



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 04:34 PM UTC

PDB ID : 6J5K / pdb_00006j5k
EMDB ID : EMD-0667
Title : Cryo-EM structure of the mammalian ATP synthase tetramer bound with inhibitory protein IF1
Authors : Gu, J.; Zhang, L.; Yi, J.; Yang, M.
Deposited on : 2019-01-11
Resolution : 6.20 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:

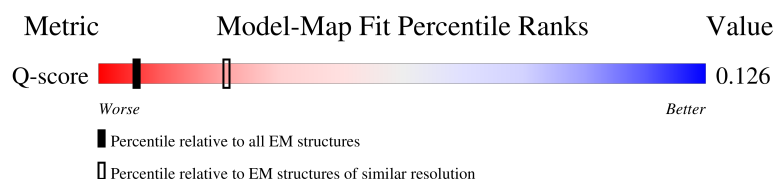
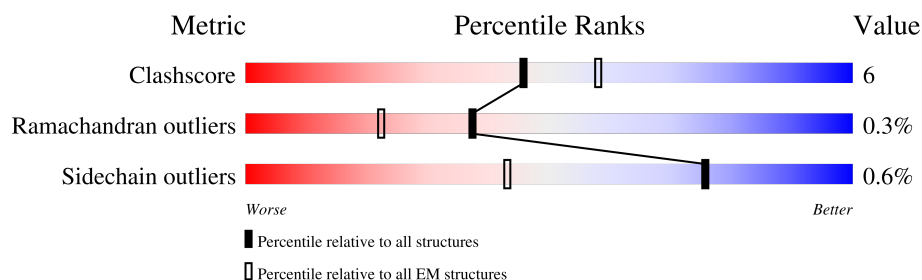
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 6.20 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	537 (5.70 - 6.70)

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.

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1	A	509	
1	AA	509	
1	AB	509	
1	AC	509	

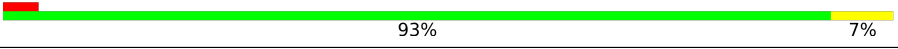
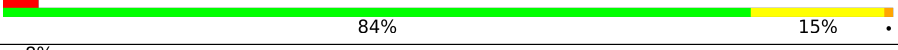
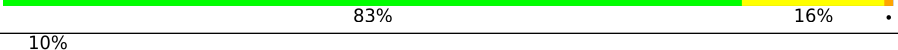
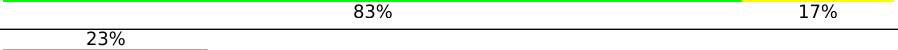
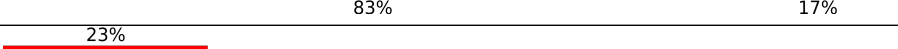
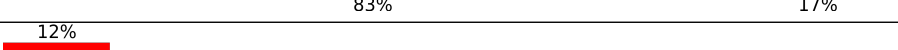
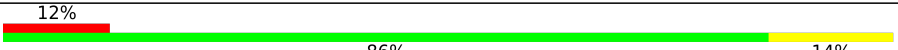
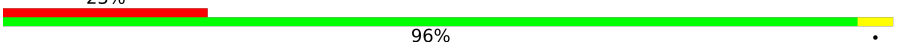
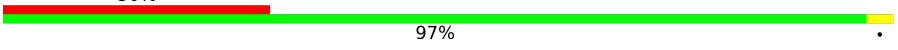
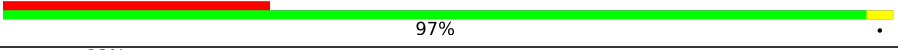
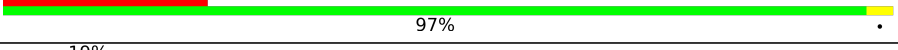
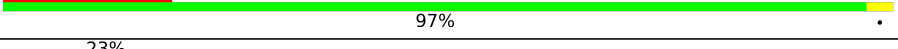
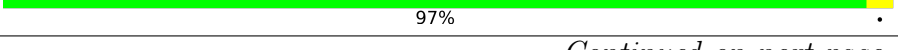
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Mol	Chain	Length	Quality of chain
1	B	509	
1	BA	509	
1	BB	509	
1	BC	509	
1	C	509	
1	CA	509	
1	CB	509	
1	CC	509	
2	AD	469	
2	AE	469	
2	AF	469	
2	BD	469	
2	BE	469	
2	BF	469	
2	CD	469	
2	CE	469	
2	CF	469	
2	D	469	
2	E	469	
2	F	469	
3	AJ	83	
3	BJ	83	
3	CJ	83	
3	J	83	
4	AG	272	

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Mol	Chain	Length	Quality of chain
4	BG	272	 84%15%
4	CG	272	 84%15%
4	G	272	 93%7%
5	AH	132	 84%15%
5	BH	132	 80%19%8%
5	CH	132	 81%18%8%
5	H	132	 83%16%5%
6	AI	48	 83%17%10%
6	BI	48	 83%17%23%
6	CI	48	 83%17%23%
6	I	48	 83%17%12%
7	AS	187	 83%16%27%
7	BS	187	 83%17%25%
7	CS	187	 82%18%25%
7	S	187	 83%16%26%
8	Ab	209	 86%14%12%
8	Bb	209	 85%14%16%
8	Cb	209	 84%15%17%
8	b	209	 88%12%12%
9	Ac	70	 96%23%
9	Bc	70	 97%30%
9	Cc	70	 97%30%
9	c	70	 97%23%
10	Ad	147	 97%19%
10	Bd	147	 97%23%

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Mol	Chain	Length	Quality of chain
10	Cd	147	
10	d	147	
11	Ae	63	
11	Be	63	
11	Ce	63	
11	e	63	
12	Af	87	
12	Bf	87	
12	Cf	87	
12	f	87	
13	Ag	84	
13	Bg	84	
13	Cg	84	
13	g	84	
14	Ai	42	
14	Bi	42	
14	Ci	42	
14	i	42	
15	Ak	29	
15	Bk	29	
15	Ck	29	
15	k	29	
16	8	67	
16	A8	67	
16	B8	67	

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Mol	Chain	Length	Quality of chain
16	C8	67	
17	Aa	226	
17	Ba	226	
17	Ca	226	
17	a	226	
18	AK	72	
18	AL	72	
18	AM	72	
18	AN	72	
18	AO	72	
18	AP	72	
18	AQ	72	
18	AR	72	
18	BK	72	
18	BL	72	
18	BM	72	
18	BN	72	
18	BO	72	
18	BP	72	
18	BQ	72	
18	BR	72	
18	CK	72	
18	CL	72	
18	CM	72	
18	CN	72	

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Mol	Chain	Length	Quality of chain
18	CO	72	
18	CP	72	
18	CQ	72	
18	CR	72	
18	K	72	
18	L	72	
18	M	72	
18	N	72	
18	O	72	
18	P	72	
18	Q	72	
18	R	72	
19	Au	42	
19	Bu	42	
19	Cu	42	
19	u	42	

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 153148 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 F1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	504	Total	C	N	O	S	0	0
			3837	2417	676	732	12		
1	B	501	Total	C	N	O	S	0	0
			3814	2400	673	729	12		
1	C	488	Total	C	N	O	S	0	0
			3722	2347	657	706	12		
1	AA	504	Total	C	N	O	S	0	0
			3837	2417	676	732	12		
1	AB	501	Total	C	N	O	S	0	0
			3814	2400	673	729	12		
1	AC	488	Total	C	N	O	S	0	0
			3722	2347	657	706	12		
1	BA	509	Total	C	N	O	S	0	0
			3873	2438	682	741	12		
1	BB	481	Total	C	N	O	S	0	0
			3669	2312	649	696	12		
1	BC	502	Total	C	N	O	S	0	0
			3821	2407	674	728	12		
1	CA	509	Total	C	N	O	S	0	0
			3873	2438	682	741	12		
1	CB	481	Total	C	N	O	S	0	0
			3669	2312	649	696	12		
1	CC	502	Total	C	N	O	S	0	0
			3821	2407	674	728	12		

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	469	Total	C	N	O	S	0	0
			3552	2252	603	685	12		
2	E	465	Total	C	N	O	S	0	0
			3522	2234	597	679	12		
2	F	466	Total	C	N	O	S	0	0
			3527	2237	598	680	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	AD	469	Total	C	N	O	S	0	0
			3555	2253	603	687	12		
2	AE	465	Total	C	N	O	S	0	0
			3522	2234	597	679	12		
2	AF	466	Total	C	N	O	S	0	0
			3527	2237	598	680	12		
2	BD	469	Total	C	N	O	S	0	0
			3555	2253	603	687	12		
2	BE	465	Total	C	N	O	S	0	0
			3522	2234	597	679	12		
2	BF	466	Total	C	N	O	S	0	0
			3527	2237	598	680	12		
2	CD	469	Total	C	N	O	S	0	0
			3555	2253	603	687	12		
2	CE	465	Total	C	N	O	S	0	0
			3522	2234	597	679	12		
2	CF	466	Total	C	N	O	S	0	0
			3527	2237	598	680	12		

- Molecule 3 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	78	Total	C	N	O	0	0
			583	354	116	113		
3	AJ	78	Total	C	N	O	0	0
			583	354	116	113		
3	BJ	75	Total	C	N	O	0	0
			561	336	112	113		
3	CJ	75	Total	C	N	O	0	0
			561	336	112	113		

- Molecule 4 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	272	Total	C	N	O	S	0	0
			2109	1331	366	405	7		
4	AG	272	Total	C	N	O	S	0	0
			2109	1331	366	405	7		
4	BG	272	Total	C	N	O	S	0	0
			2112	1332	366	407	7		
4	CG	272	Total	C	N	O	S	0	0
			2109	1331	366	405	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	132	Total	C	N	O	S	0	0
			970	607	165	196	2		
5	AH	132	Total	C	N	O	S	0	0
			970	607	165	196	2		
5	BH	132	Total	C	N	O	S	0	0
			973	610	165	196	2		
5	CH	132	Total	C	N	O	S	0	0
			973	610	165	196	2		

- Molecule 6 is a protein called ATP synthase F1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	48	Total	C	N	O	S	0	0
			377	241	69	66	1		
6	AI	48	Total	C	N	O	S	0	0
			377	241	69	66	1		
6	BI	48	Total	C	N	O	S	0	0
			377	241	69	66	1		
6	CI	48	Total	C	N	O	S	0	0
			377	241	69	66	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	187	Total	C	N	O	S	0	0
			1429	910	244	266	9		
7	AS	187	Total	C	N	O	S	0	0
			1429	910	244	266	9		
7	BS	187	Total	C	N	O	S	0	0
			1435	913	247	266	9		
7	CS	187	Total	C	N	O	S	0	0
			1435	913	247	266	9		

- Molecule 8 is a protein called ATP synthase peripheral stalk-membrane subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	209	Total	C	N	O	S	0	0
			1478	916	277	280	5		
8	Ab	209	Total	C	N	O	S	0	0
			1478	916	277	280	5		
8	Bb	209	Total	C	N	O	S	0	0
			1476	915	278	278	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	Cb	209	Total	C	N	O	S	0	0
			1476	915	278	278	5		

- Molecule 9 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	c	70	Total	C	N	O	0	0
			428	263	84	81		
9	Ac	70	Total	C	N	O	0	0
			428	263	84	81		
9	Bc	70	Total	C	N	O	0	0
			428	263	84	81		
9	Cc	70	Total	C	N	O	0	0
			428	263	84	81		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	d	147	Total	C	N	O	0	0
			741	446	148	147		
10	Ad	147	Total	C	N	O	0	0
			741	446	148	147		
10	Bd	147	Total	C	N	O	0	0
			741	446	148	147		
10	Cd	147	Total	C	N	O	0	0
			741	446	148	147		

- Molecule 11 is a protein called ATP synthase subunit e.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	63	Total	C	N	O	0	0
			315	189	63	63		
11	Ae	63	Total	C	N	O	0	0
			315	189	63	63		
11	Be	63	Total	C	N	O	0	0
			315	189	63	63		
11	Ce	63	Total	C	N	O	0	0
			315	189	63	63		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	87	Total	C	N	O	S	0	0
			530	327	103	98	2		
12	Af	87	Total	C	N	O	S	0	0
			530	327	103	98	2		
12	Bf	80	Total	C	N	O	S	0	0
			495	306	96	91	2		
12	Cf	80	Total	C	N	O	S	0	0
			486	300	93	91	2		

- Molecule 13 is a protein called ATP synthase subunit g.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	g	84	Total	C	N	O		0	0
			420	252	84	84			
13	Ag	84	Total	C	N	O		0	0
			420	252	84	84			
13	Bg	79	Total	C	N	O		0	0
			395	237	79	79			
13	Cg	80	Total	C	N	O		0	0
			400	240	80	80			

- Molecule 14 is a protein called ATP synthase membrane subunit DAPIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	i	42	Total	C	N	O	S	0	0
			306	202	49	53	2		
14	Ai	42	Total	C	N	O	S	0	0
			306	202	49	53	2		
14	Bi	42	Total	C	N	O	S	0	0
			303	199	49	53	2		
14	Ci	42	Total	C	N	O	S	0	0
			303	199	49	53	2		

- Molecule 15 is a protein called subunit k analog.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	k	29	Total	C	N	O	0	0
			145	87	29	29		
15	Ak	29	Total	C	N	O	0	0
			145	87	29	29		
15	Bk	29	Total	C	N	O	0	0
			145	87	29	29		

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Mol	Chain	Residues	Atoms				AltConf	Trace
15	Ck	29	Total	C	N	O	0	0
			145	87	29	29		

- Molecule 16 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	8	56	Total	C	N	O	S	0	0
			374	242	60	70	2		
16	A8	56	Total	C	N	O	S	0	0
			374	242	60	70	2		
16	B8	56	Total	C	N	O	S	0	0
			374	242	60	70	2		
16	C8	56	Total	C	N	O	S	0	0
			374	242	60	70	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	223	Total	C	N	O	S	0	0
			1699	1128	269	290	12		
17	Aa	223	Total	C	N	O	S	0	0
			1699	1128	269	290	12		
17	Ba	223	Total	C	N	O	S	0	0
			1684	1116	266	291	11		
17	Ca	223	Total	C	N	O	S	0	0
			1684	1116	266	291	11		

