C	496/510 (97%)	449 (90%)	44 (9%)	3 (1%)	21	54
11	K	495/510 (97%)	434 (88%)	56 (11%)	5 (1%)	12	45
11	W	486/510 (95%)	439 (90%)	45 (9%)	2 (0%)	30	61
11	X	496/510 (97%)	449 (90%)	44 (9%)	3 (1%)	21	54
11	n	495/510 (97%)	434 (88%)	56 (11%)	5 (1%)	12	45
12	D	468/478 (98%)	429 (92%)	37 (8%)	2 (0%)	30	61
12	E	466/478 (98%)	424 (91%)	36 (8%)	6 (1%)	9	39
12	F	467/478 (98%)	417 (89%)	42 (9%)	8 (2%)	7	35
12	Y	468/478 (98%)	429 (92%)	37 (8%)	2 (0%)	30	61
12	Z	466/478 (98%)	424 (91%)	36 (8%)	6 (1%)	9	39
12	c	467/478 (98%)	417 (89%)	42 (9%)	8 (2%)	7	35
13	G	261/278 (94%)	229 (88%)	25 (10%)	7 (3%)	4	27
13	j	261/278 (94%)	230 (88%)	24 (9%)	7 (3%)	4	27
14	H	109/138 (79%)	89 (82%)	15 (14%)	5 (5%)	2	17
14	l	109/138 (79%)	89 (82%)	15 (14%)	5 (5%)	2	17
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	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	o	157/195 (80%)	126 (80%)	24 (15%)	7 (4%)	2	17
All	All	9946/10594 (94%)	9045 (91%)	785 (8%)	116 (1%)	13	41

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%)	54 (98%)	1 (2%)	51	68
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%)	54 (98%)	1 (2%)	51	68
1	5	55/56 (98%)	53 (96%)	2 (4%)	31	56
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%)	54 (98%)	1 (2%)	51	68
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%)	54 (98%)	1 (2%)	51	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	55/56 (98%)	53 (96%)	2 (4%)	31	56
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%)	215 (99%)	2 (1%)	70	76
3	p	217/217 (100%)	215 (99%)	2 (1%)	70	76
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%)	41 (98%)	1 (2%)	43	63
5	r	42/158 (27%)	41 (98%)	1 (2%)	43	63
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
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%)	345 (90%)	39 (10%)	7	30
11	C	384/412 (93%)	349 (91%)	35 (9%)	9	33
11	K	384/412 (93%)	359 (94%)	25 (6%)	15	43
11	W	384/412 (93%)	345 (90%)	39 (10%)	7	30
11	X	384/412 (93%)	349 (91%)	35 (9%)	9	33
11	n	384/412 (93%)	359 (94%)	25 (6%)	15	43
12	D	380/384 (99%)	350 (92%)	30 (8%)	11	37
12	E	378/384 (98%)	355 (94%)	23 (6%)	17	45
12	F	379/384 (99%)	352 (93%)	27 (7%)	13	40
12	Y	380/384 (99%)	350 (92%)	30 (8%)	11	37
12	Z	378/384 (98%)	355 (94%)	23 (6%)	17	45
12	c	379/384 (99%)	352 (93%)	27 (7%)	13	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	G	218/236 (92%)	185 (85%)	33 (15%)	3	17
13	j	218/236 (92%)	185 (85%)	33 (15%)	3	17
14	H	54/112 (48%)	41 (76%)	13 (24%)	1	5
14	l	54/112 (48%)	41 (76%)	13 (24%)	1	5
15	I	23/48 (48%)	19 (83%)	4 (17%)	2	12
15	m	23/48 (48%)	19 (83%)	4 (17%)	2	12
All	All	7194/8260 (87%)	6722 (93%)	472 (7%)	17	43

5 of 472 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	H	86	THR
13	j	216	ASN
11	W	233	ILE
13	j	155	LYS
12	c	163	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
11	n	454	HIS
11	X	217	GLN
11	W	67	ASN
11	W	343	ASN
12	Z	43	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	c	501	19	33,33,33	2.88	11 (33%)	45,52,52	2.08	15 (33%)
18	ANP	n	601	19	33,33,33	2.89	11 (33%)	45,52,52	1.90	12 (26%)
18	ANP	K	601	19	33,33,33	2.88	11 (33%)	45,52,52	1.90	12 (26%)
18	ANP	D	501	19	33,33,33	2.95	11 (33%)	45,52,52	2.15	16 (35%)
18	ANP	C	601	19	33,33,33	2.80	12 (36%)	45,52,52	2.24	14 (31%)
18	ANP	W	601	19	33,33,33	2.90	10 (30%)	45,52,52	1.85	11 (24%)
18	ANP	Y	501	19	33,33,33	2.96	11 (33%)	45,52,52	2.14	17 (37%)
18	ANP	X	601	19	33,33,33	2.81	12 (36%)	45,52,52	2.23	14 (31%)
18	ANP	F	501	19	33,33,33	2.88	11 (33%)	45,52,52	2.08	15 (33%)
18	ANP	B	601	19	33,33,33	2.90	11 (33%)	45,52,52	1.86	11 (24%)

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

The worst 5 of 111 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 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	X	601	ANP	O4'-C1'-N9	6.66	120.89	108.09
18	C	601	ANP	O4'-C1'-N9	6.64	120.83	108.09
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

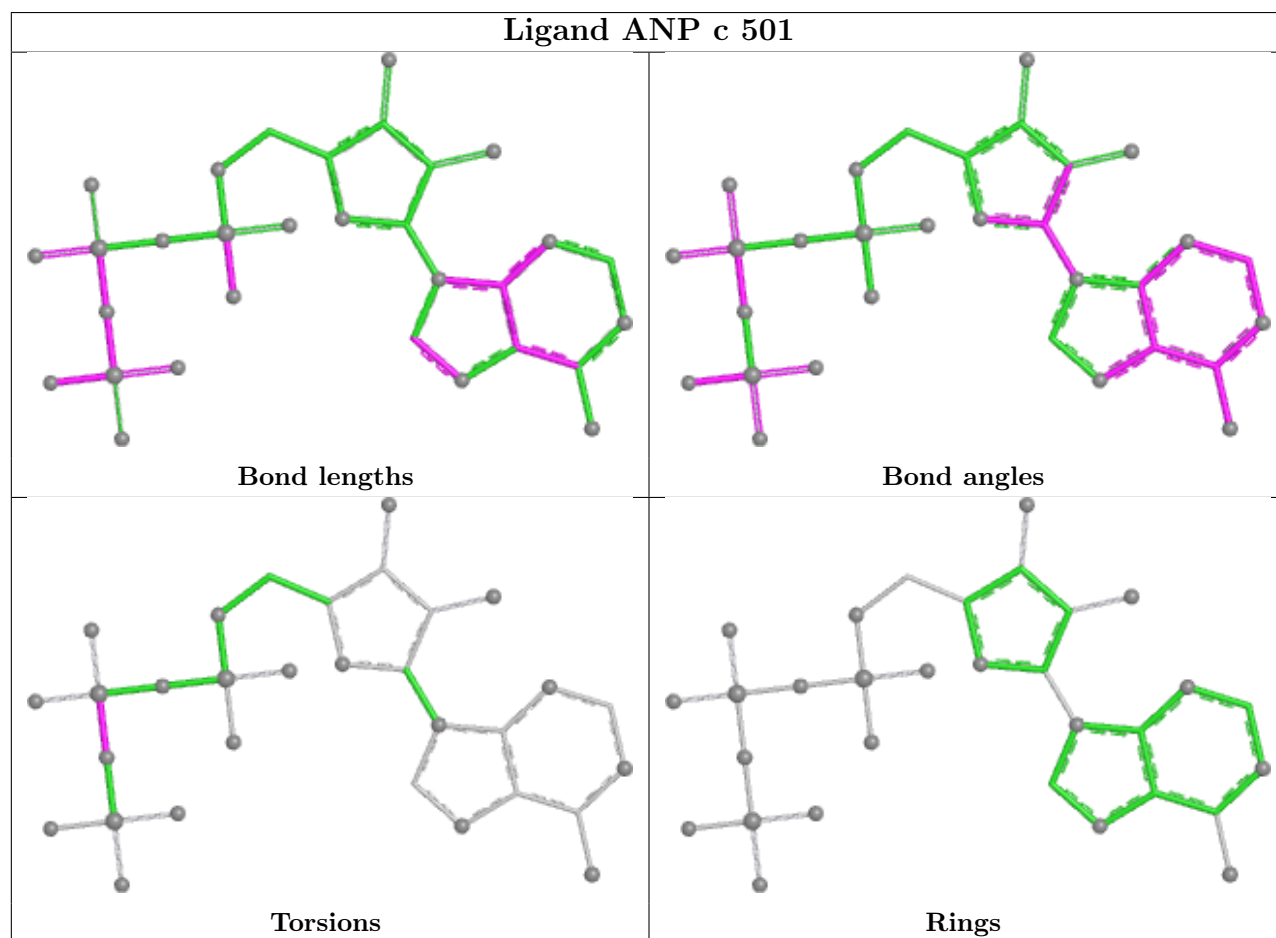
There are no ring outliers.