- Molecule 18 is a protein called Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	72	Total	C	N	O	S	0	0
			513	340	80	89	4		
18	L	72	Total	C	N	O	S	0	0
			513	340	80	89	4		
18	M	72	Total	C	N	O	S	0	0
			513	340	80	89	4		
18	N	72	Total	C	N	O	S	0	0
			510	338	80	89	3		
18	O	72	Total	C	N	O	S	0	0
			510	339	79	88	4		
18	P	72	Total	C	N	O	S	0	0
			513	340	80	89	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	72	Total 513	C 340	N 80	O 89	S 4	0	0
18	R	72	Total 513	C 340	N 80	O 89	S 4	0	0
18	AK	72	Total 513	C 340	N 80	O 89	S 4	0	0
18	AL	72	Total 513	C 340	N 80	O 89	S 4	0	0
18	AM	72	Total 513	C 340	N 80	O 89	S 4	0	0
18	AN	72	Total 510	C 338	N 80	O 89	S 3	0	0
18	AO	72	Total 510	C 339	N 79	O 88	S 4	0	0
18	AP	72	Total 513	C 340	N 80	O 89	S 4	0	0
18	AQ	72	Total 513	C 340	N 80	O 89	S 4	0	0
18	AR	72	Total 513	C 340	N 80	O 89	S 4	0	0
18	BK	72	Total 513	C 340	N 80	O 89	S 4	0	0
18	BL	72	Total 513	C 340	N 80	O 89	S 4	0	0
18	BM	72	Total 513	C 340	N 80	O 89	S 4	0	0
18	BN	72	Total 510	C 338	N 80	O 89	S 3	0	0
18	BO	72	Total 510	C 338	N 80	O 89	S 3	0	0
18	BP	72	Total 513	C 340	N 80	O 89	S 4	0	0
18	BQ	72	Total 513	C 340	N 80	O 89	S 4	0	0
18	BR	72	Total 510	C 337	N 80	O 89	S 4	0	0
18	CK	72	Total 513	C 340	N 80	O 89	S 4	0	0
18	CL	72	Total 513	C 340	N 80	O 89	S 4	0	0
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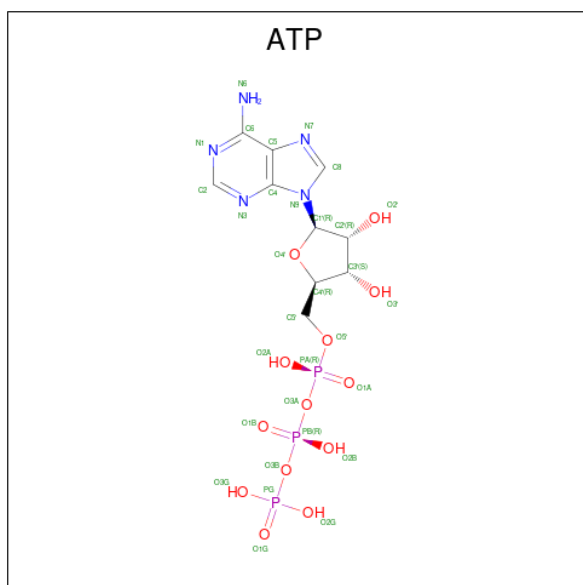
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Mol	Chain	Residues	Atoms					AltConf	Trace
18	CN	72	Total	C	N	O	S	0	0
			510	338	80	89	3		
18	CO	72	Total	C	N	O	S	0	0
			510	338	80	89	3		
18	CP	72	Total	C	N	O	S	0	0
			513	340	80	89	4		
18	CQ	72	Total	C	N	O	S	0	0
			513	340	80	89	4		
18	CR	72	Total	C	N	O	S	0	0
			510	337	80	89	4		

- Molecule 19 is a protein called ATP synthase membrane subunit 6.8PL.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	u	42	Total	C	N	O	0	0
			210	126	42	42		
19	Au	42	Total	C	N	O	0	0
			210	126	42	42		
19	Bu	42	Total	C	N	O	0	0
			210	126	42	42		
19	Cu	42	Total	C	N	O	0	0
			210	126	42	42		

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	AA	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	AB	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	AC	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	BA	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	BB	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	BC	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	CA	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	CB	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	CC	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

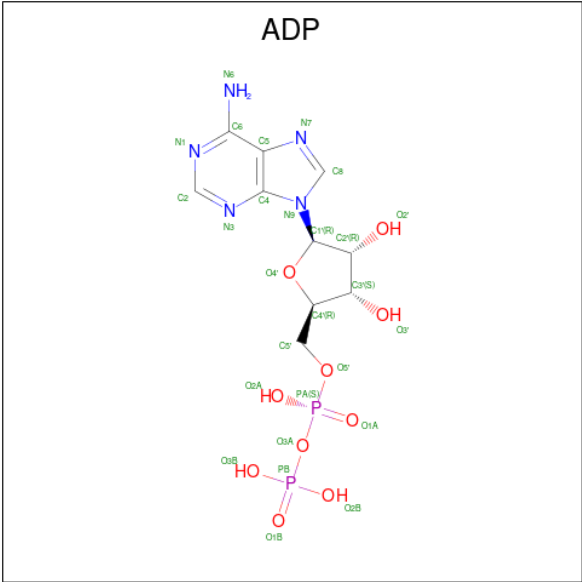
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Mg	0
			1	1	
21	B	1	Total	Mg	0
			1	1	
21	C	1	Total	Mg	0
			1	1	
21	D	1	Total	Mg	0
			1	1	
21	F	1	Total	Mg	0
			1	1	
21	AA	1	Total	Mg	0
			1	1	
21	AB	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
21	AC	1	Total 1	Mg 1	0
21	AD	1	Total 1	Mg 1	0
21	AF	1	Total 1	Mg 1	0
21	BA	1	Total 1	Mg 1	0
21	BB	1	Total 1	Mg 1	0
21	BC	1	Total 1	Mg 1	0
21	BD	1	Total 1	Mg 1	0
21	BF	1	Total 1	Mg 1	0
21	CA	1	Total 1	Mg 1	0
21	CB	1	Total 1	Mg 1	0
21	CC	1	Total 1	Mg 1	0
21	CD	1	Total 1	Mg 1	0
21	CF	1	Total 1	Mg 1	0

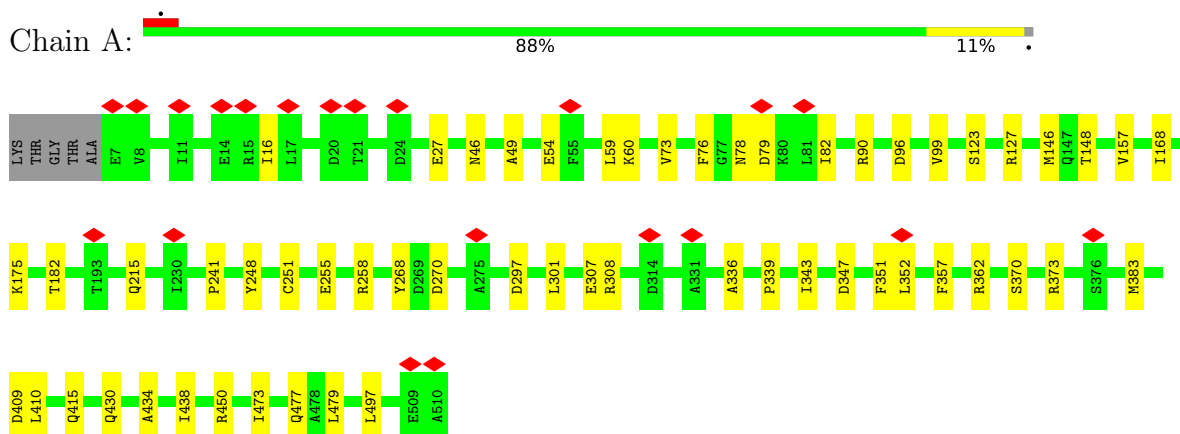
- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



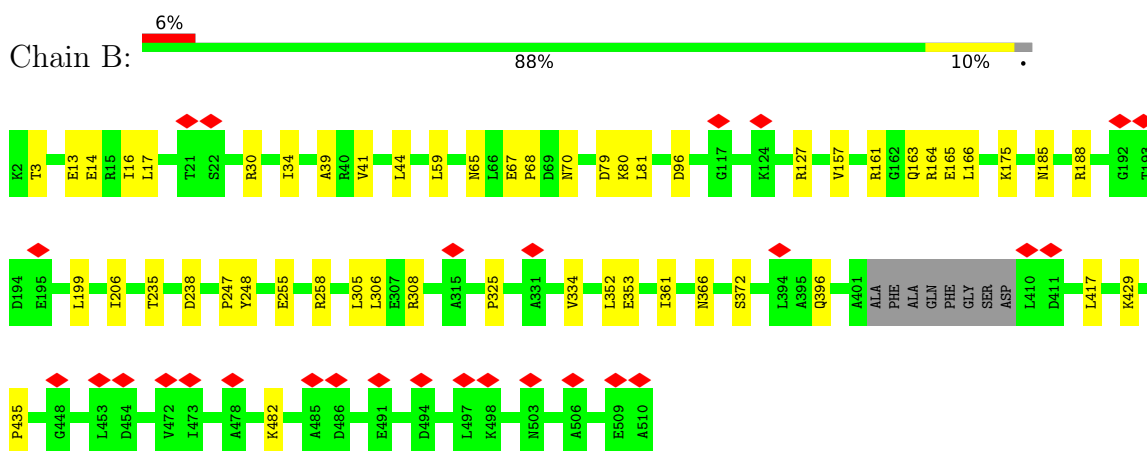
3 Residue-property plots [i](#)

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.

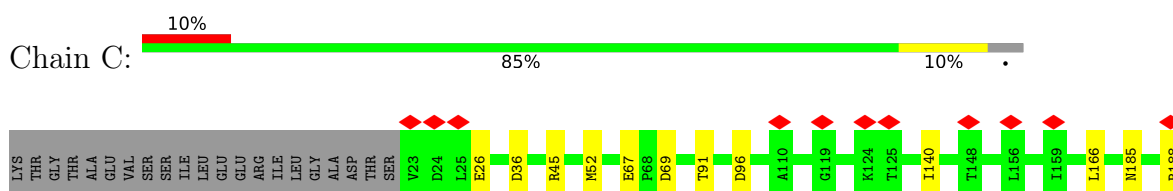
- Molecule 1: ATP synthase F1 subunit alpha

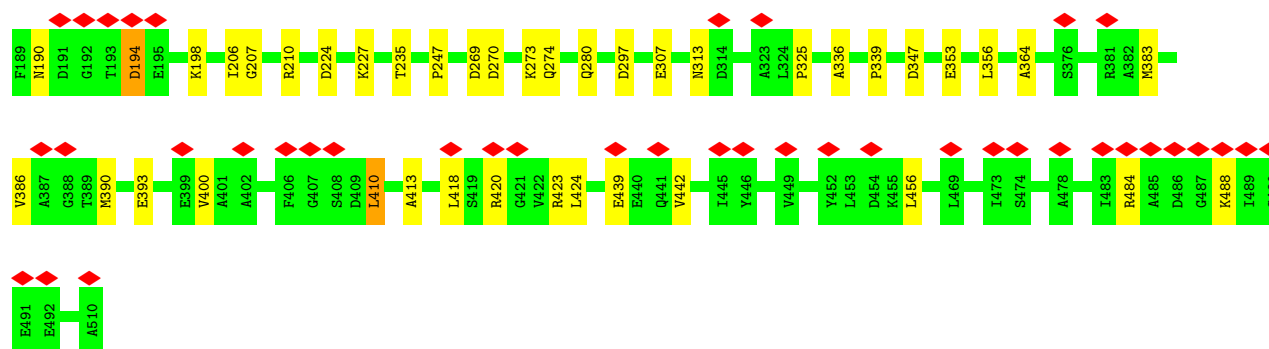


- Molecule 1: ATP synthase F1 subunit alpha



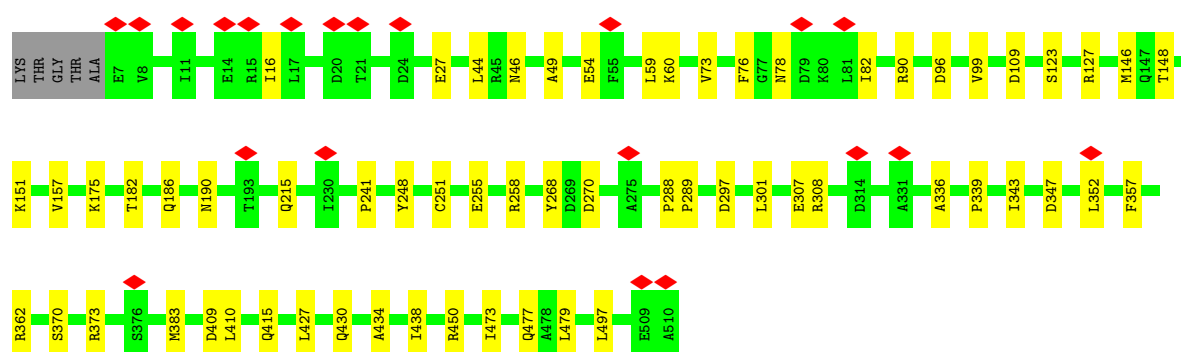
- Molecule 1: ATP synthase F1 subunit alpha





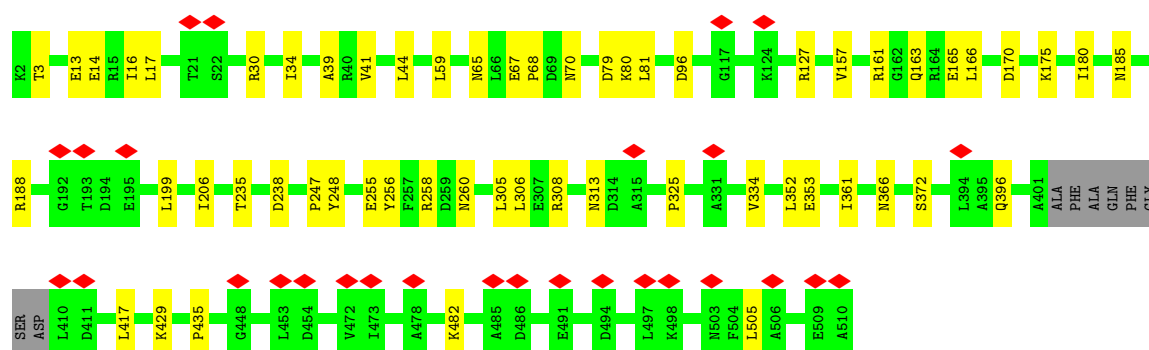
- Molecule 1: ATP synthase F1 subunit alpha

Chain AA: 87% 12% .



- Molecule 1: ATP synthase F1 subunit alpha

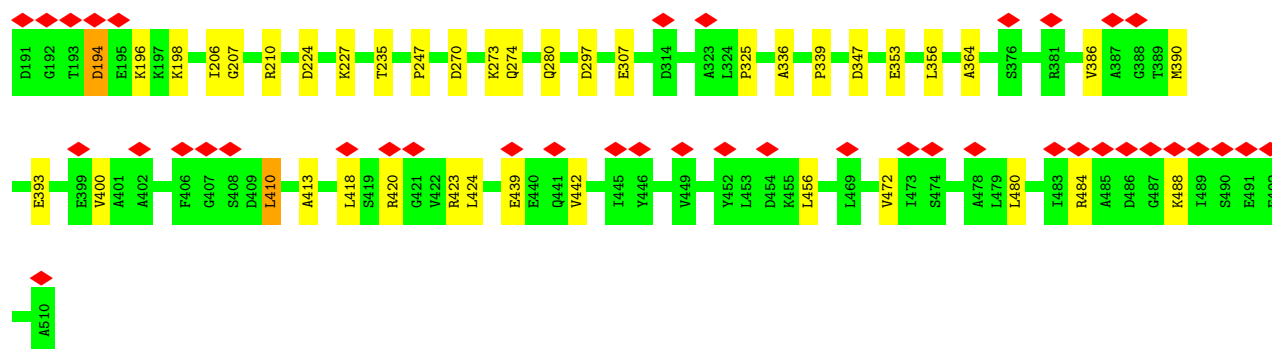
Chain AB: 6% 87% 11% .



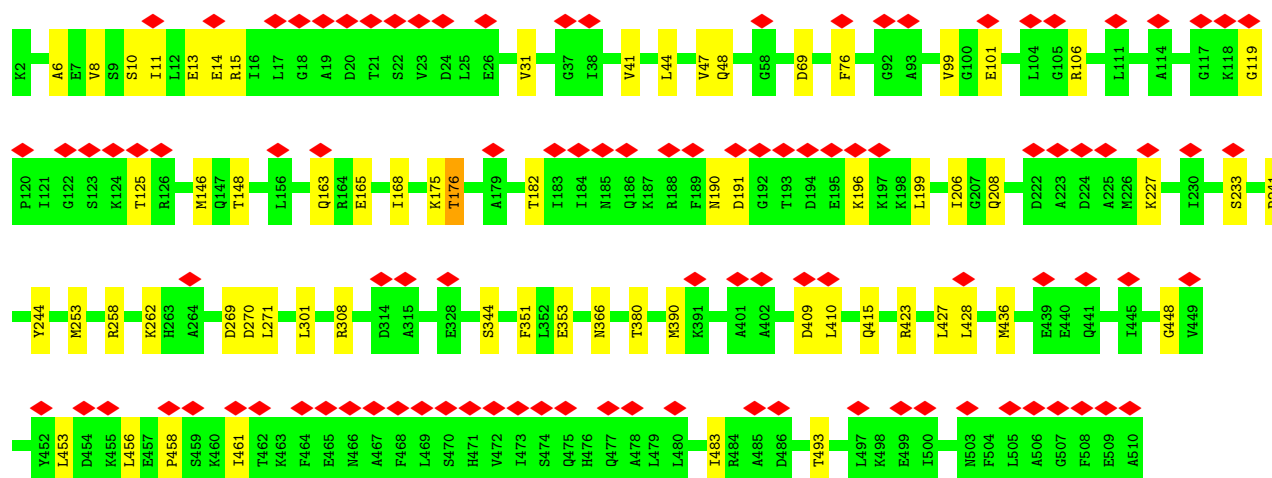
- Molecule 1: ATP synthase F1 subunit alpha

Chain AC: 10% 86% 10% .

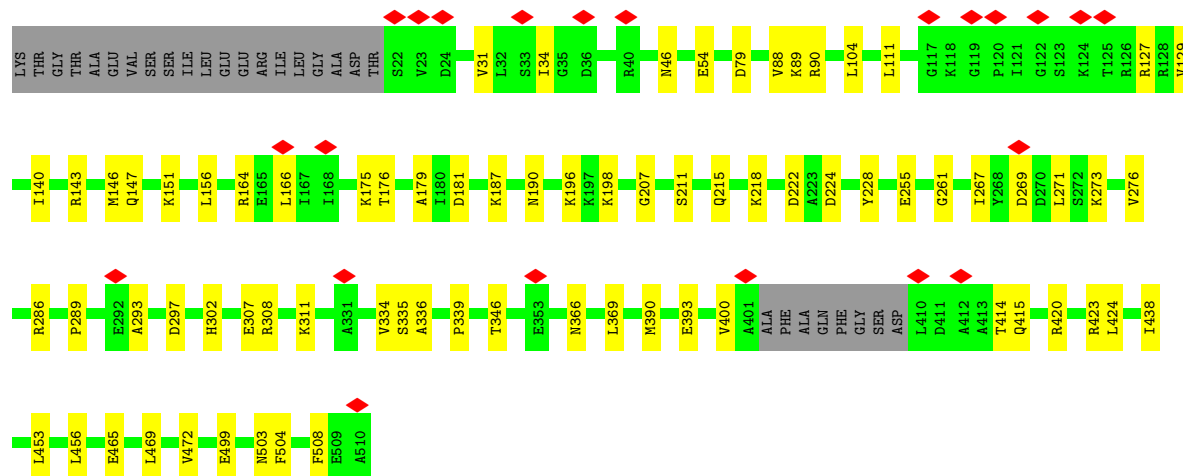
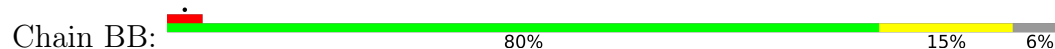




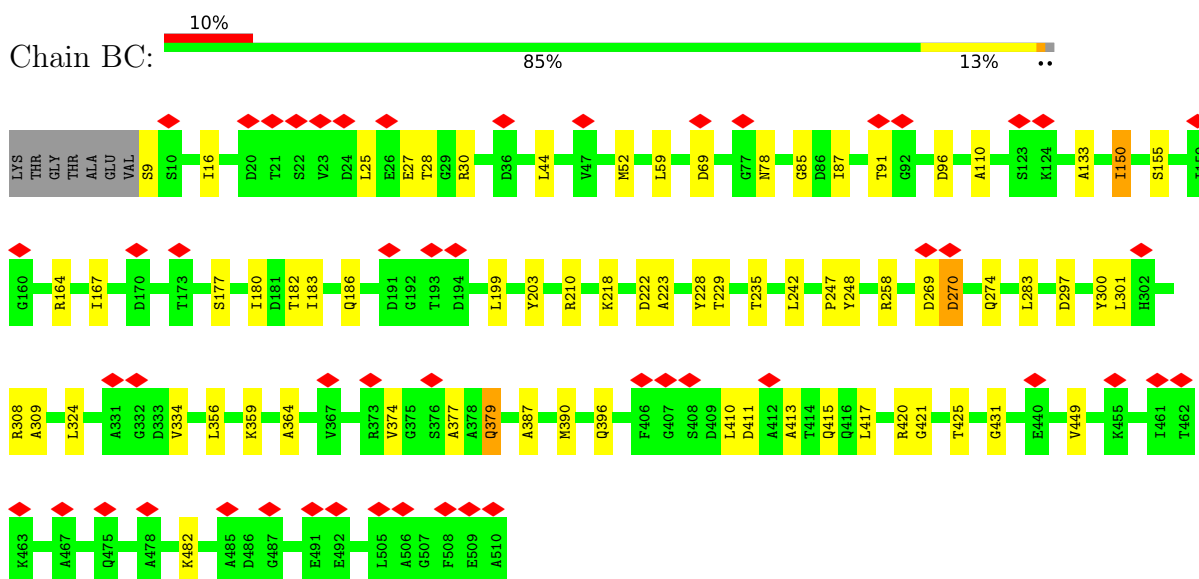
- Molecule 1: ATP synthase F1 subunit alpha



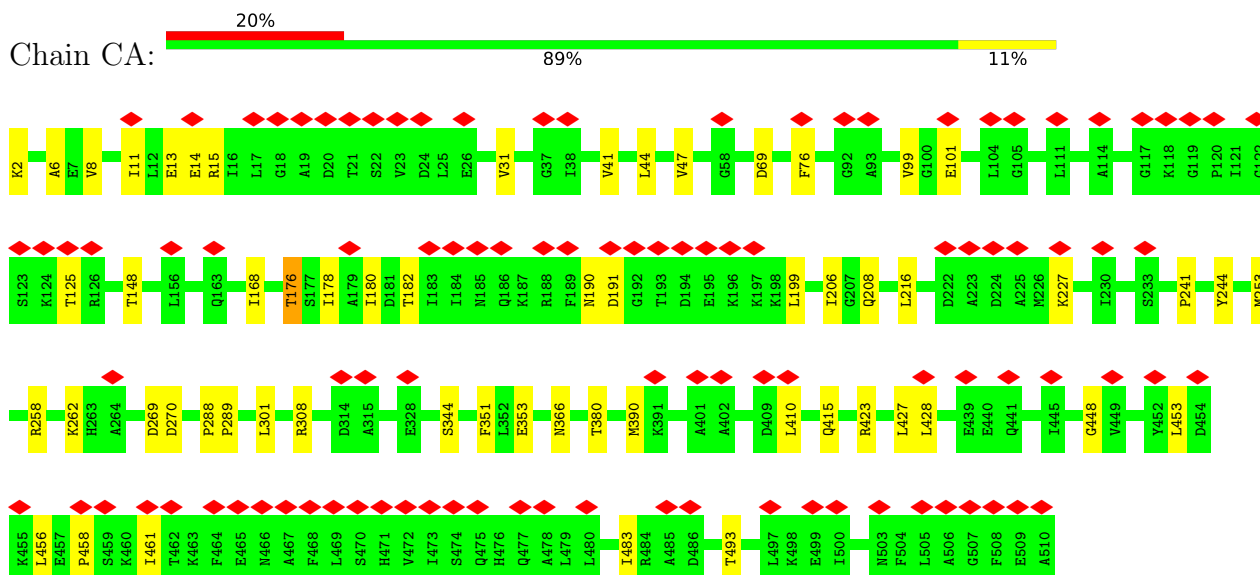
- Molecule 1: ATP synthase F1 subunit alpha



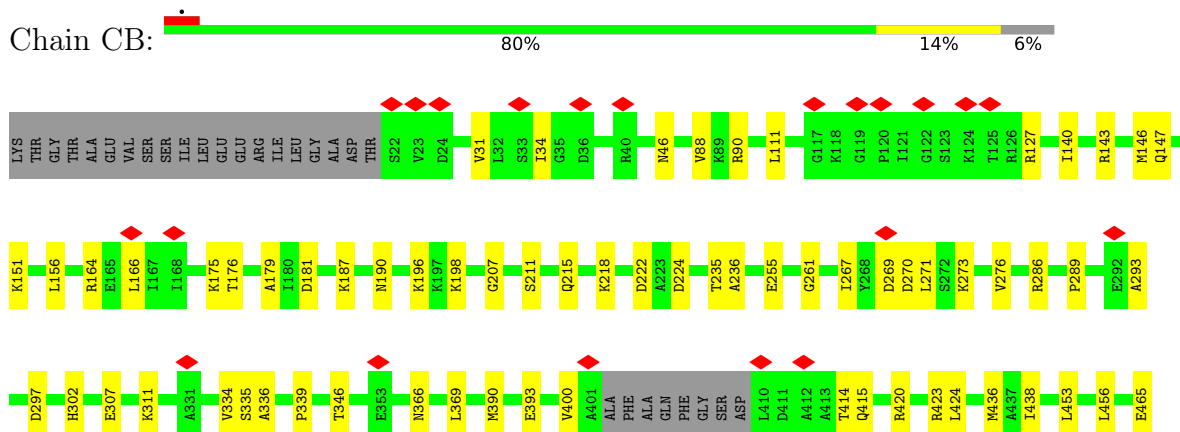
- Molecule 1: ATP synthase F1 subunit alpha



• Molecule 1: ATP synthase F1 subunit alpha

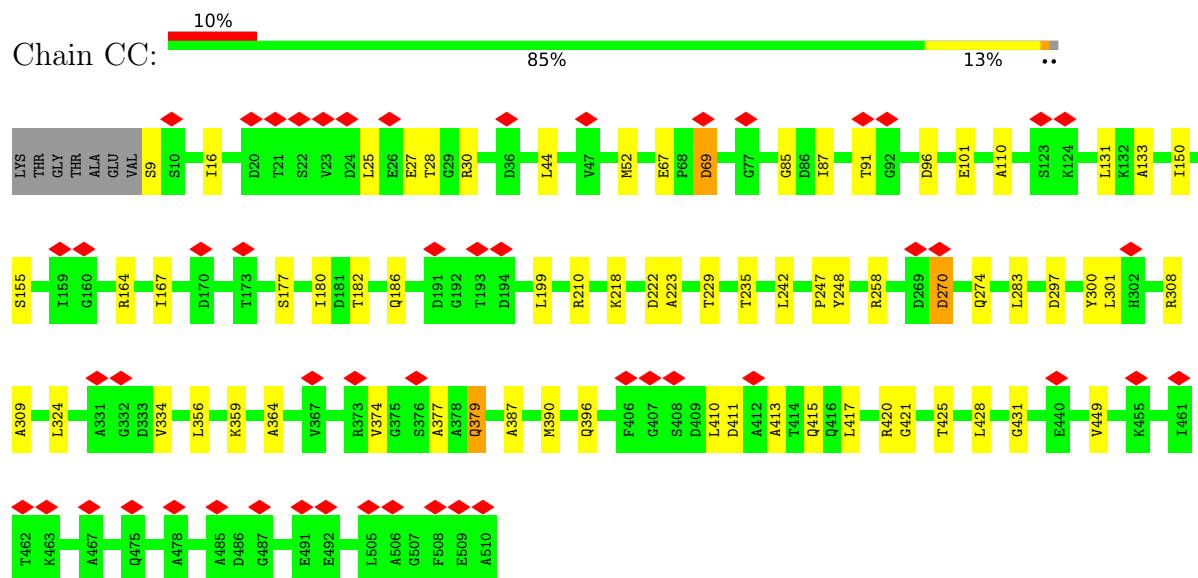


• Molecule 1: ATP synthase F1 subunit alpha

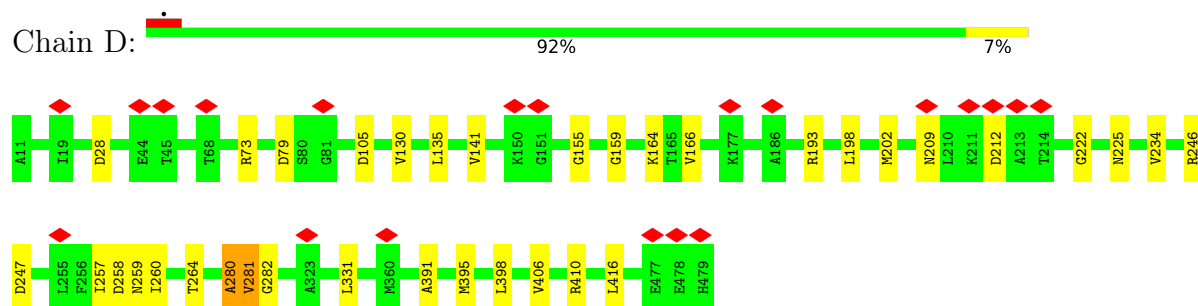




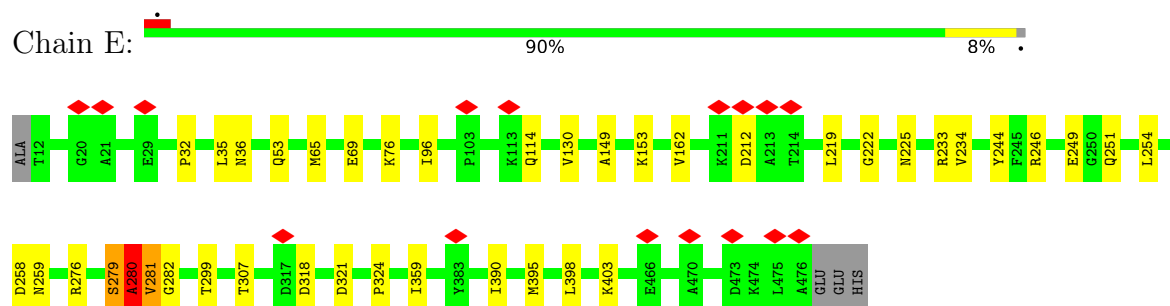
• Molecule 1: ATP synthase F1 subunit alpha