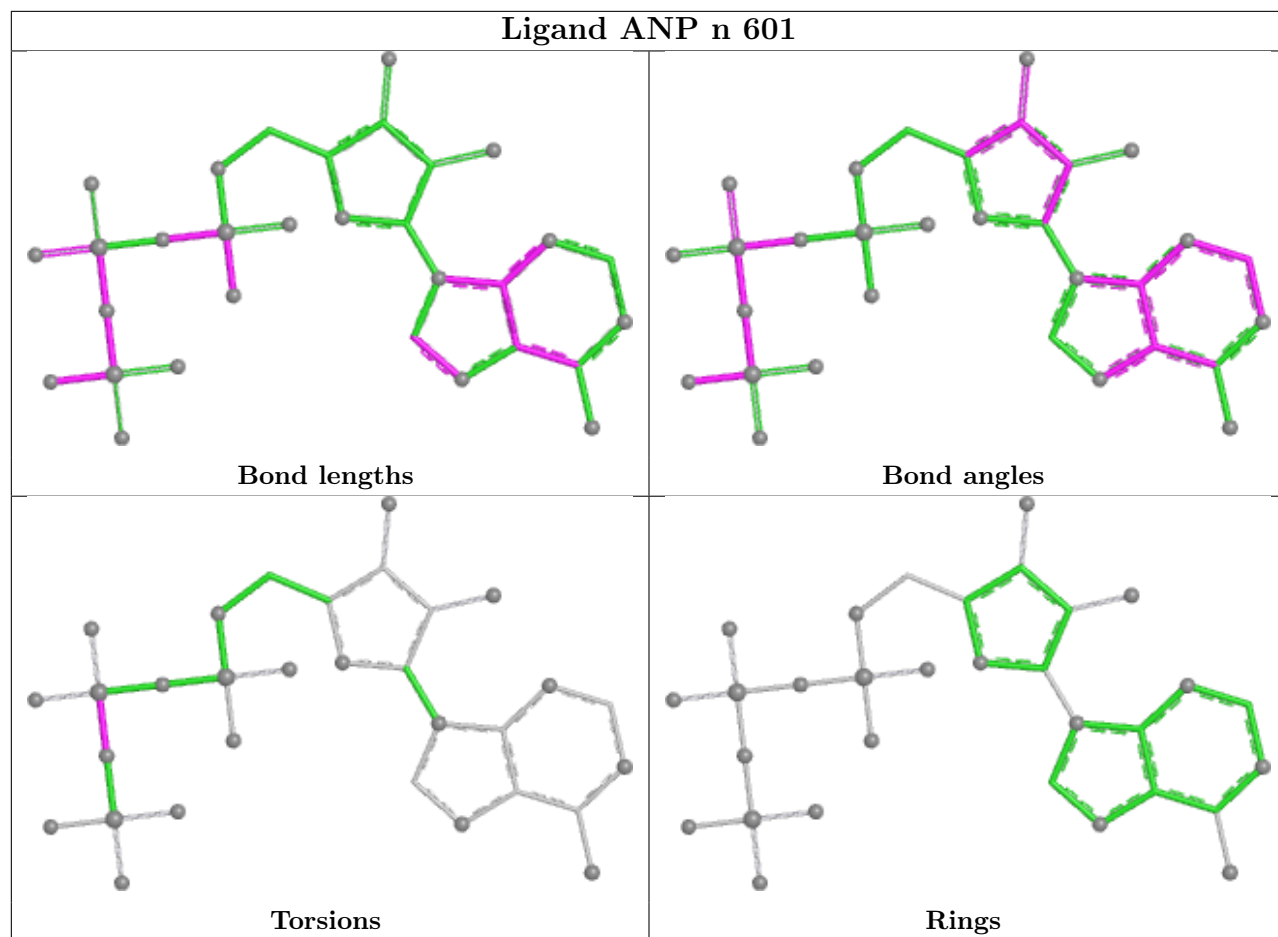
10 monomers are involved in 30 short contacts:

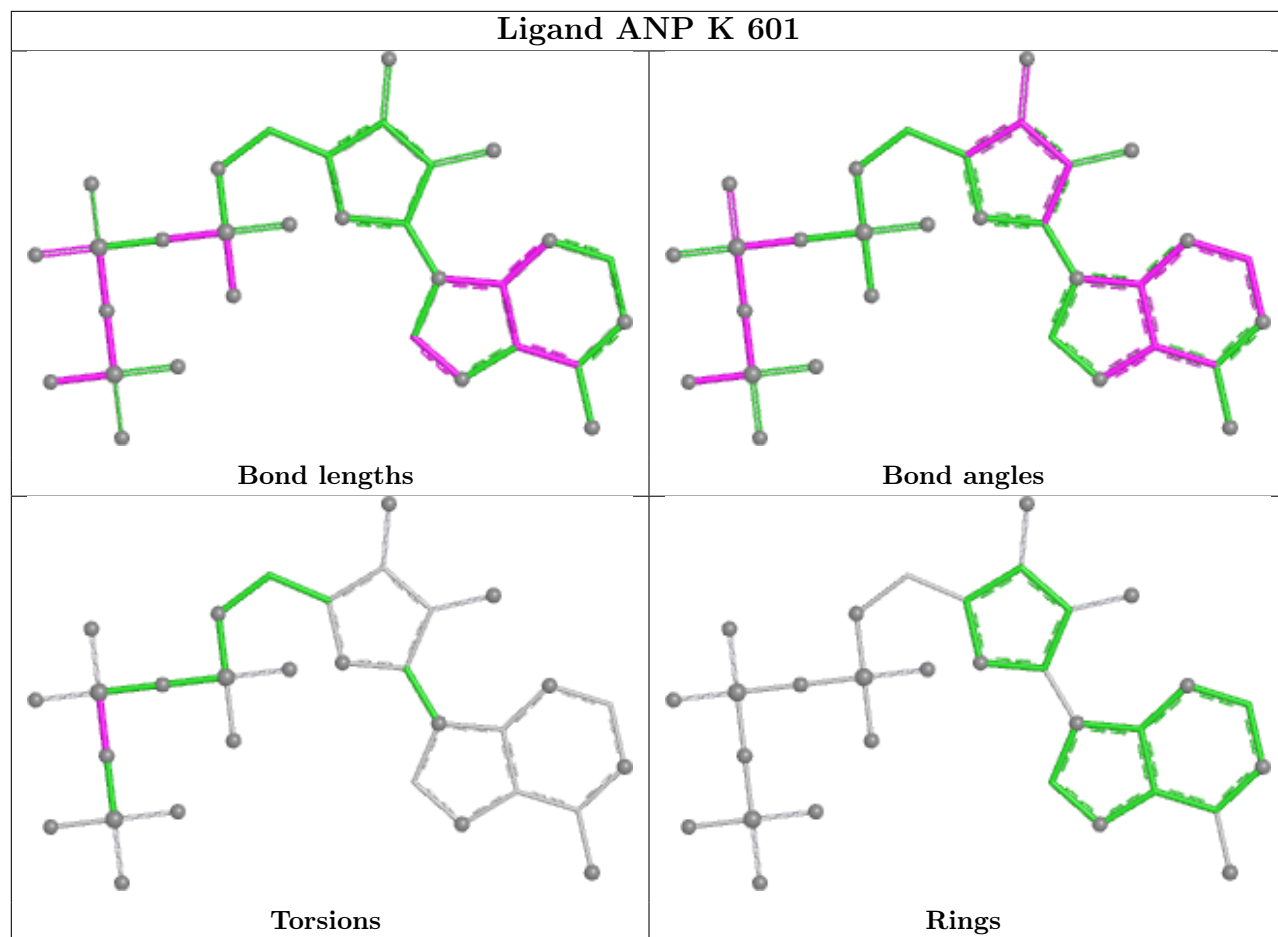
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	c	501	ANP	7	0
18	n	601	ANP	1	0
18	K	601	ANP	1	0
18	D	501	ANP	3	0
18	C	601	ANP	3	0
18	W	601	ANP	1	0
18	Y	501	ANP	3	0
18	X	601	ANP	3	0
18	F	501	ANP	7	0
18	B	601	ANP	1	0

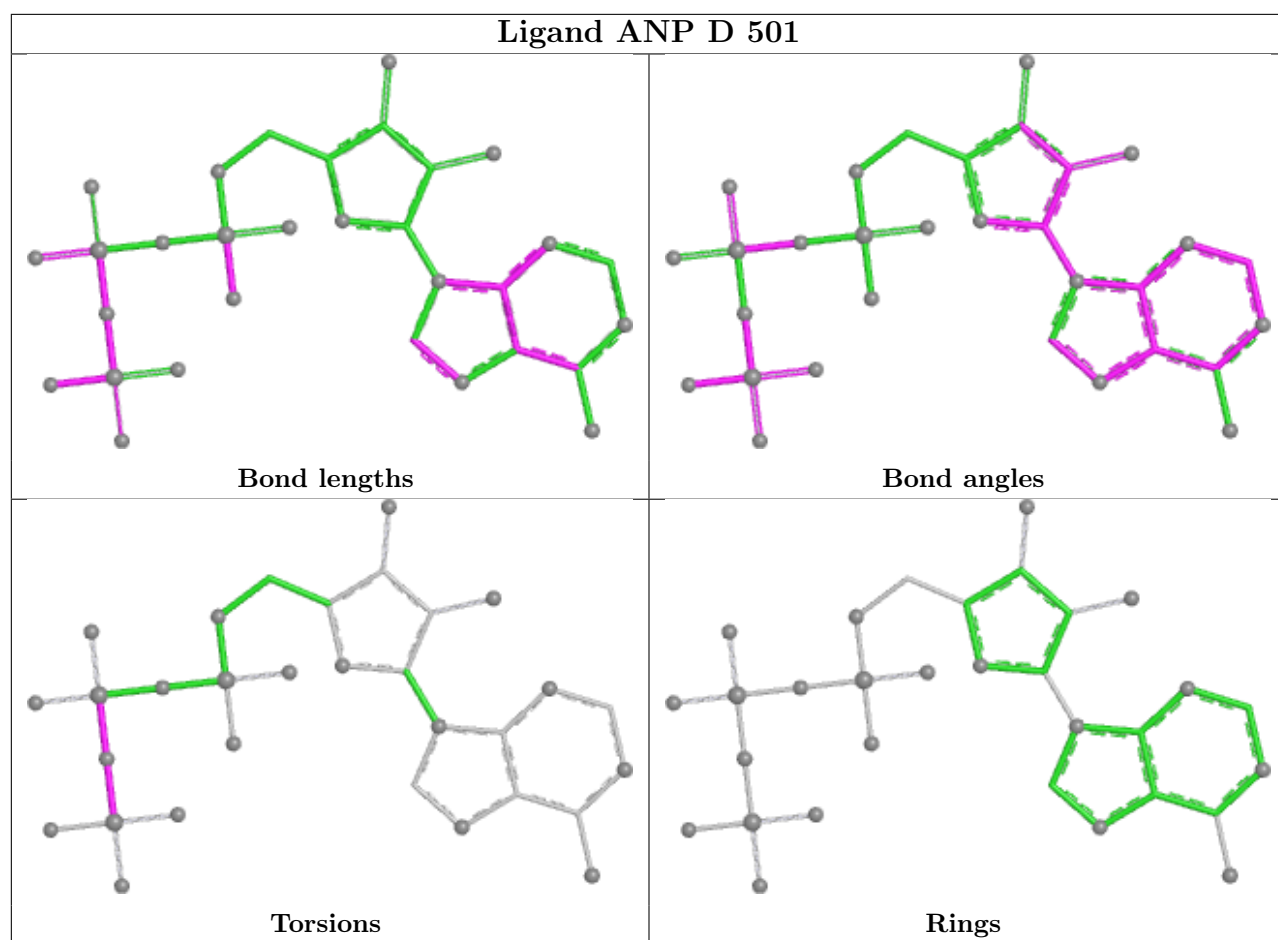
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