• Molecule 2: ATP synthase subunit beta

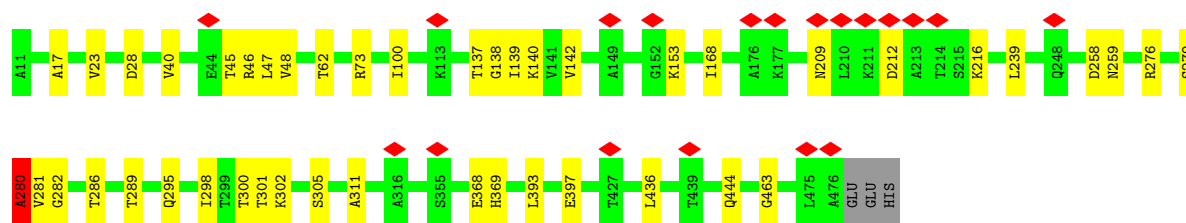


• Molecule 2: ATP synthase subunit beta

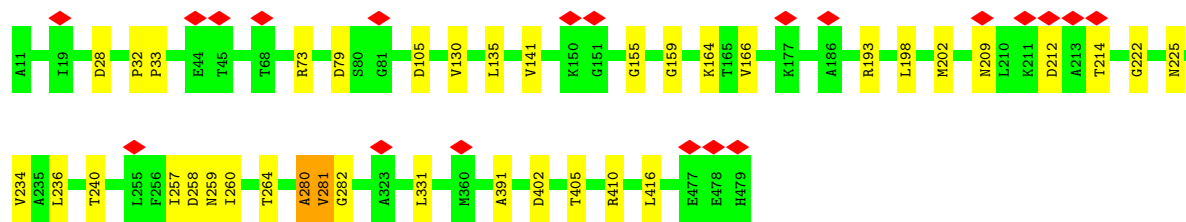


• Molecule 2: ATP synthase subunit beta

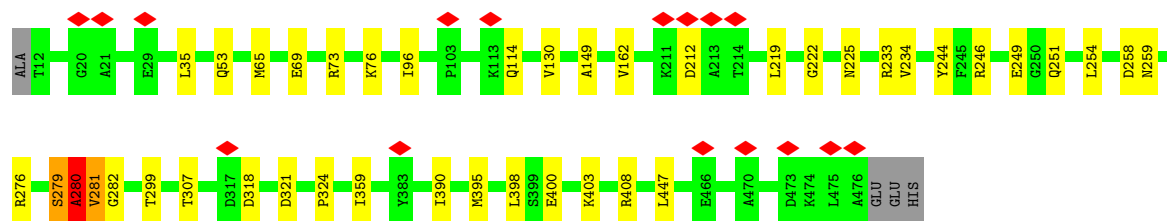
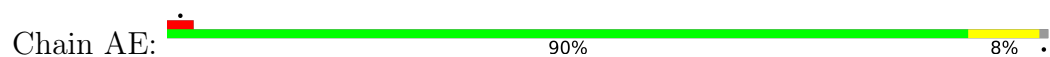




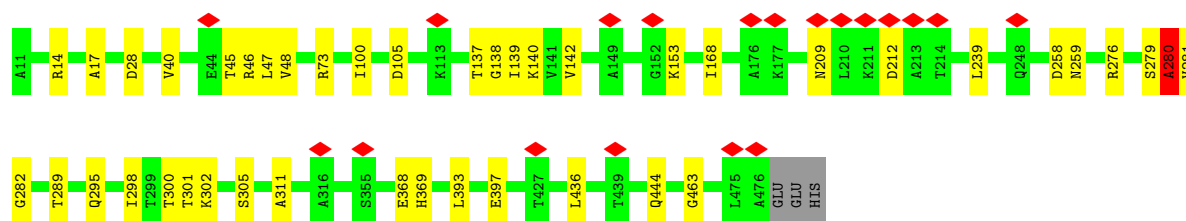
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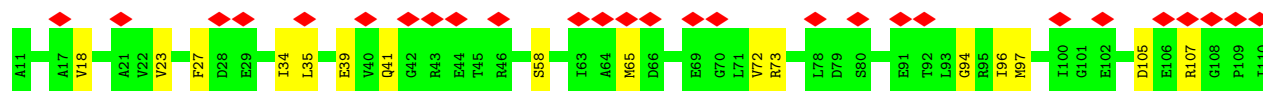
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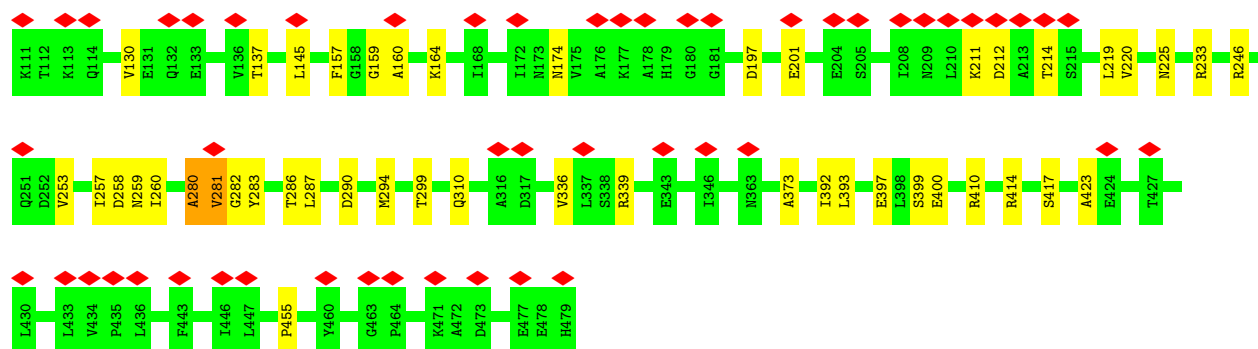


- Molecule 2: ATP synthase subunit beta

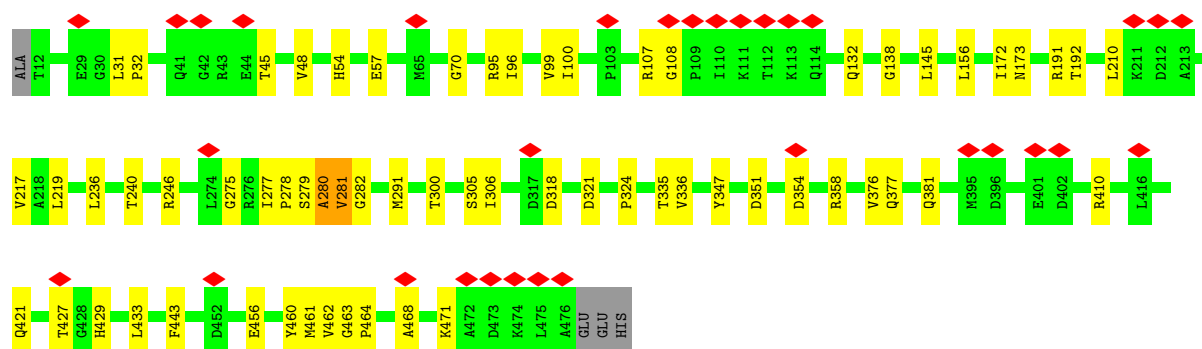
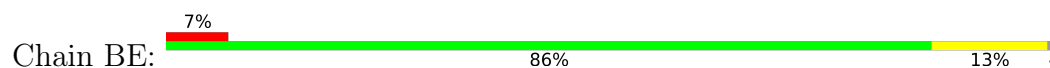


- Molecule 2: ATP synthase subunit beta

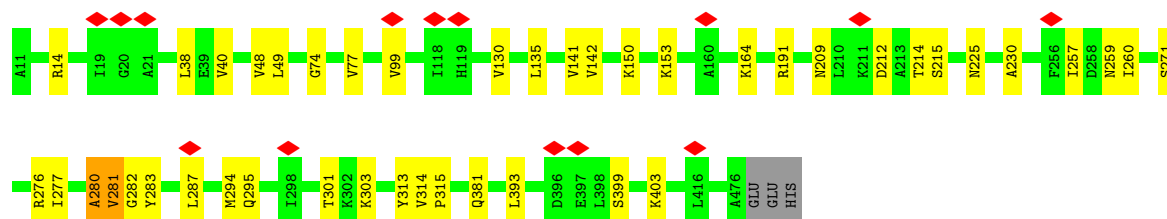
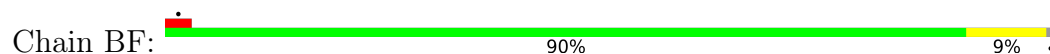




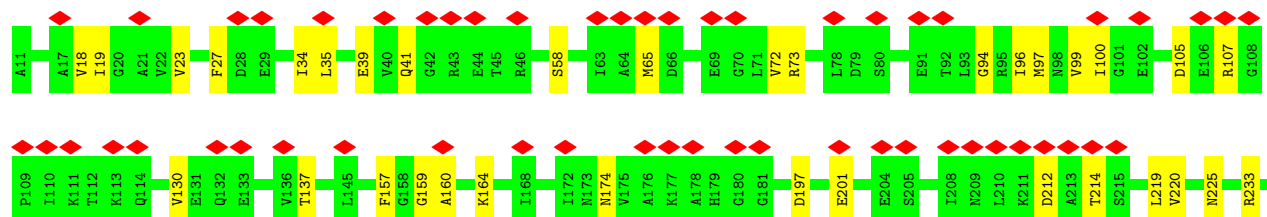
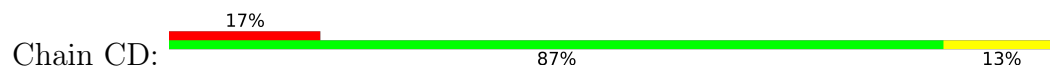
• Molecule 2: ATP synthase subunit beta

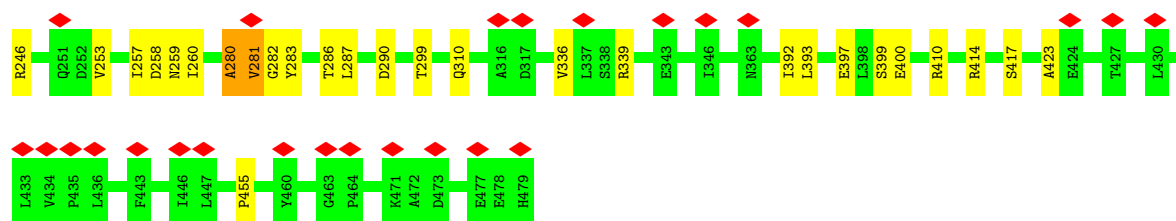


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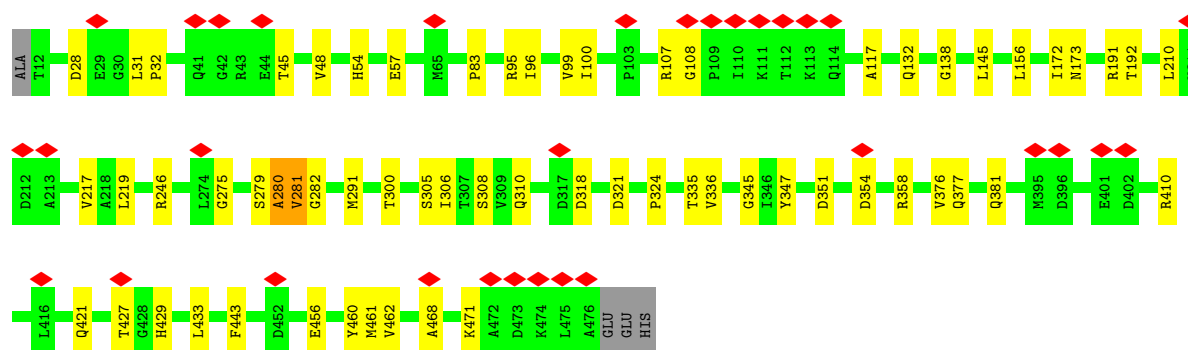
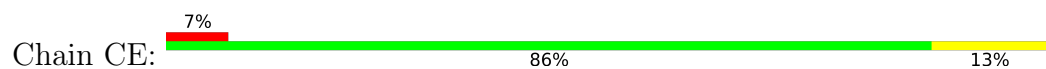


• Molecule 2: ATP synthase subunit beta

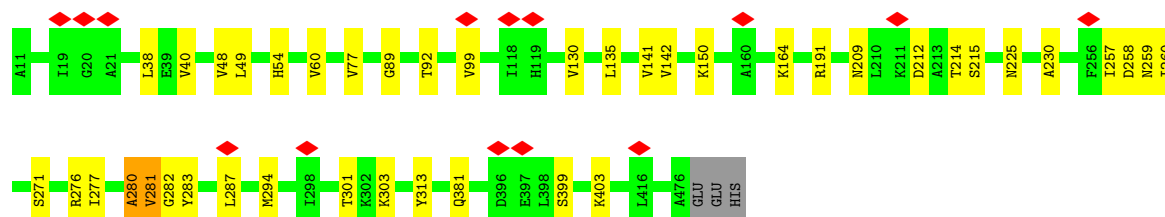




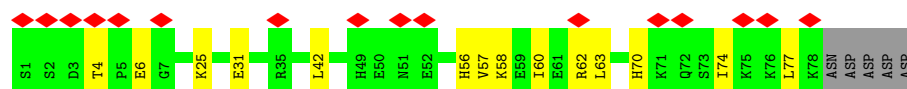
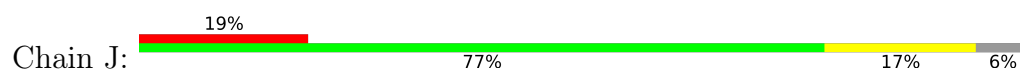
- Molecule 2: ATP synthase subunit beta



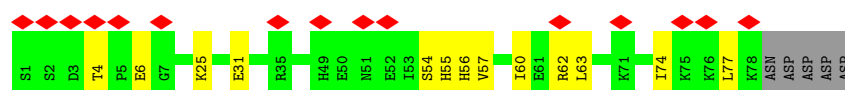
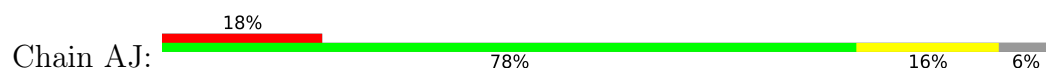
- Molecule 2: ATP synthase subunit beta



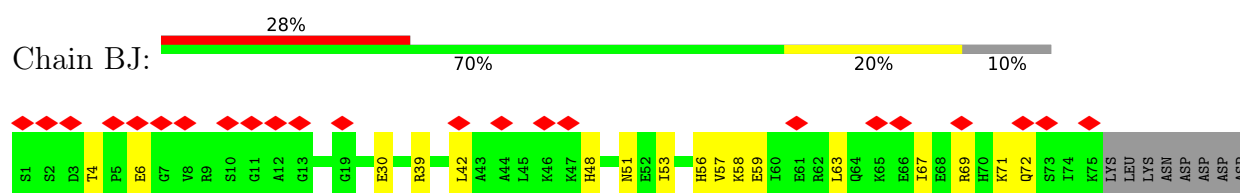
- Molecule 3: ATPase inhibitor, mitochondrial



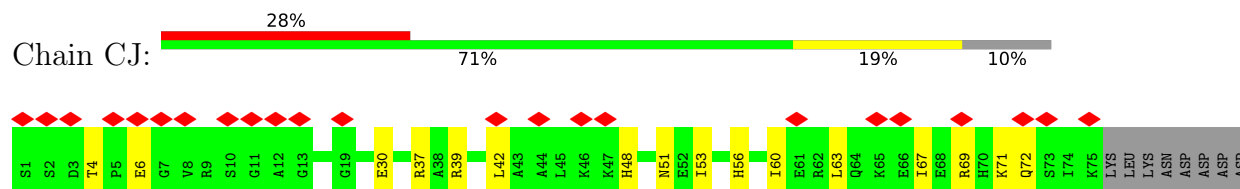
- Molecule 3: ATPase inhibitor, mitochondrial



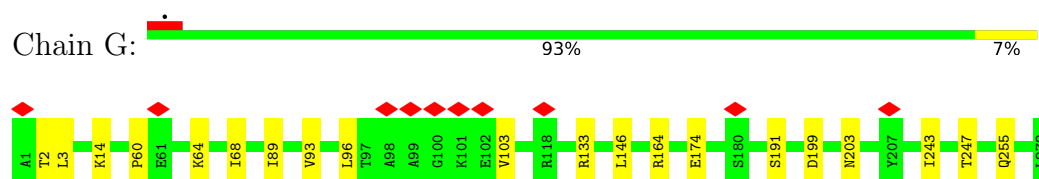
- Molecule 3: ATPase inhibitor, mitochondrial



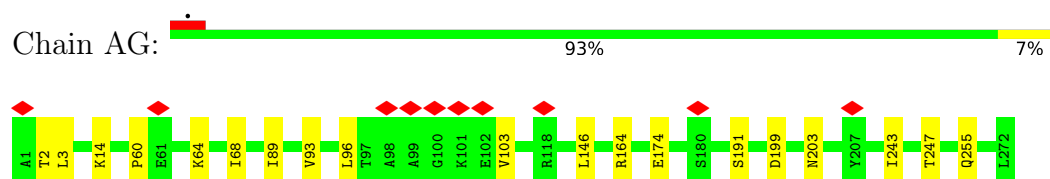
- Molecule 3: ATPase inhibitor, mitochondrial



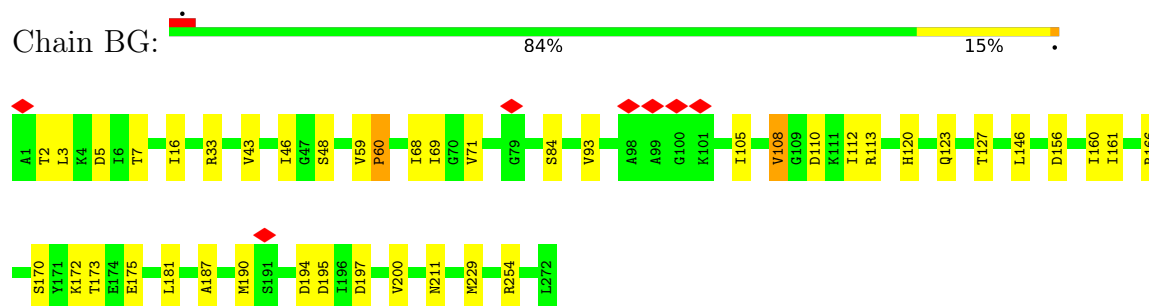
- Molecule 4: ATP synthase subunit gamma



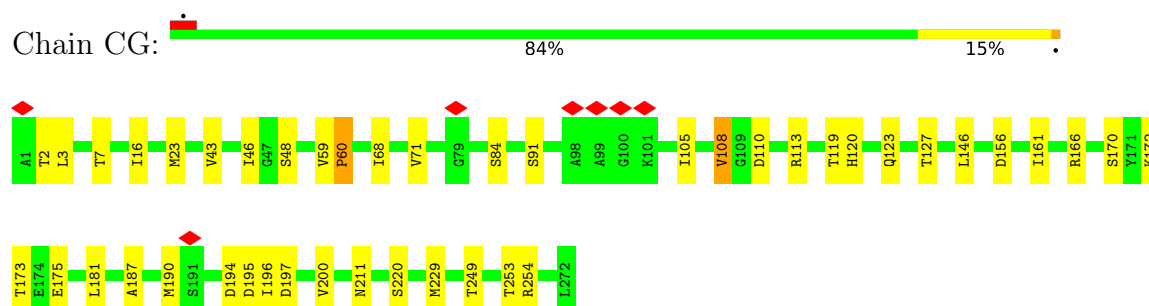
- Molecule 4: ATP synthase subunit gamma



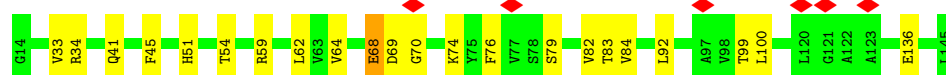
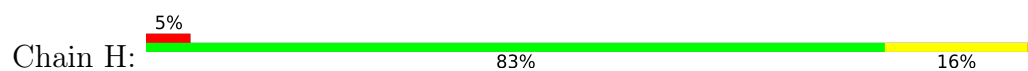
- Molecule 4: ATP synthase subunit gamma



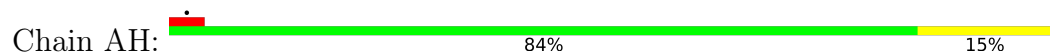
- Molecule 4: ATP synthase subunit gamma



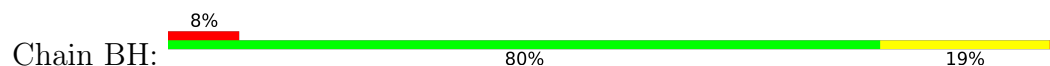
- Molecule 5: ATP synthase subunit delta, mitochondrial



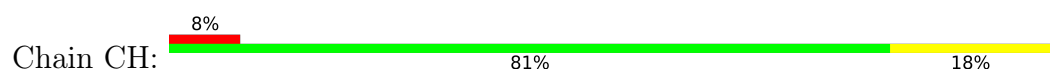
- Molecule 5: ATP synthase subunit delta, mitochondrial



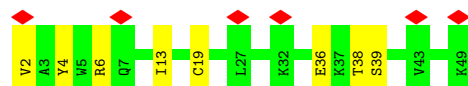
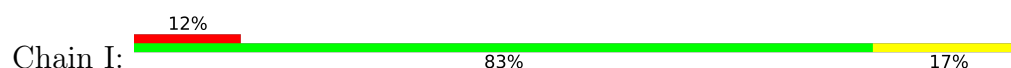
- Molecule 5: ATP synthase subunit delta, mitochondrial



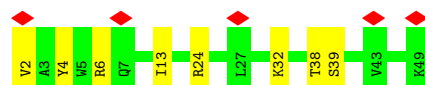
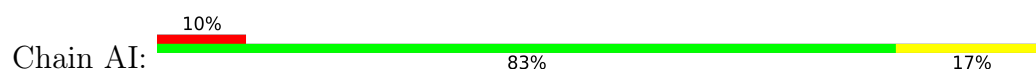
- Molecule 5: ATP synthase subunit delta, mitochondrial



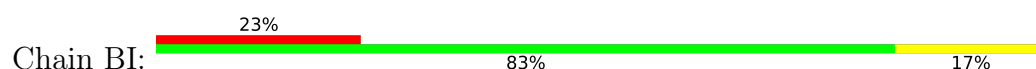
- Molecule 6: ATP synthase F1 subunit epsilon

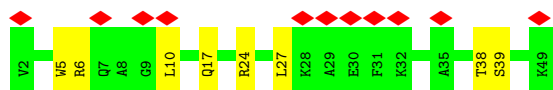


- Molecule 6: ATP synthase F1 subunit epsilon

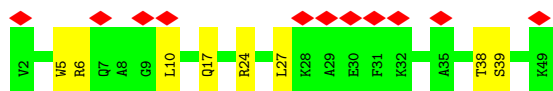
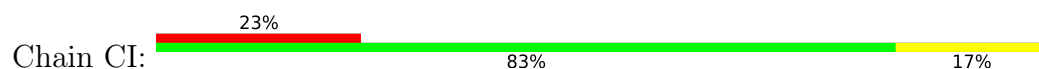


- Molecule 6: ATP synthase F1 subunit epsilon

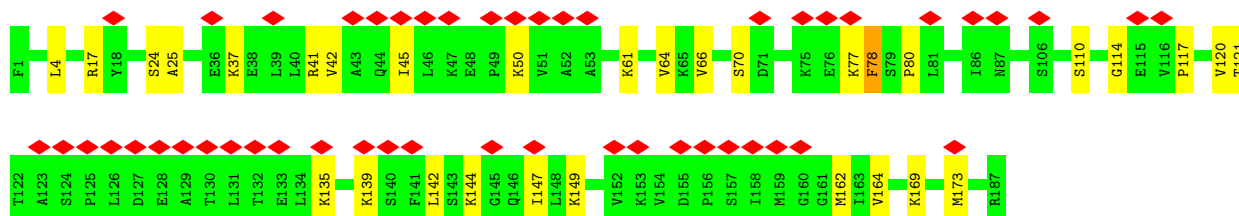
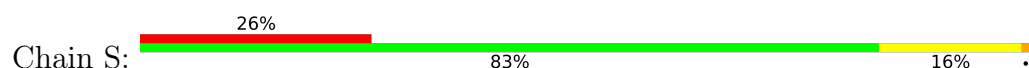




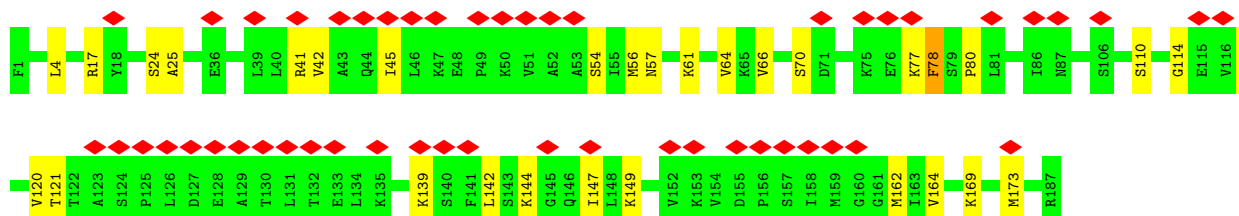
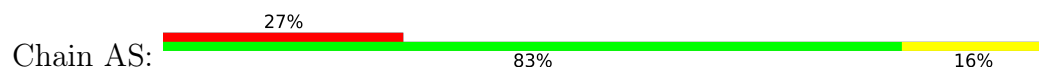
- Molecule 6: ATP synthase F1 subunit epsilon



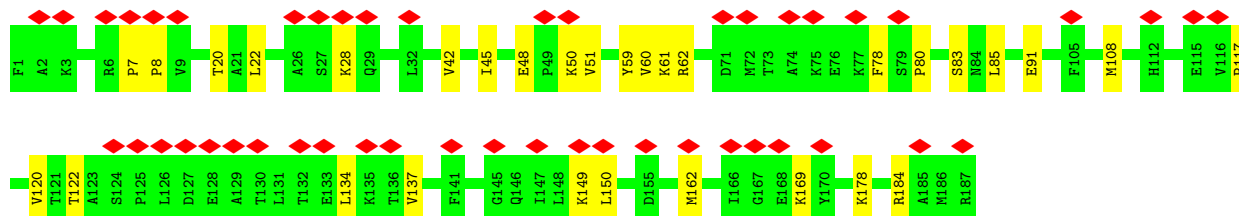
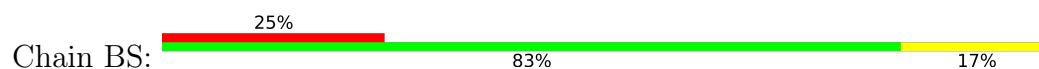
- Molecule 7: ATP synthase subunit O, mitochondrial