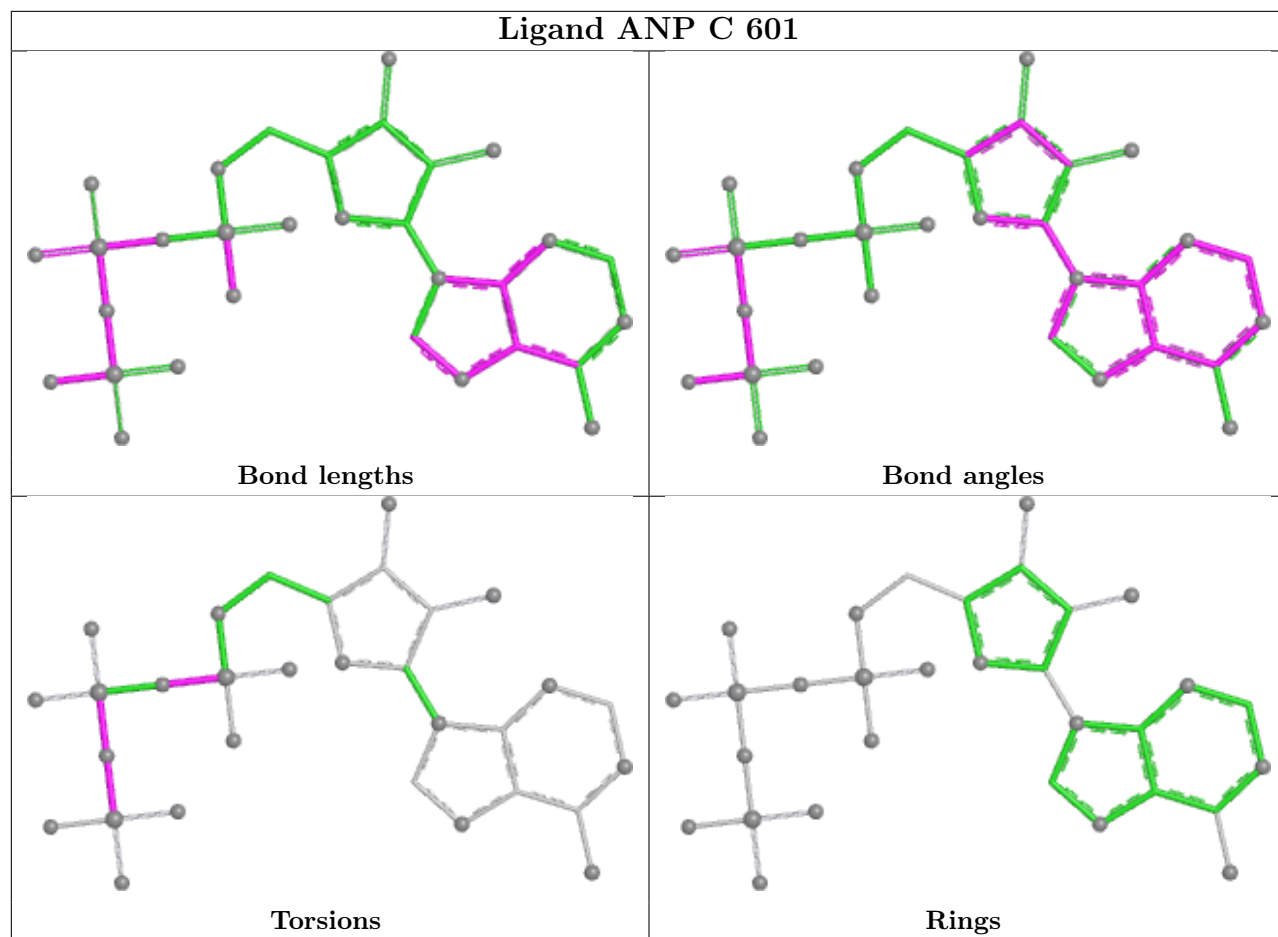
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