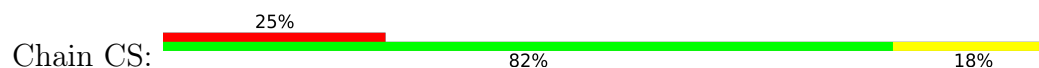
- Molecule 7: ATP synthase subunit O, mitochondrial

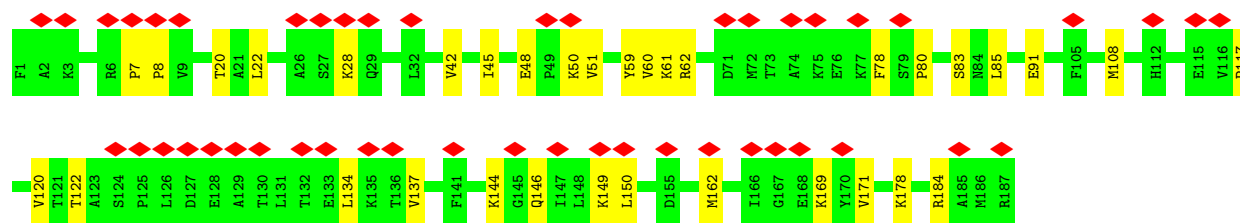


- Molecule 7: ATP synthase subunit O, mitochondrial

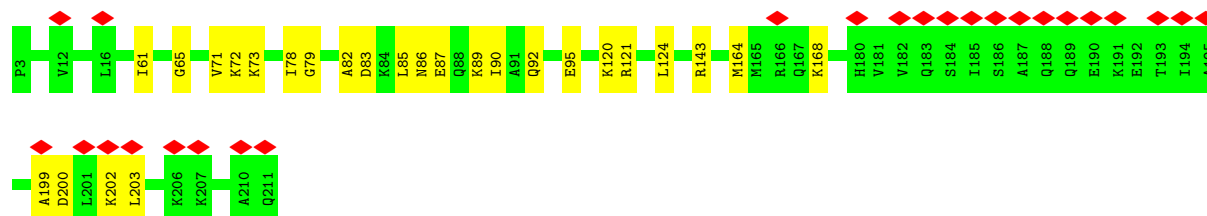
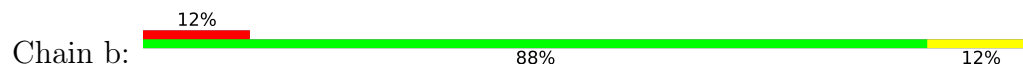


- Molecule 7: ATP synthase subunit O, mitochondrial

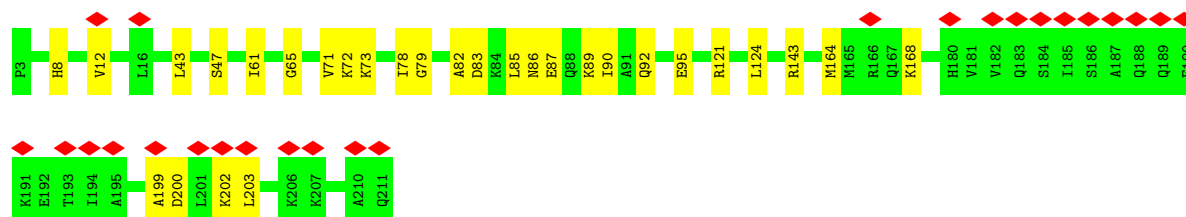
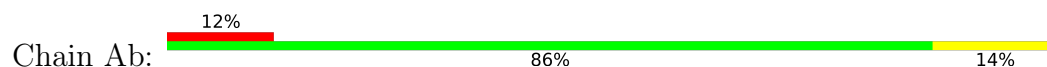




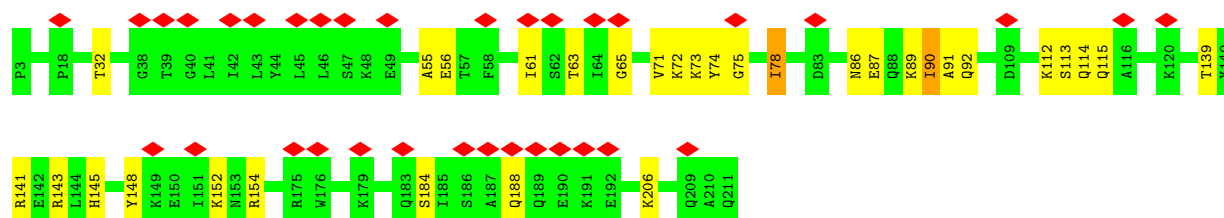
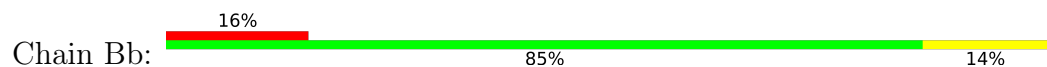
- Molecule 8: ATP synthase peripheral stalk-membrane subunit b



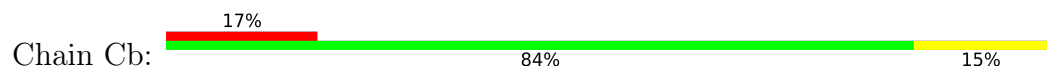
- Molecule 8: ATP synthase peripheral stalk-membrane subunit b

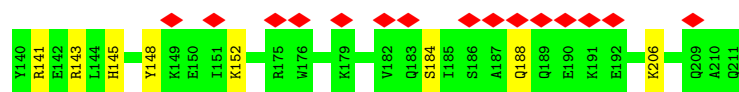


- Molecule 8: ATP synthase peripheral stalk-membrane subunit b

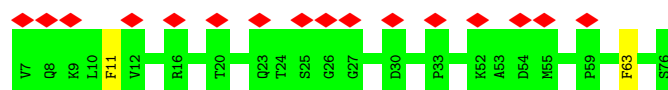


- Molecule 8: ATP synthase peripheral stalk-membrane subunit b

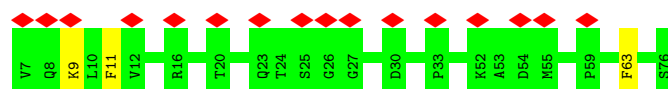




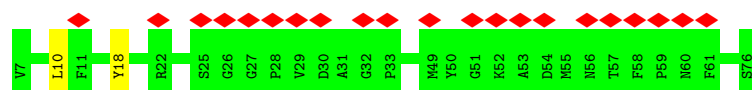
- Molecule 9: ATP synthase-coupling factor 6, mitochondrial



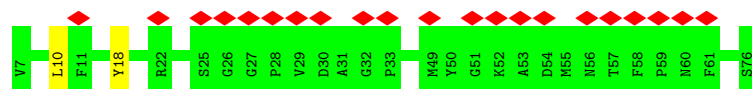
- Molecule 9: ATP synthase-coupling factor 6, mitochondrial



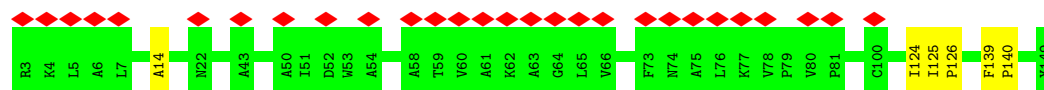
- Molecule 9: ATP synthase-coupling factor 6, mitochondrial



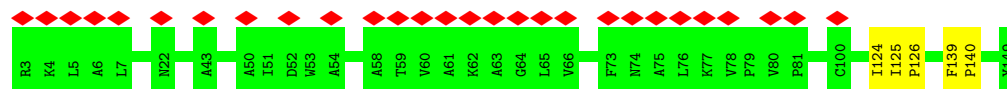
- Molecule 9: ATP synthase-coupling factor 6, mitochondrial



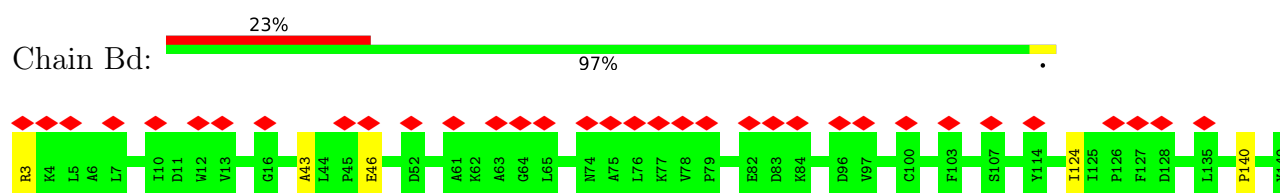
- Molecule 10: ATP synthase subunit d, mitochondrial



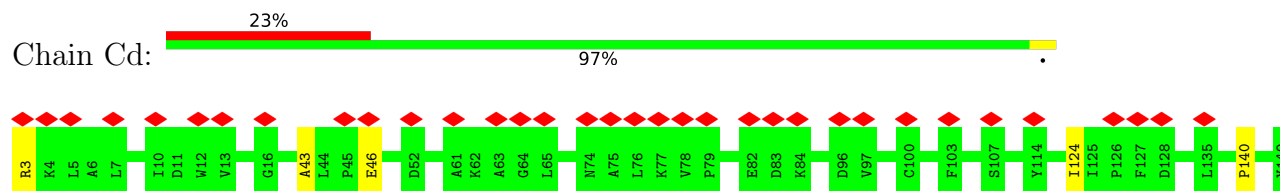
- Molecule 10: ATP synthase subunit d, mitochondrial



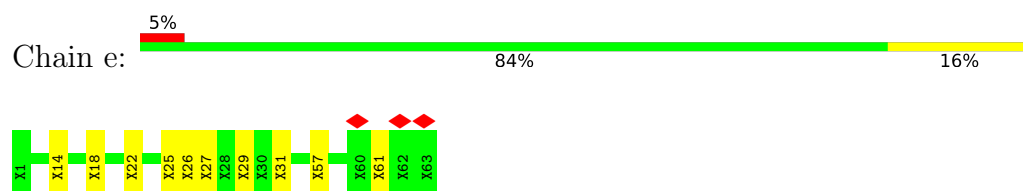
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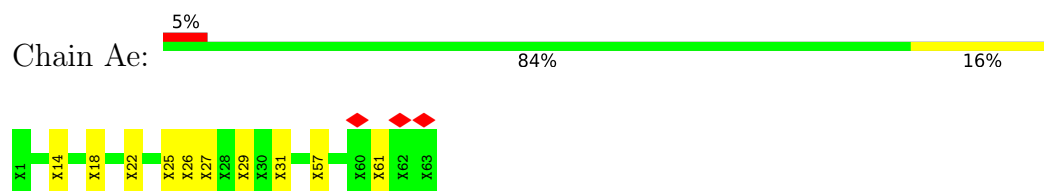
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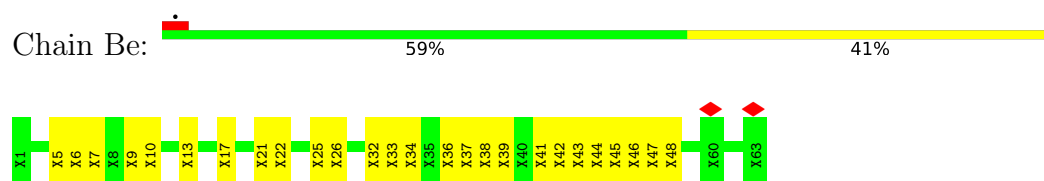
- Molecule 11: ATP synthase subunit e



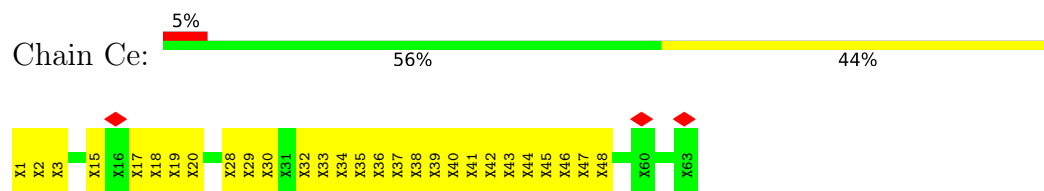
- Molecule 11: ATP synthase subunit e



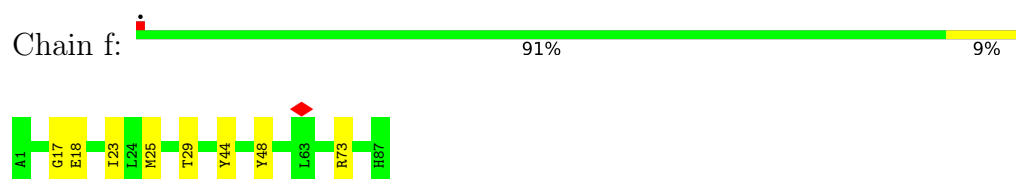
- Molecule 11: ATP synthase subunit e



- Molecule 11: ATP synthase subunit e



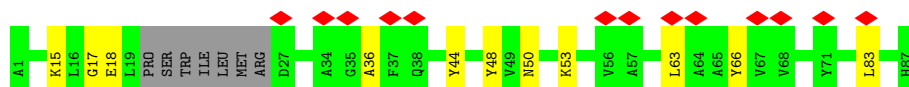
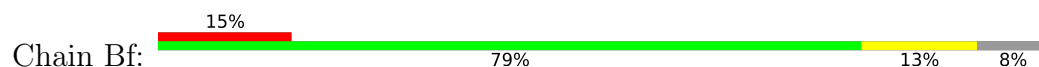
- Molecule 12: ATP synthase subunit f, mitochondrial



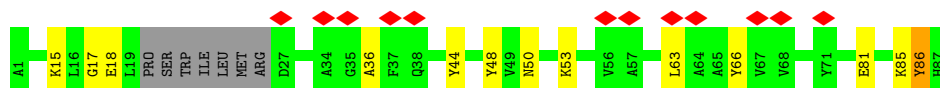
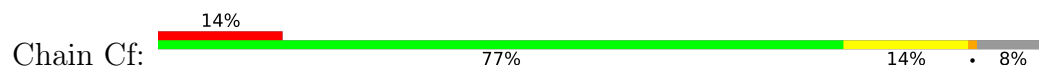
- Molecule 12: ATP synthase subunit f, mitochondrial



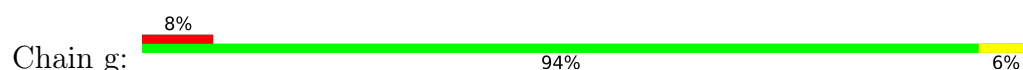
- Molecule 12: ATP synthase subunit f, mitochondrial