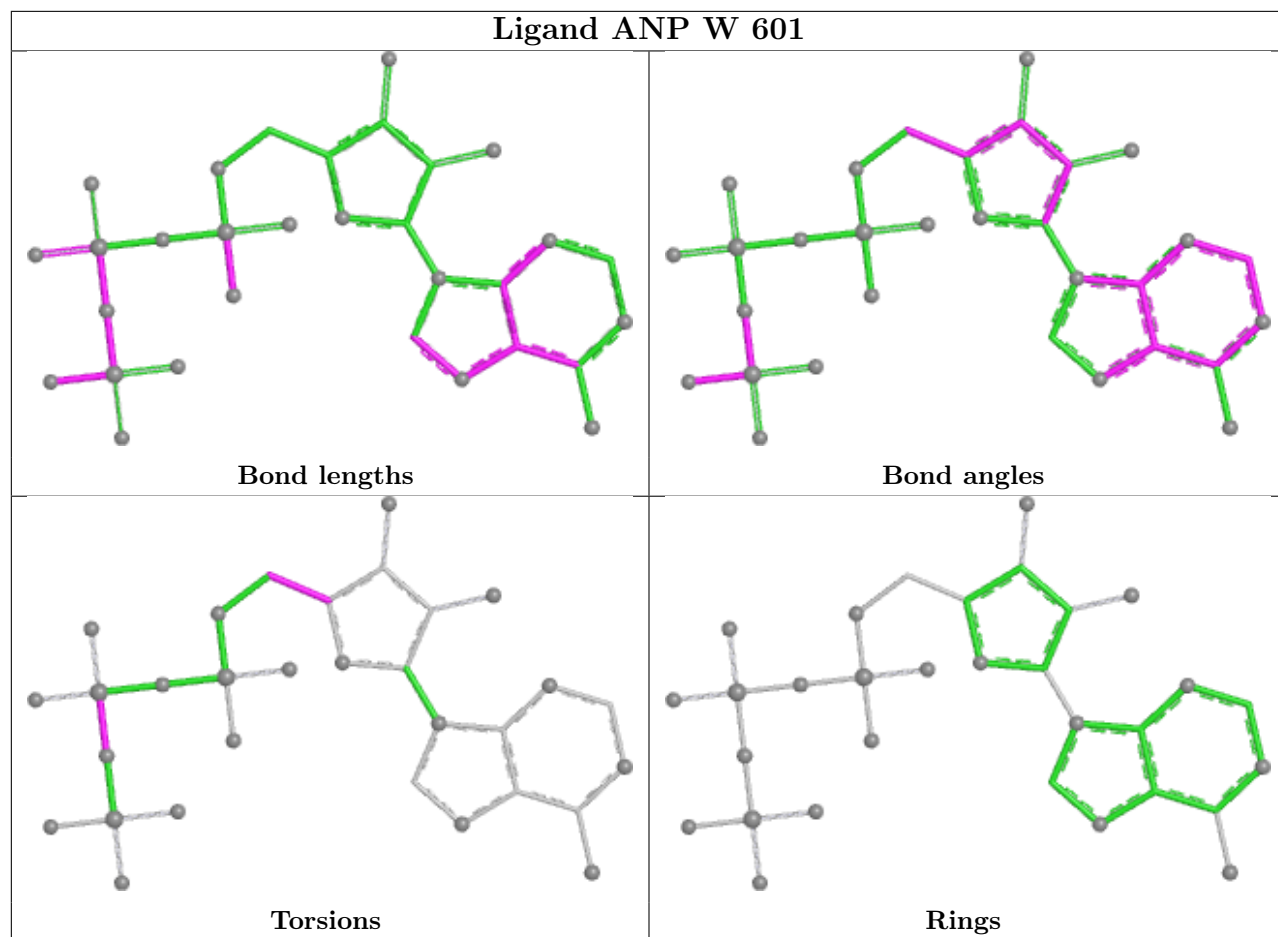


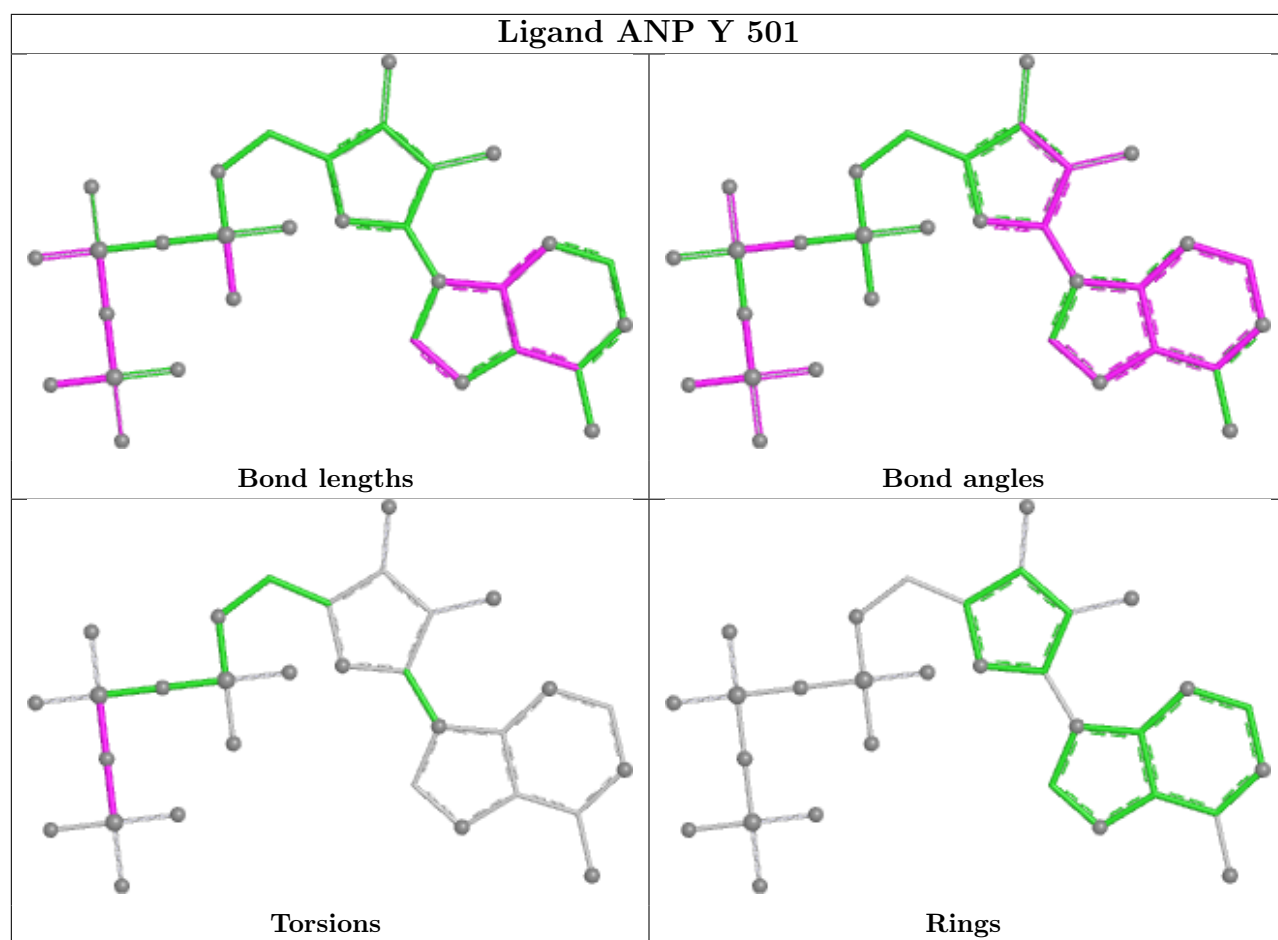


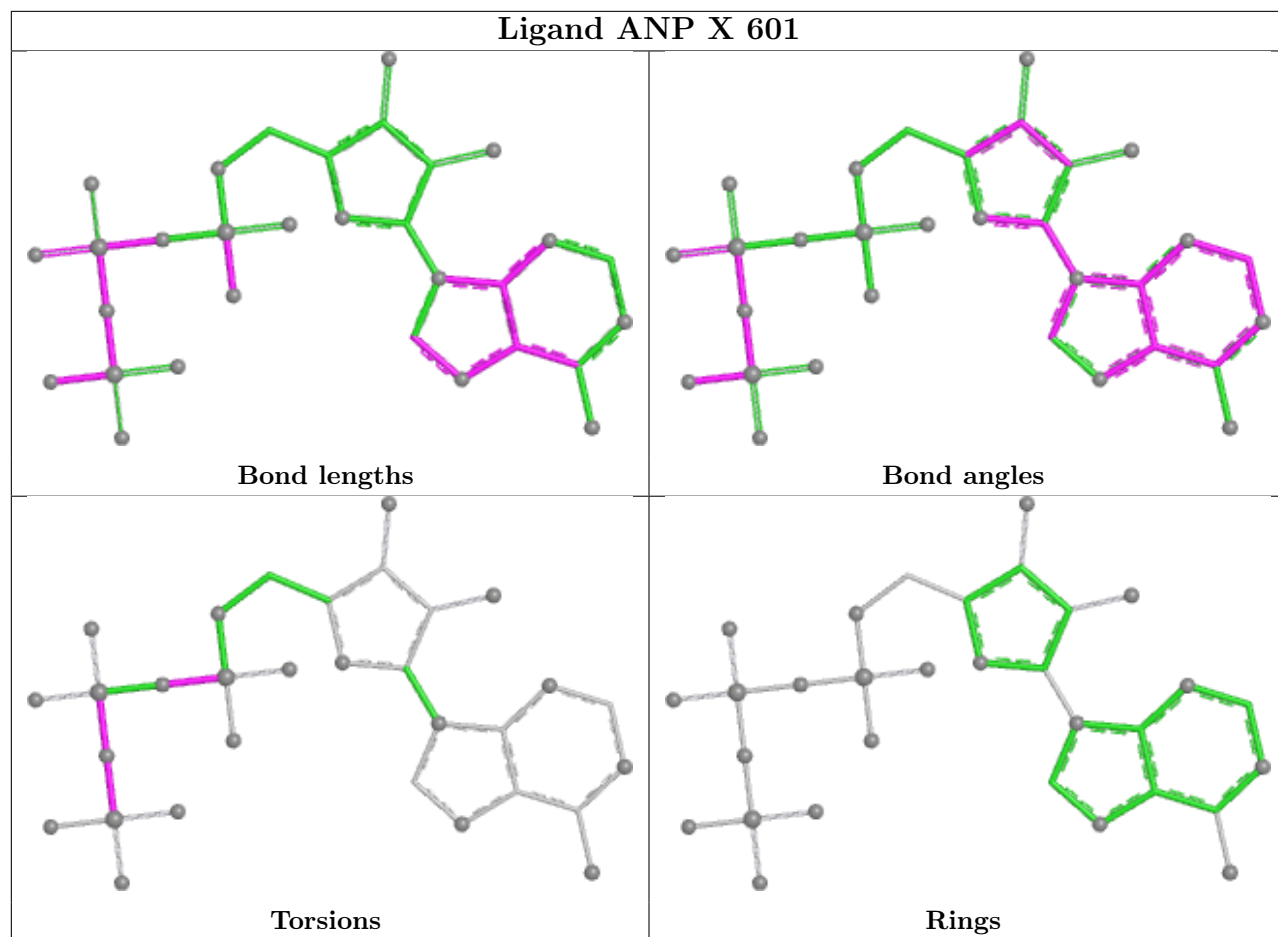


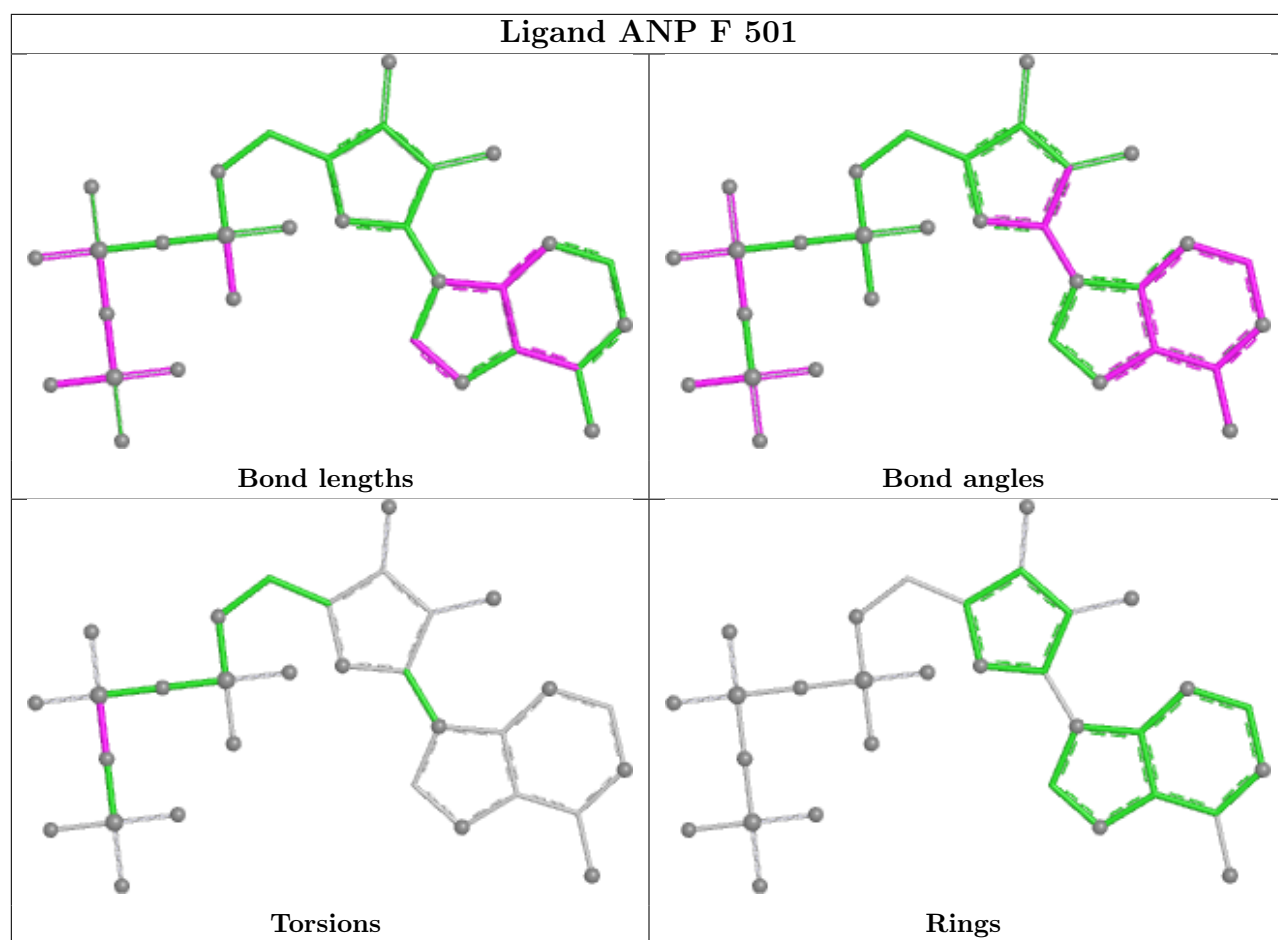


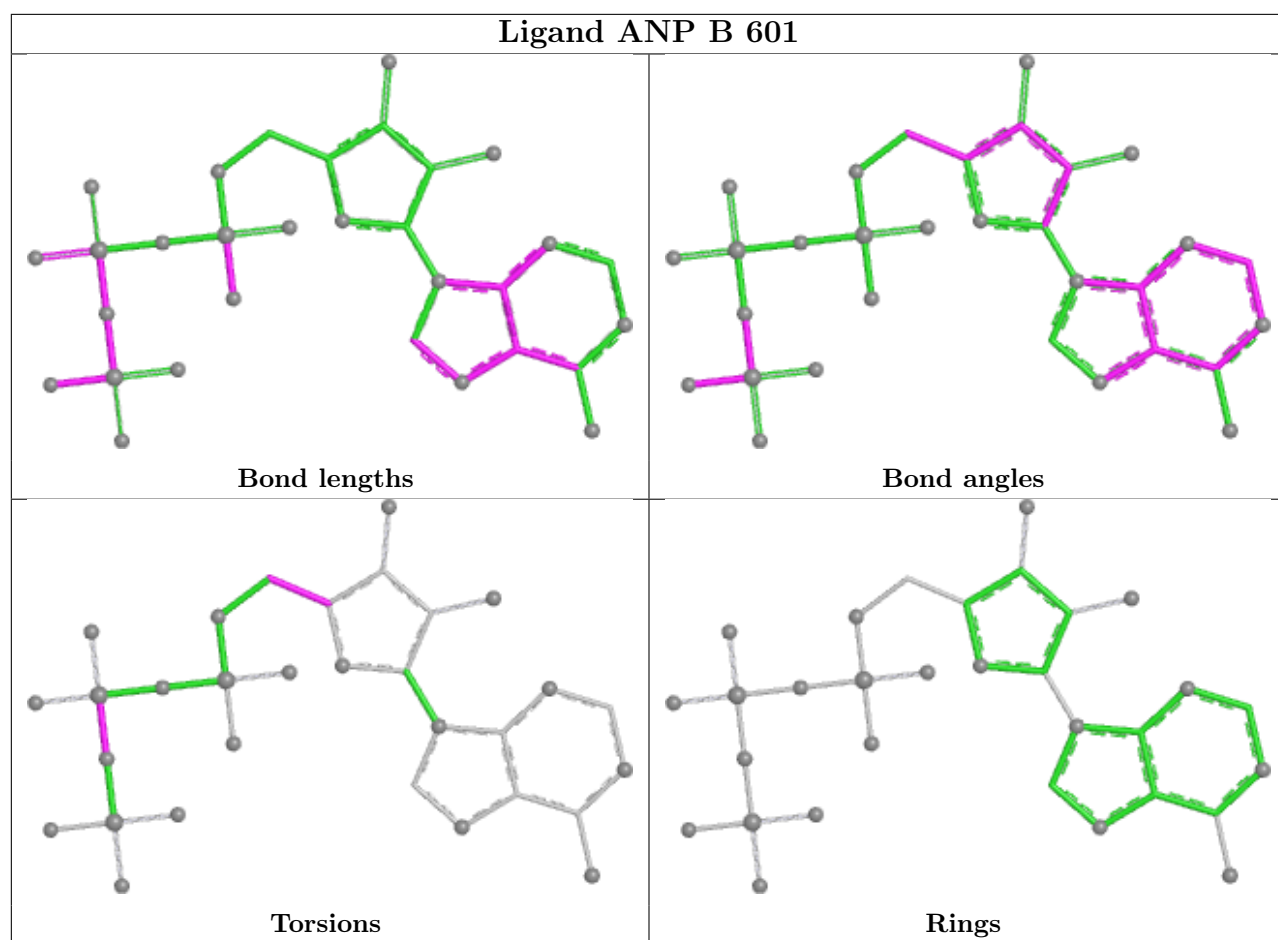












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

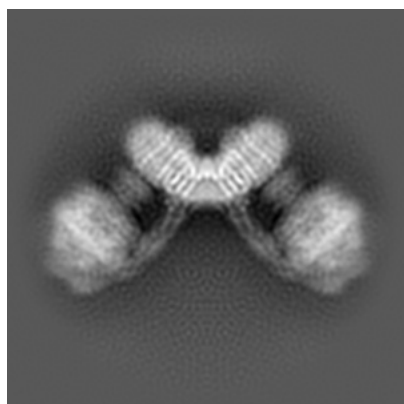
6 Map visualisation [i](#)

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

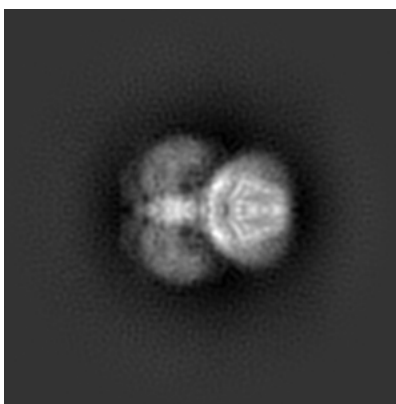
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

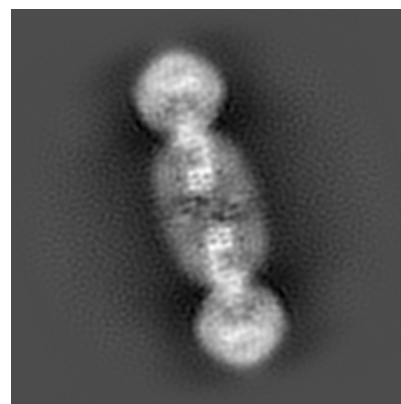
6.1.1 Primary map



X

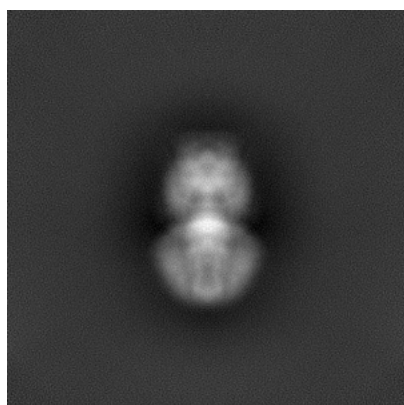


Y

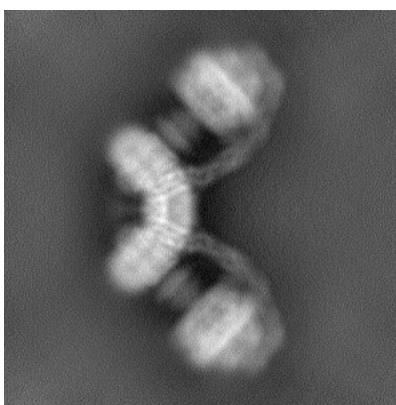


Z

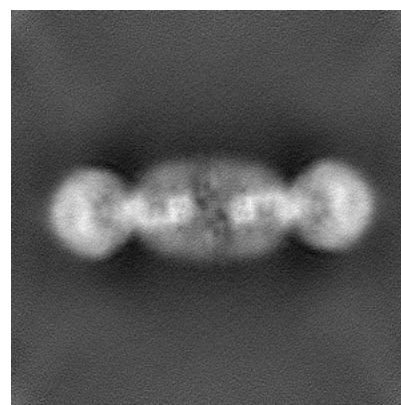
6.1.2 Raw map



X



Y

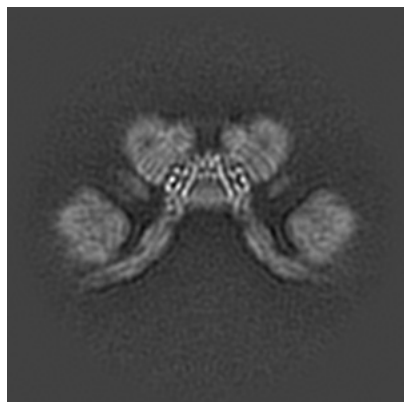


Z

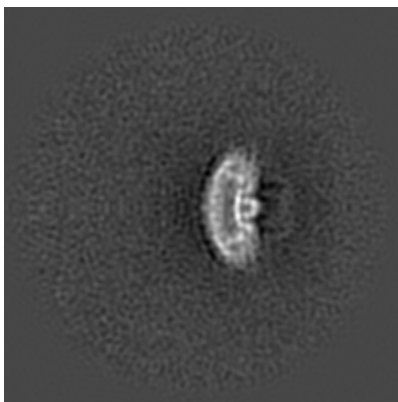
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

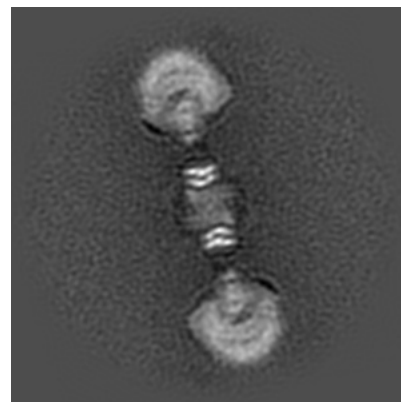
6.2.1 Primary map



X Index: 160

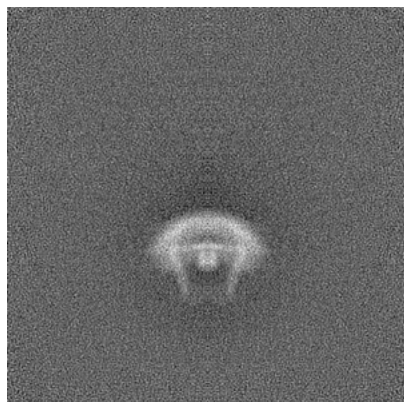


Y Index: 160

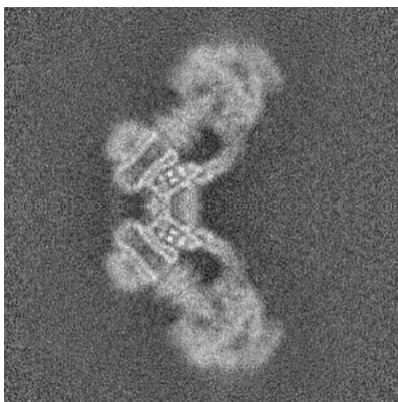


Z Index: 160

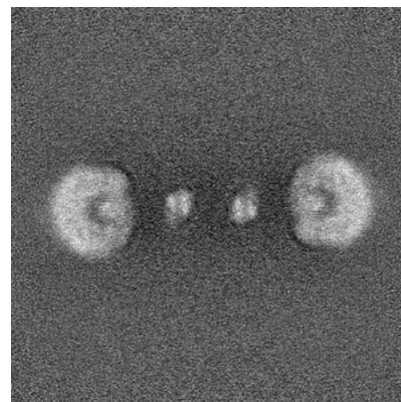
6.2.2 Raw map



X Index: 160



Y Index: 160

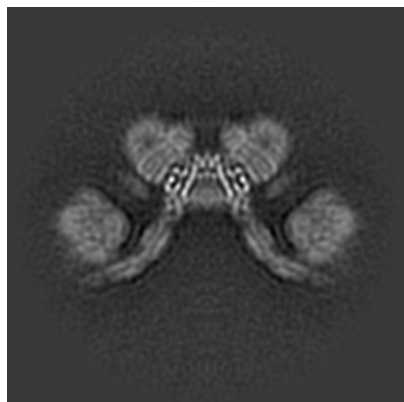


Z Index: 160

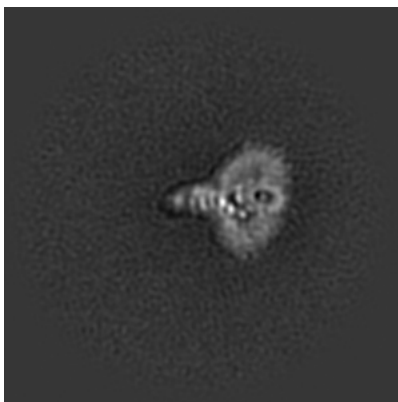
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

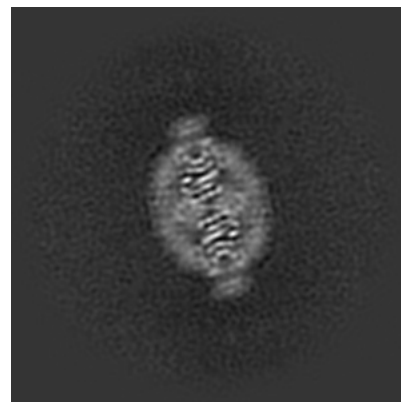
6.3.1 Primary map



X Index: 159

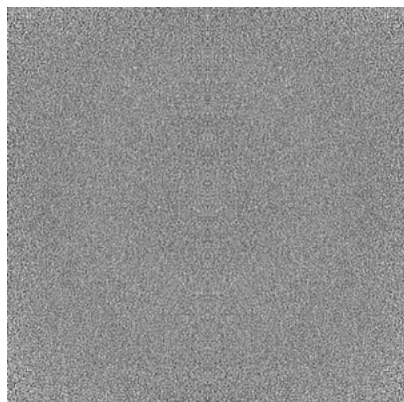


Y Index: 130

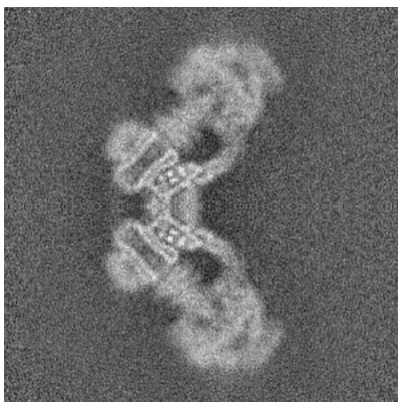


Z Index: 188

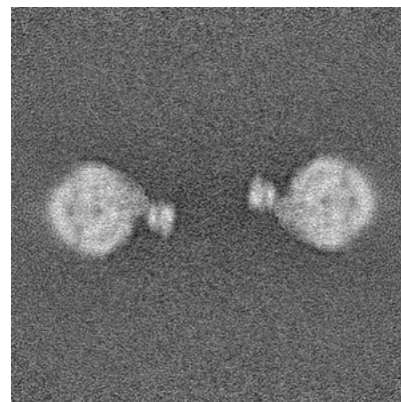
6.3.2 Raw map



X Index: 0



Y Index: 160

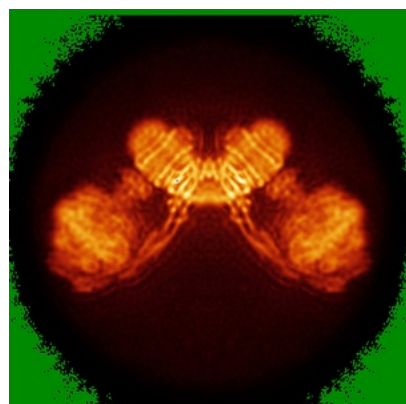


Z Index: 181

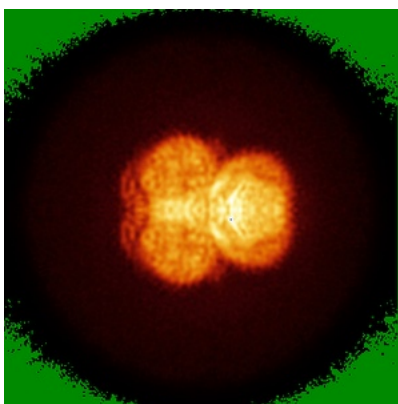
The images above show the largest variance slices of the map in three orthogonal directions.

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

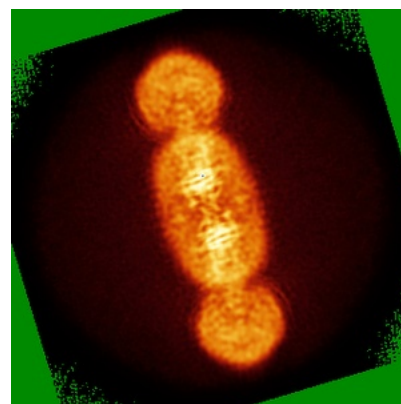
6.4.1 Primary map



X

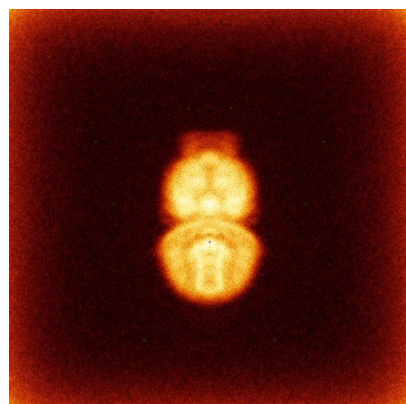


Y

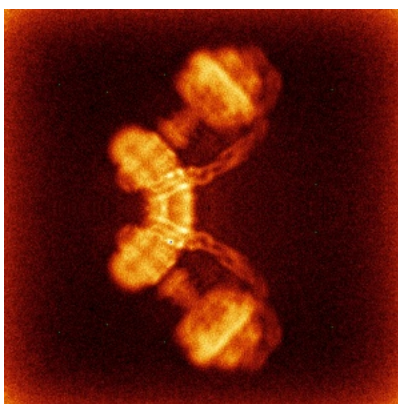


Z

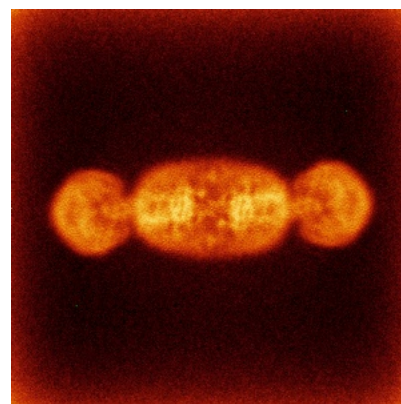
6.4.2 Raw map



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.

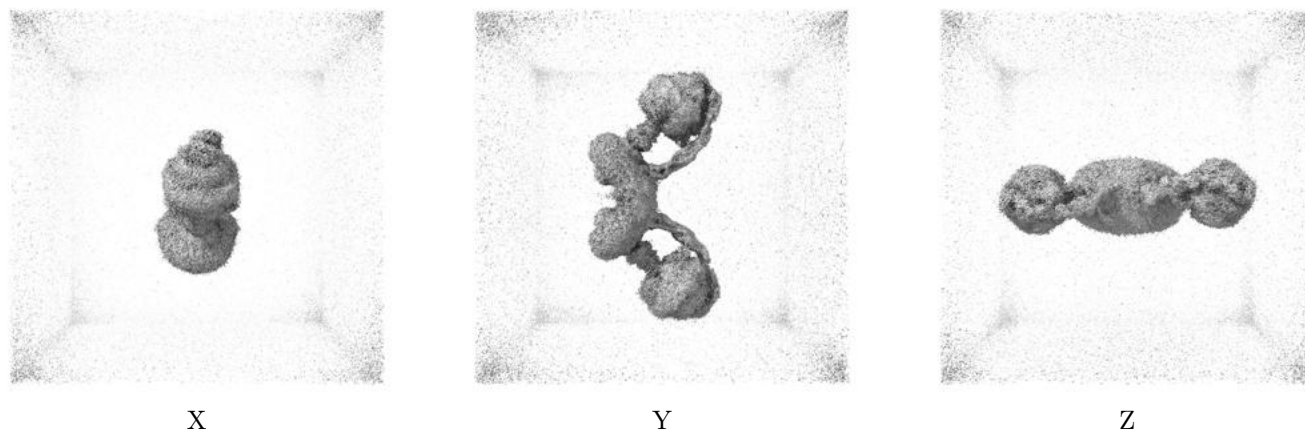
6.5 Orthogonal surface views [i](#)

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.

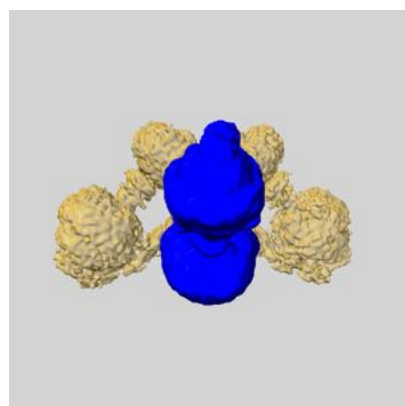
6.6 Mask visualisation [i](#)

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

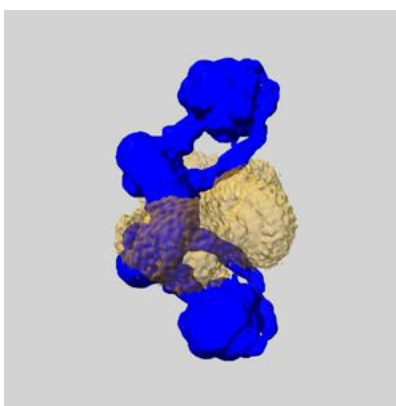
A mask typically either:

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

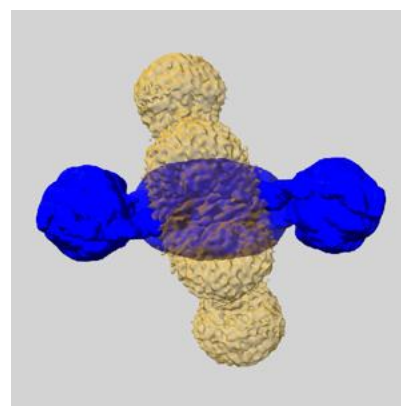
6.6.1 emd_7067_msk_1.map [i](#)



X



Y

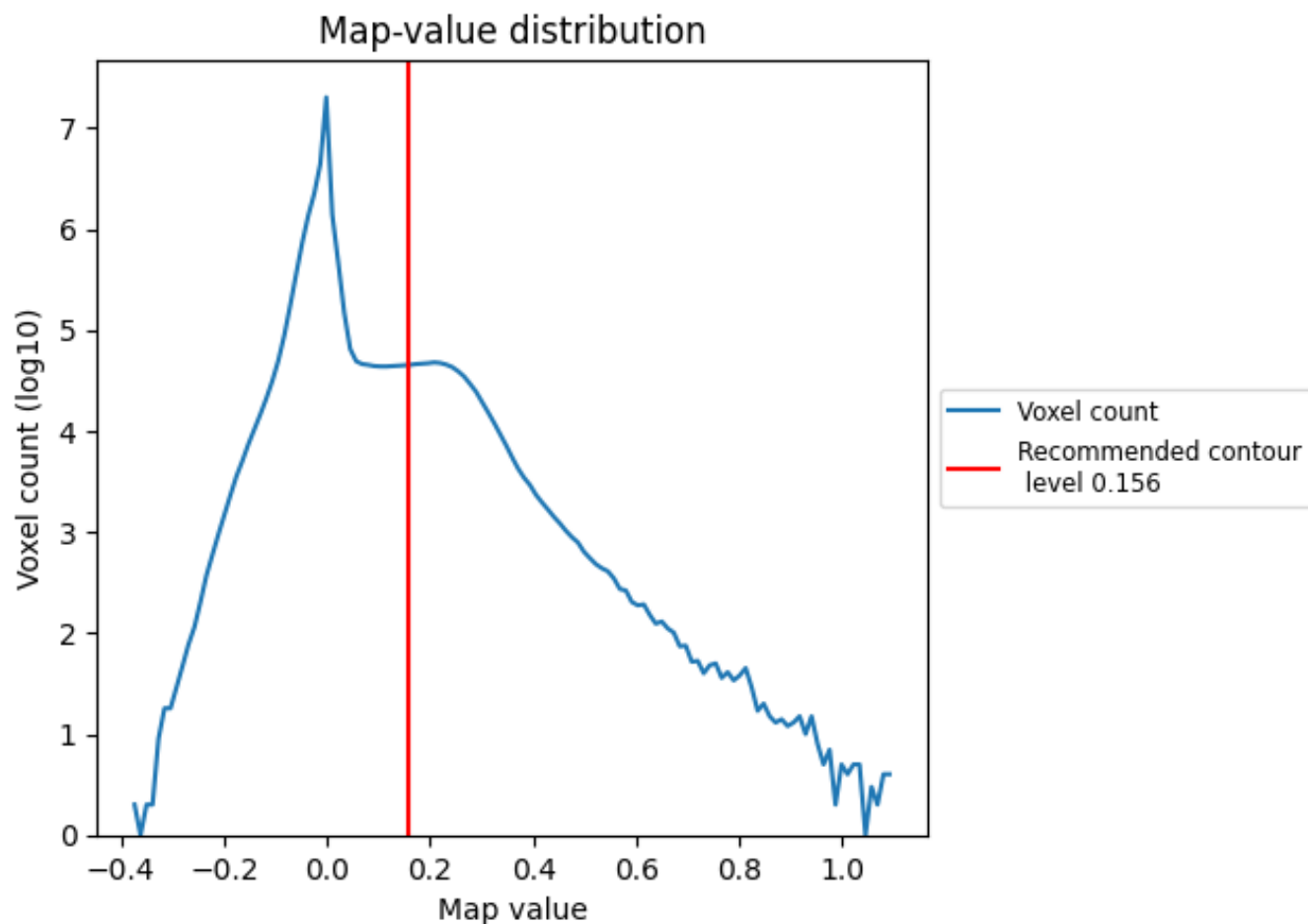


Z

7 Map analysis [i](#)

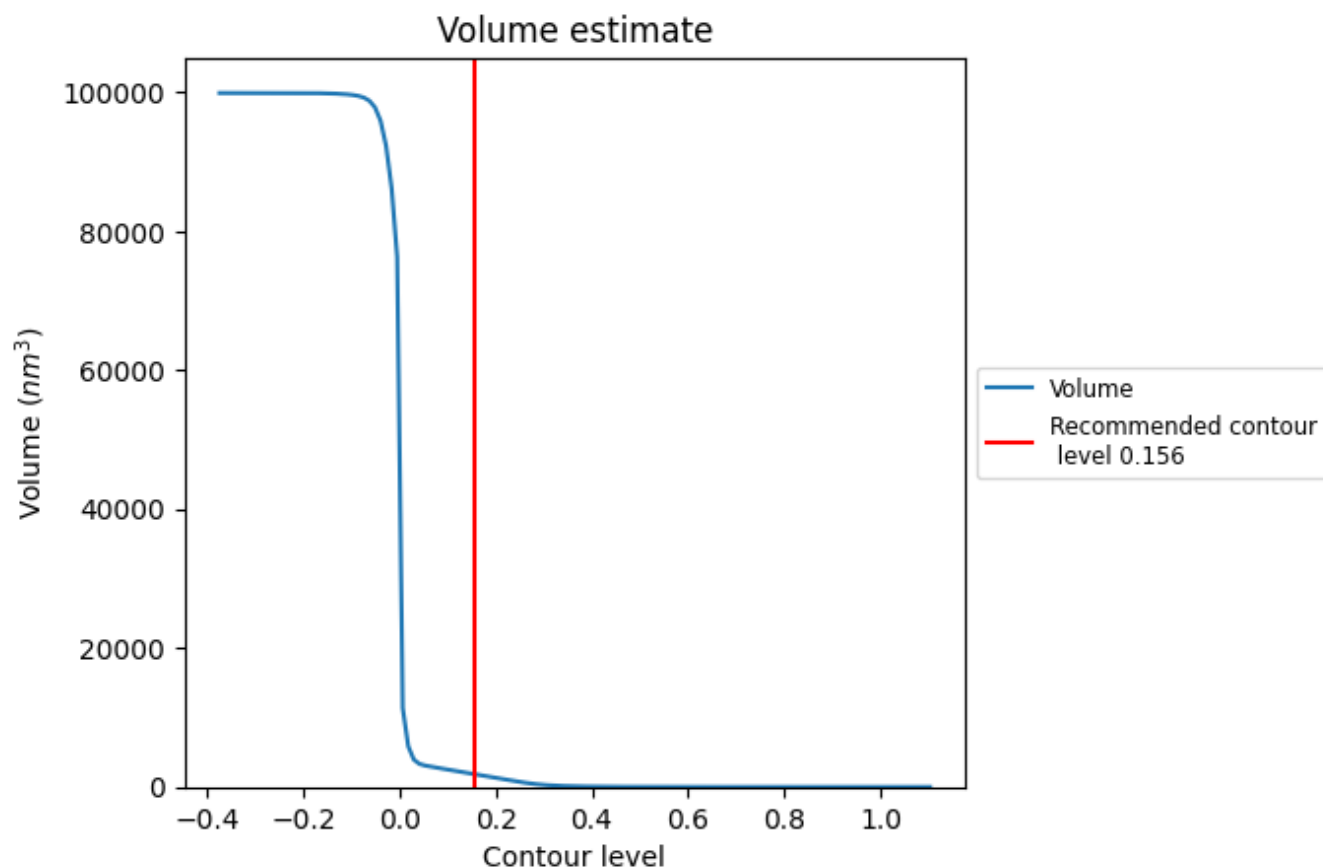
This section contains the results of statistical analysis of the map.

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.

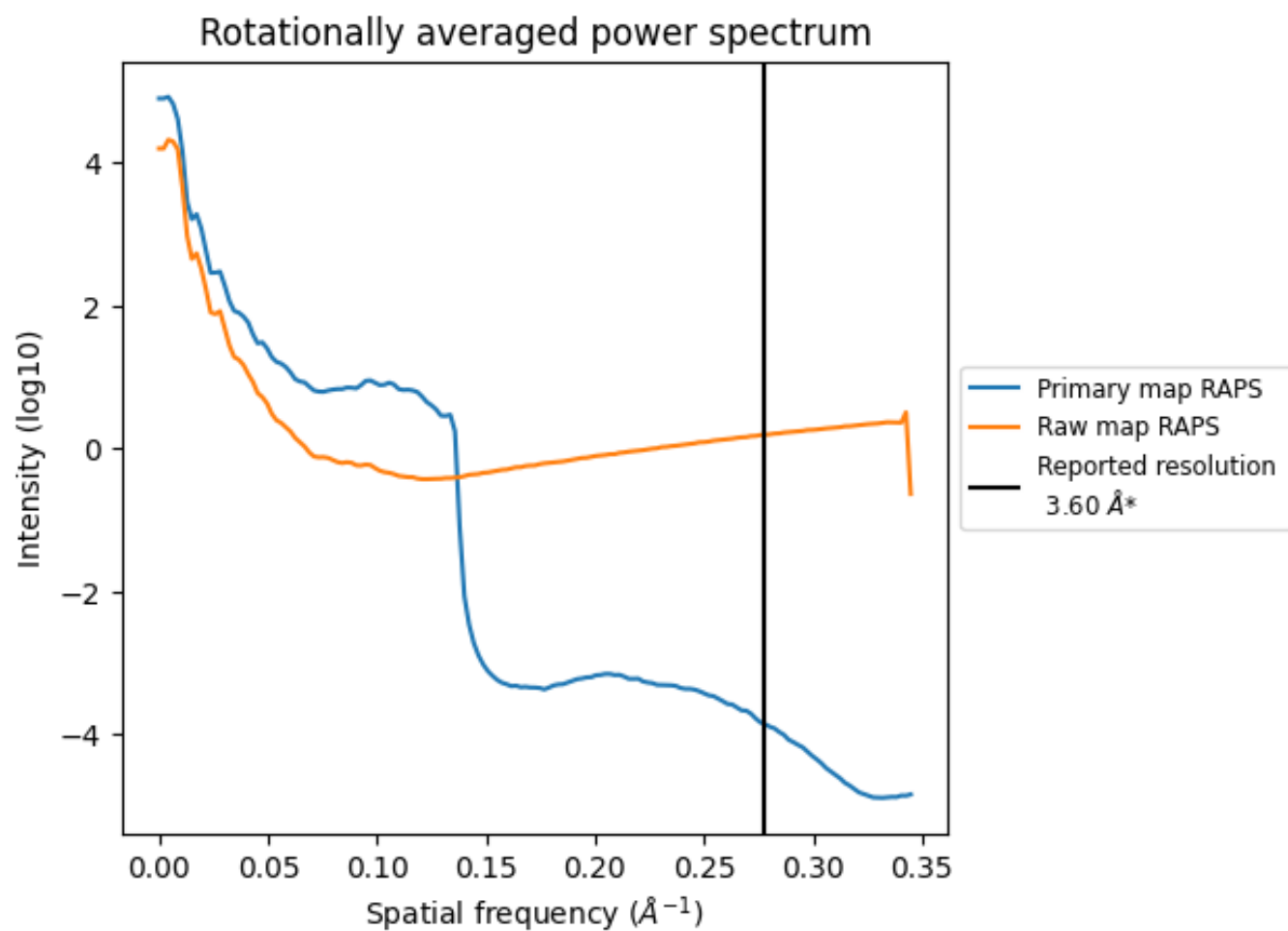
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1866 nm^3 ; 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 ⓘ

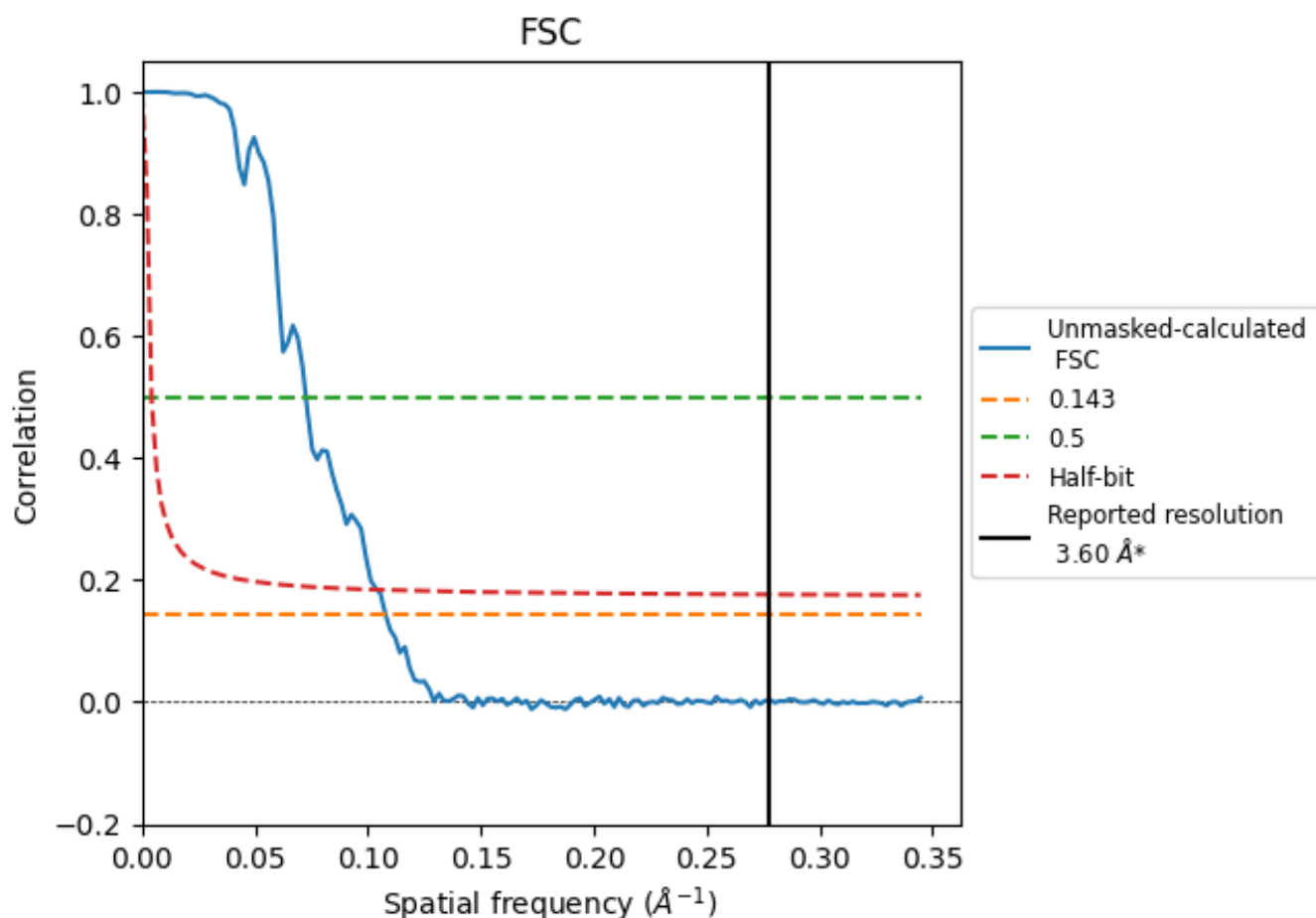


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

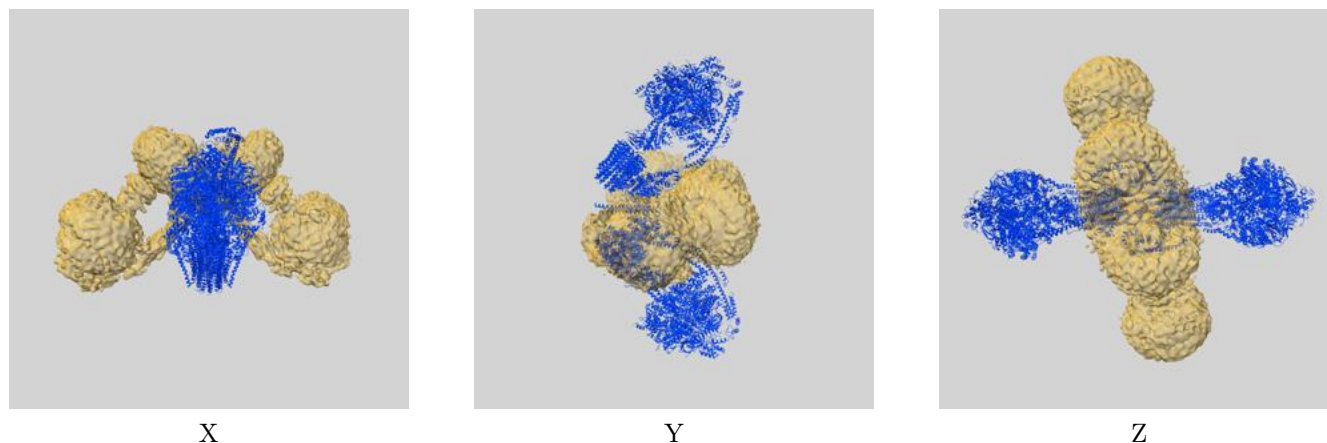
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.28	13.77	9.61

*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](#)

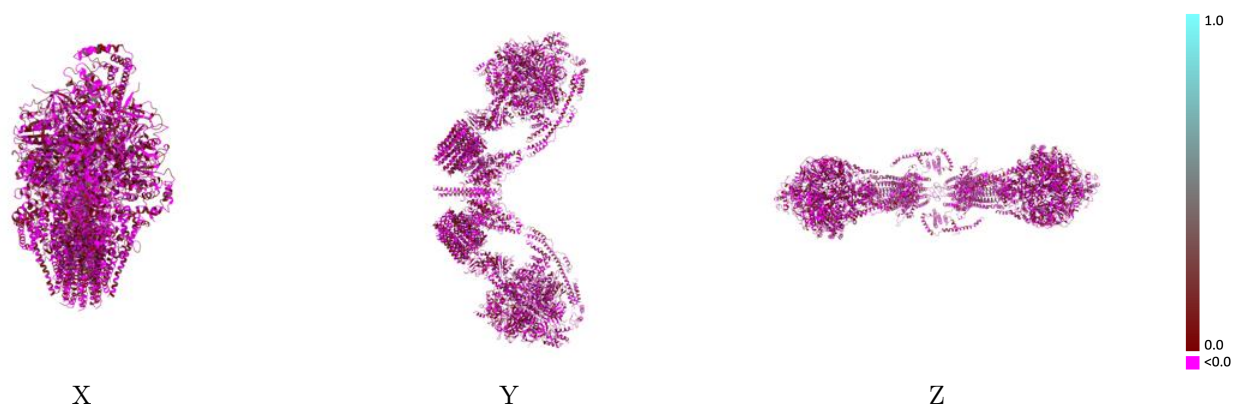
This section contains information regarding the fit between EMDB map EMD-7067 and PDB model 6B8H. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



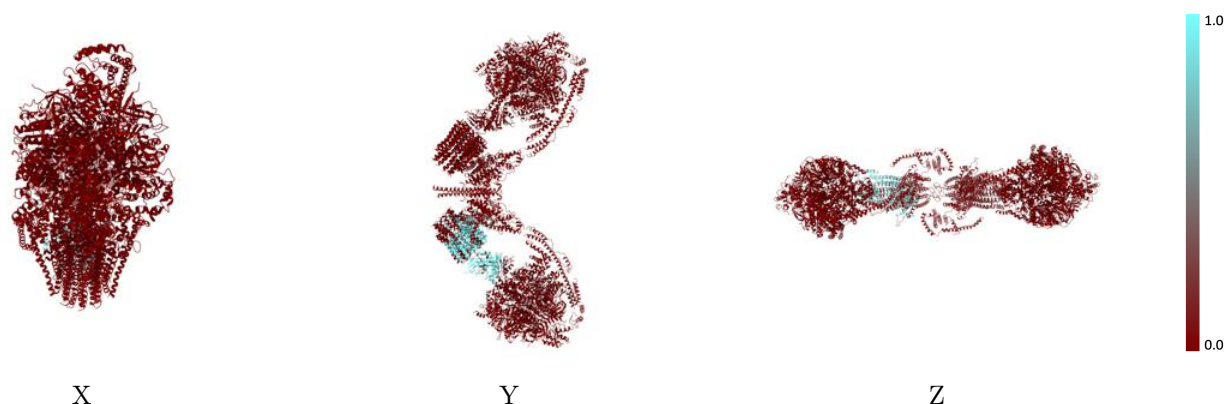
The images above show the 3D surface view of the map at the recommended contour level 0.156 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



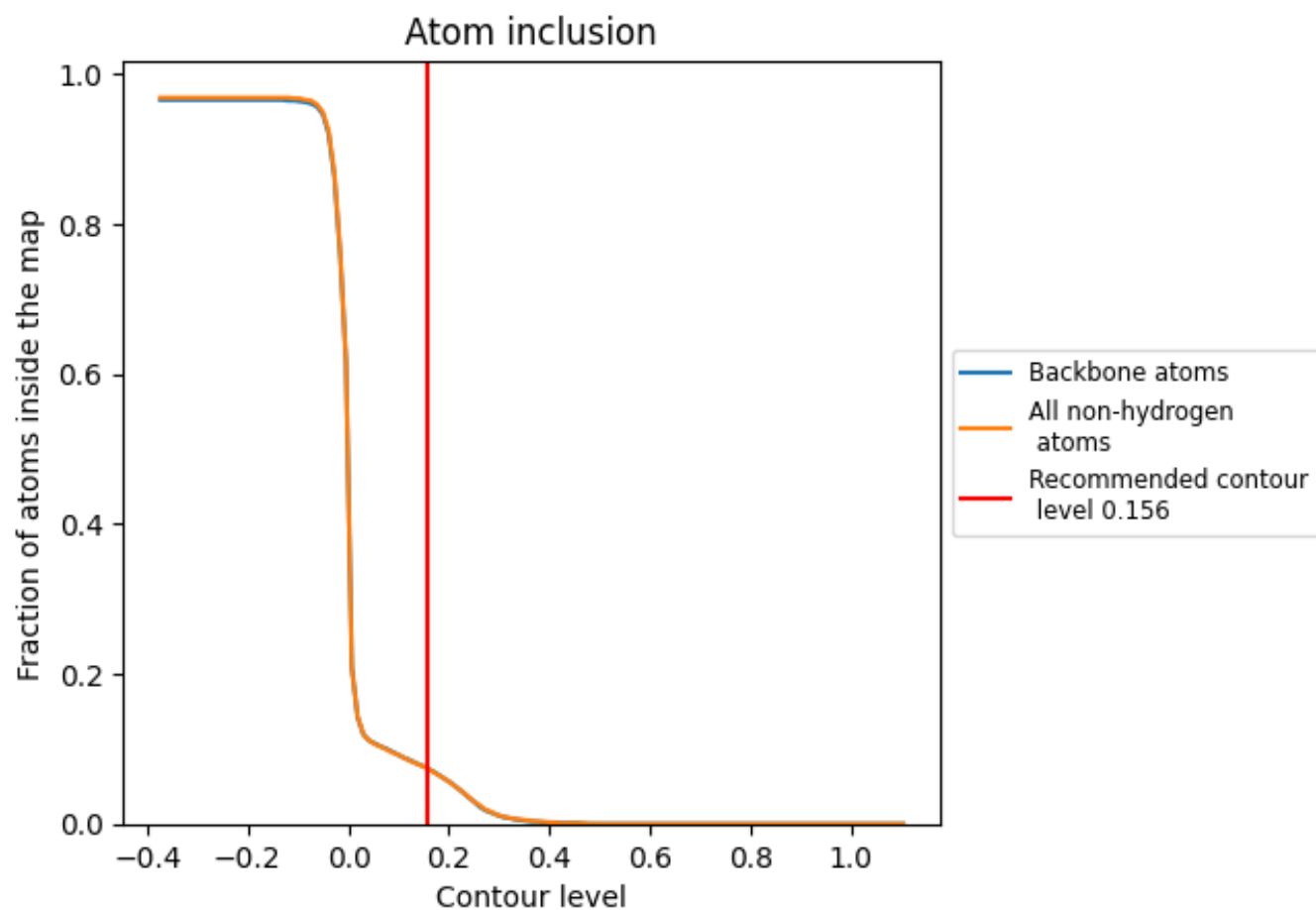
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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



Continued on next page...

Continued from previous page...

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