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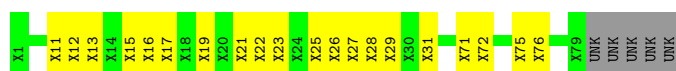
- Molecule 13: ATP synthase subunit g



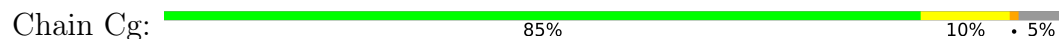
- Molecule 13: ATP synthase subunit g



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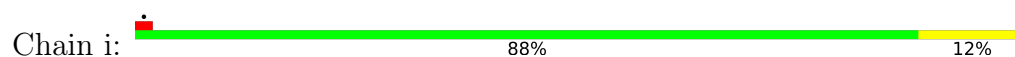


- Molecule 13: ATP synthase subunit g

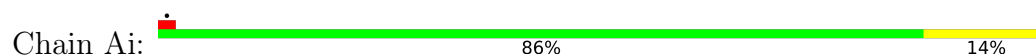




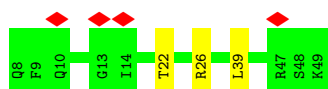
- Molecule 14: ATP synthase membrane subunit DAPIT



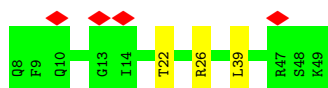
- Molecule 14: ATP synthase membrane subunit DAPIT



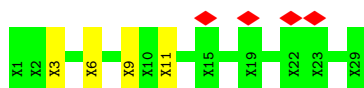
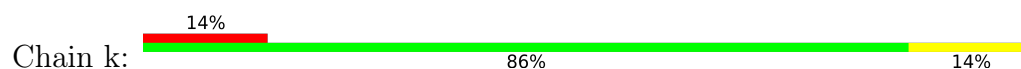
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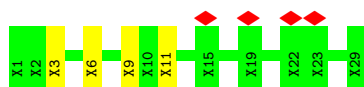
- Molecule 14: ATP synthase membrane subunit DAPIT



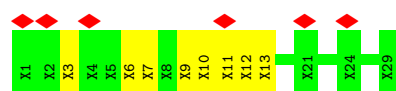
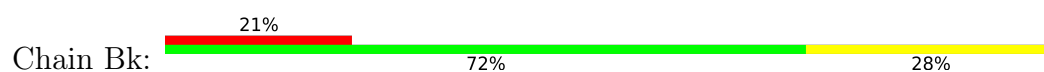
- Molecule 15: subunit k analog



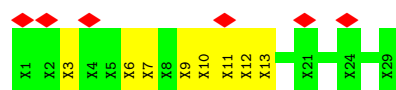
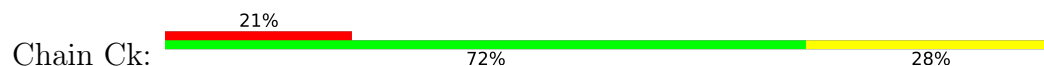
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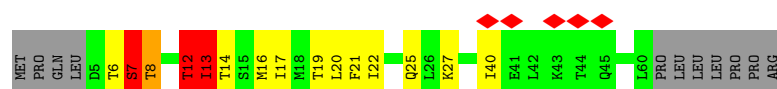
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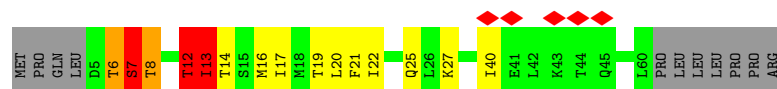
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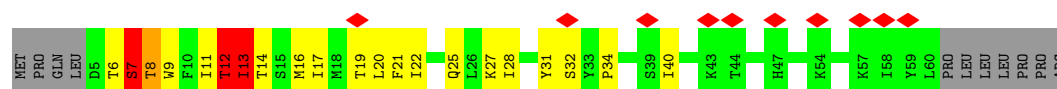
- Molecule 16: ATP synthase protein 8



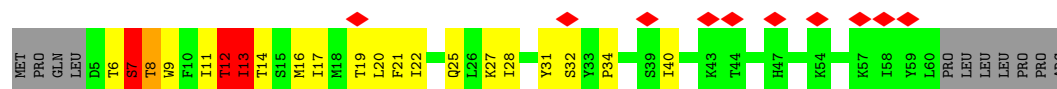
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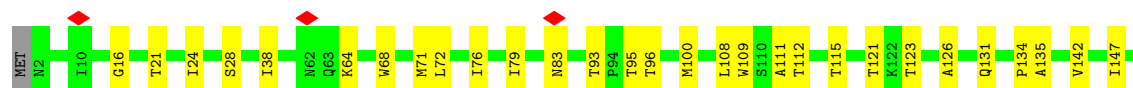
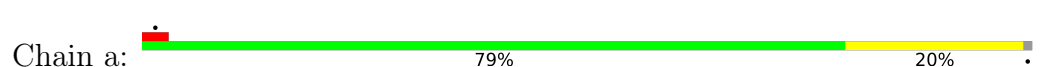
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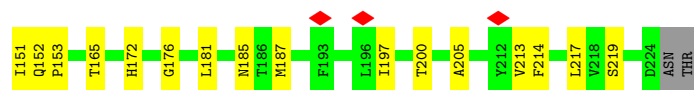


- Molecule 16: ATP synthase protein 8

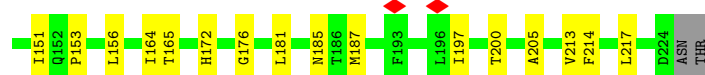
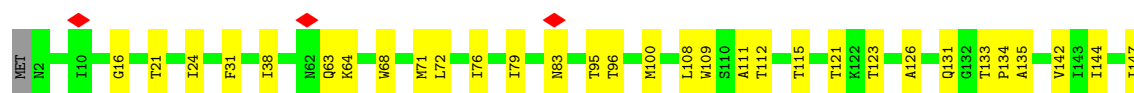
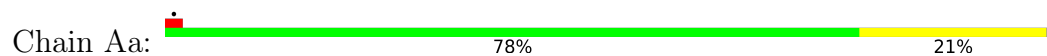


- Molecule 17: ATP synthase subunit a

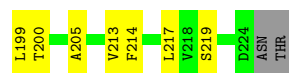
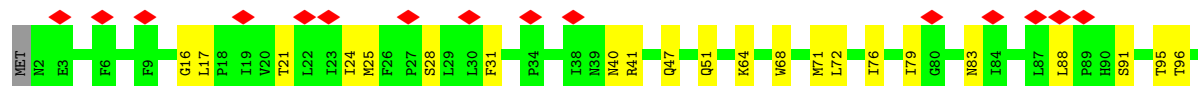
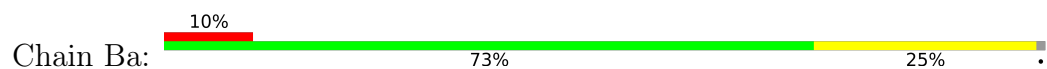




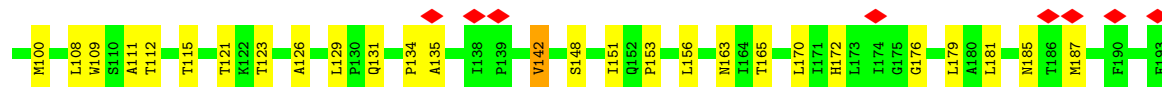
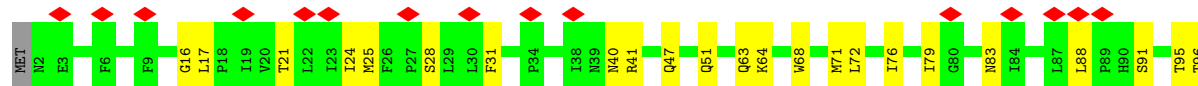
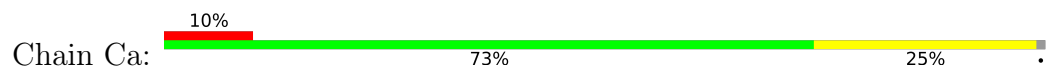
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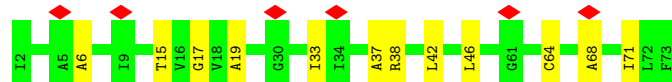
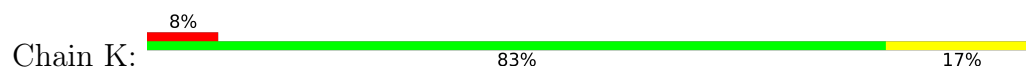
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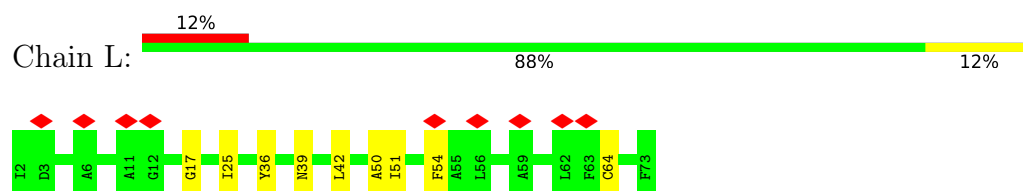
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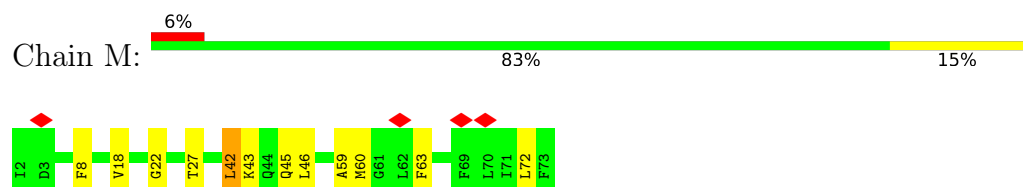
- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1



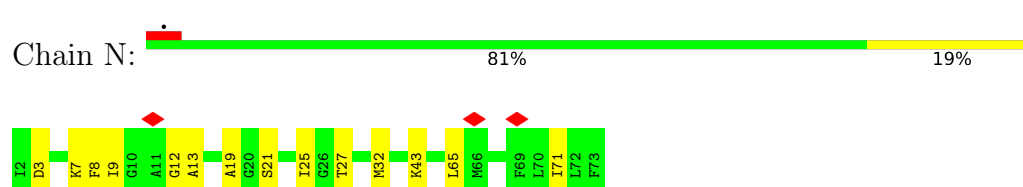
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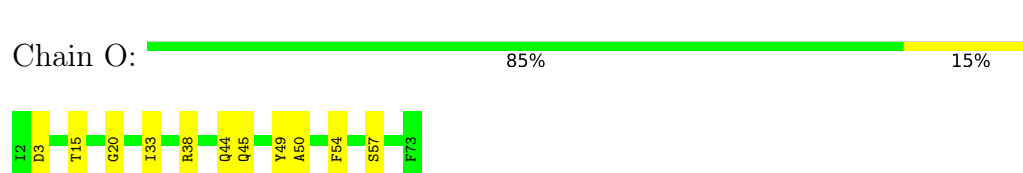
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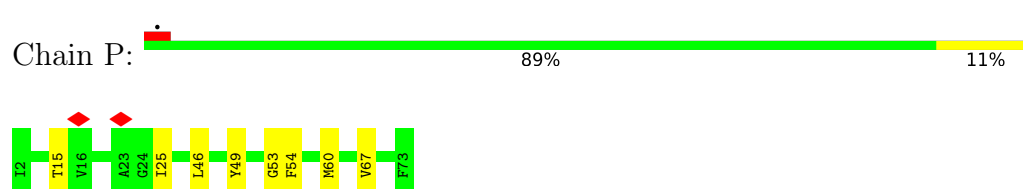
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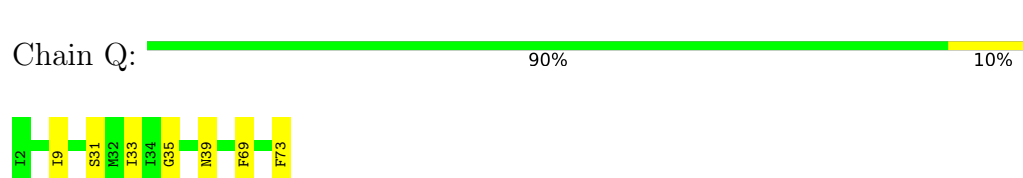
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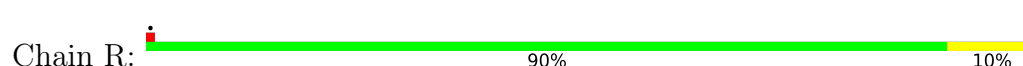
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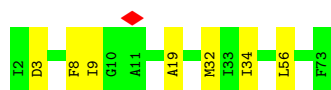


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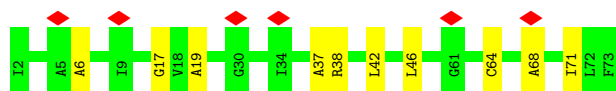
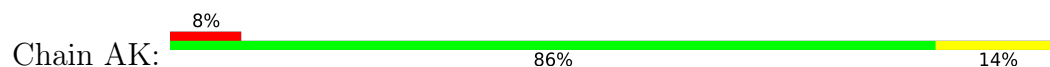


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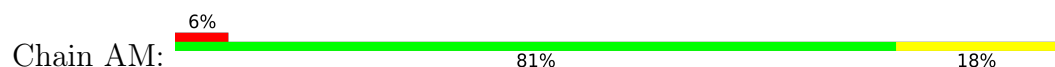
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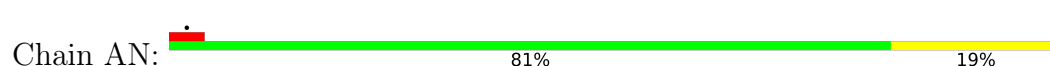
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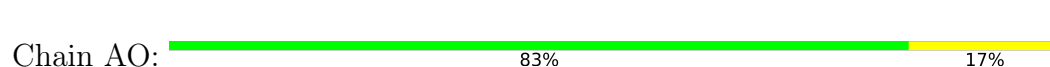
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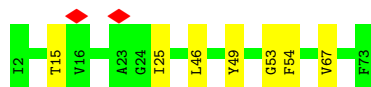
- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1



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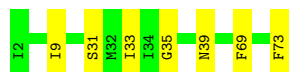


- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1



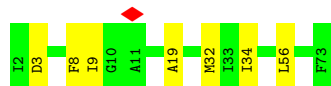
- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1

Chain AQ:  90% 10%



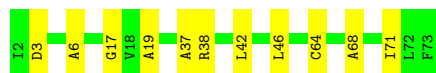
- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1

Chain AR:  90% 10%



- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1

Chain BK:  85% 15%



- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1

Chain BL:  8% 89% 11%



- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1

Chain BM:  11% 75% 24%



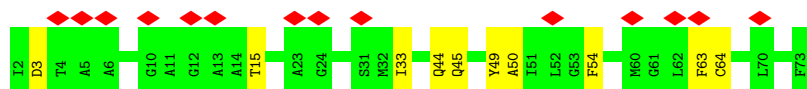
- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1

Chain BN:  14% 79% 21%

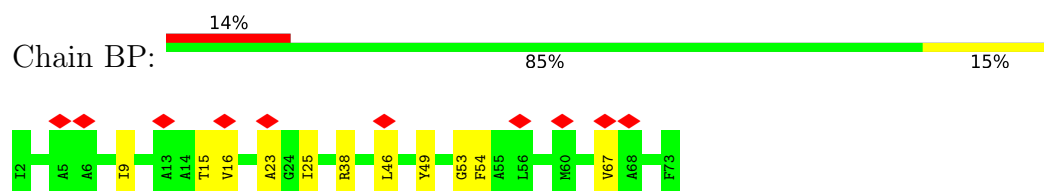


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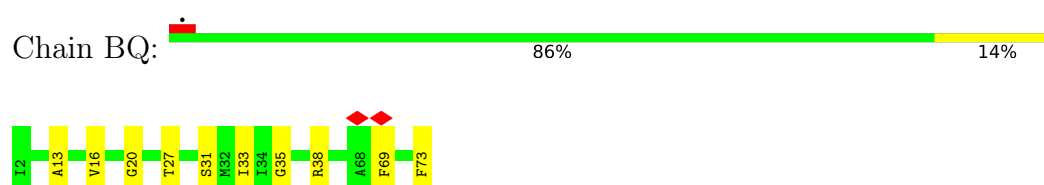
Chain BO:  19% 86% 14%



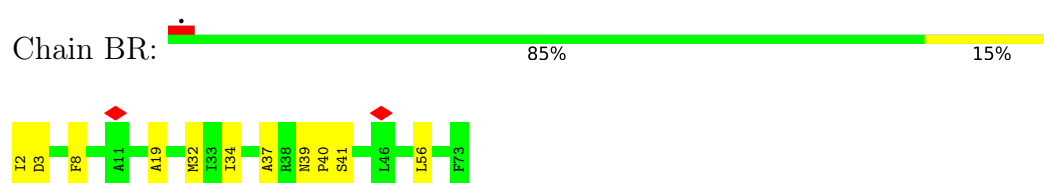
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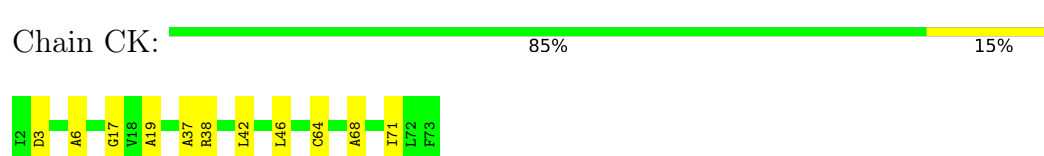
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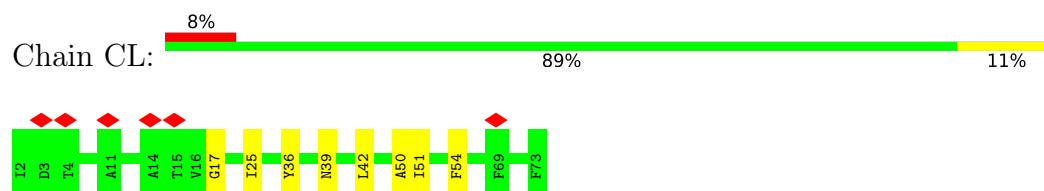
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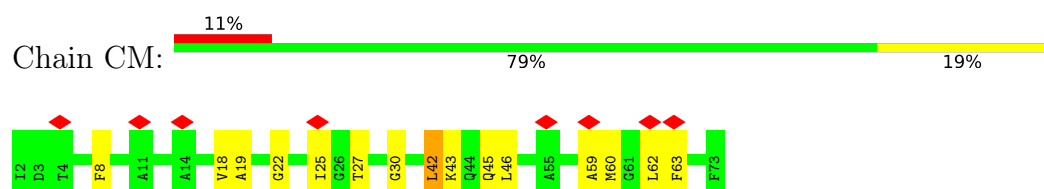
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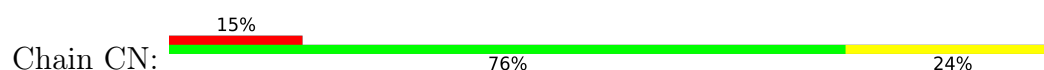
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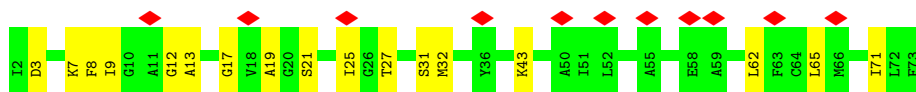


- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1

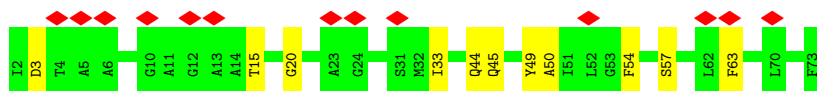
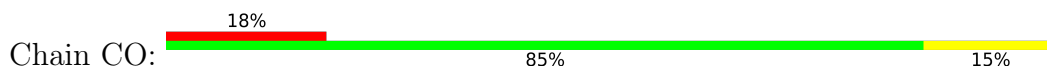


- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1

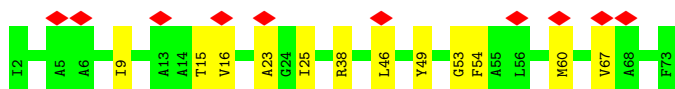
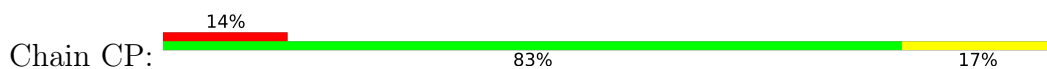




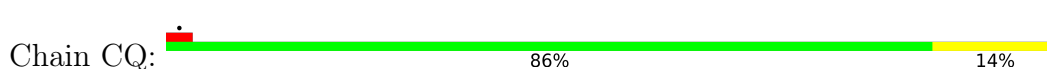
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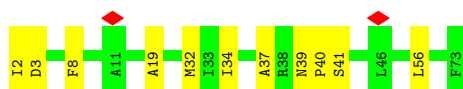
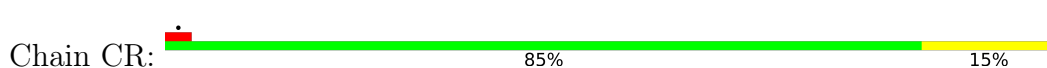
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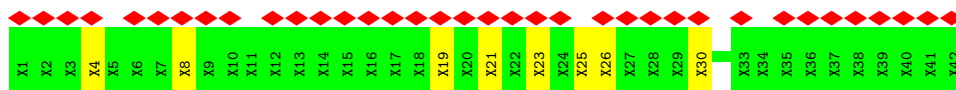
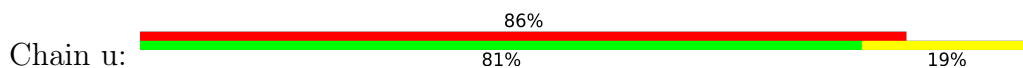
- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1



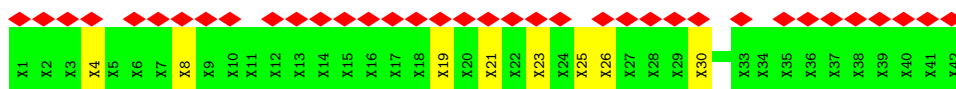
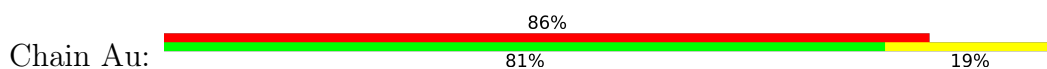
- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1



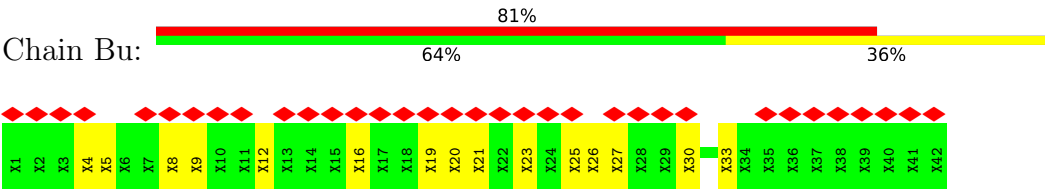
- Molecule 19: ATP synthase membrane subunit 6.8PL



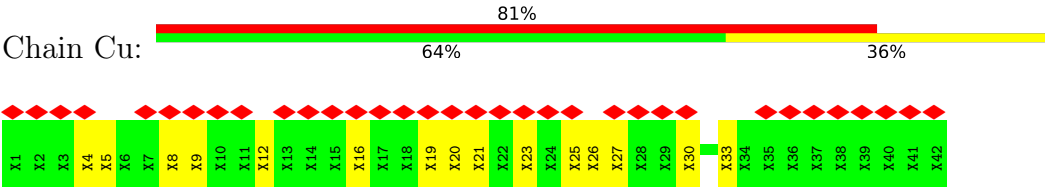
- Molecule 19: ATP synthase membrane subunit 6.8PL



- Molecule 19: ATP synthase membrane subunit 6.8PL



● Molecule 19: ATP synthase membrane subunit 6.8PL



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.571	Depositor
Minimum map value	-0.528	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.315	Depositor
Map size ($\text{\AA}$)	662.4, 662.4, 662.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.38, 1.38, 1.38	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, 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	A	0.26	0/3888	0.56	0/5247
1	AA	0.26	0/3888	0.56	0/5247
1	AB	0.23	0/3862	0.50	1/5210 (0.0%)
1	AC	0.24	0/3773	0.55	2/5091 (0.0%)
1	B	0.23	0/3862	0.50	1/5210 (0.0%)
1	BA	0.38	0/3924	0.62	0/5295
1	BB	0.38	0/3717	0.62	1/5014 (0.0%)
1	BC	0.44	0/3872	0.69	2/5225 (0.0%)
1	C	0.24	0/3773	0.55	2/5091 (0.0%)
1	CA	0.38	0/3924	0.62	0/5295
1	CB	0.38	0/3717	0.62	1/5014 (0.0%)
1	CC	0.44	0/3872	0.69	2/5225 (0.0%)
2	AD	0.27	0/3613	0.53	1/4900 (0.0%)
2	AE	0.23	0/3579	0.49	1/4854 (0.0%)
2	AF	0.24	0/3584	0.51	0/4861
2	BD	0.41	0/3613	0.63	1/4900 (0.0%)
2	BE	0.35	0/3579	0.58	1/4854 (0.0%)
2	BF	0.44	0/3584	0.61	1/4861 (0.0%)
2	CD	0.41	0/3613	0.63	1/4900 (0.0%)
2	CE	0.35	0/3579	0.58	1/4854 (0.0%)
2	CF	0.44	0/3584	0.61	1/4861 (0.0%)
2	D	0.27	0/3610	0.53	1/4896 (0.0%)
2	E	0.23	0/3579	0.49	1/4854 (0.0%)
2	F	0.24	0/3584	0.51	0/4861
3	AJ	0.36	0/587	0.81	1/780 (0.1%)
3	BJ	0.43	0/565	0.74	0/752
3	CJ	0.43	0/565	0.75	1/752 (0.1%)
3	J	0.37	0/587	0.79	0/780
4	AG	0.22	0/2135	0.59	0/2870
4	BG	0.30	0/2138	0.63	0/2874
4	CG	0.30	0/2135	0.63	0/2870
4	G	0.22	0/2135	0.59	0/2870

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	AH	0.24	0/983	0.66	0/1338
5	BH	0.27	0/986	0.65	0/1342
5	CH	0.27	0/986	0.65	0/1342
5	H	0.24	0/983	0.67	0/1338
6	AI	0.22	0/382	0.60	0/511
6	BI	0.25	0/382	0.61	0/511
6	CI	0.25	0/382	0.61	0/511
6	I	0.23	0/382	0.60	0/511
7	AS	0.20	0/1447	0.59	0/1947
7	BS	0.29	0/1453	0.61	0/1954
7	CS	0.29	0/1453	0.61	0/1954
7	S	0.20	0/1447	0.59	0/1947
8	Ab	0.23	0/1489	0.63	0/2010
8	Bb	0.28	0/1487	0.79	3/2006 (0.1%)
8	Cb	0.28	0/1487	0.79	3/2006 (0.1%)
8	b	0.23	0/1489	0.63	0/2010
9	Ac	0.17	0/431	0.49	0/587
9	Bc	0.20	0/431	0.58	0/587
9	Cc	0.20	0/431	0.58	0/587
9	c	0.17	0/431	0.50	0/587
10	Ad	0.21	0/742	0.72	2/1036 (0.2%)
10	Bd	0.23	0/742	0.75	1/1036 (0.1%)
10	Cd	0.23	0/742	0.75	1/1036 (0.1%)
10	d	0.20	0/742	0.72	2/1036 (0.2%)
12	Af	0.30	0/535	0.88	0/730
12	Bf	0.30	0/499	0.85	0/678
12	Cf	0.30	0/490	0.87	0/667
12	f	0.30	0/535	0.88	0/730
14	Ai	0.29	0/311	0.65	0/421
14	Bi	0.34	0/308	0.73	0/417
14	Ci	0.34	0/308	0.73	0/417
14	i	0.29	0/311	0.65	0/421
16	8	0.43	0/380	1.08	4/522 (0.8%)
16	A8	0.43	0/380	1.08	4/522 (0.8%)
16	B8	0.45	0/380	1.11	4/522 (0.8%)
16	C8	0.45	0/380	1.11	4/522 (0.8%)
17	Aa	0.44	0/1736	0.82	3/2375 (0.1%)
17	Ba	0.44	0/1721	0.82	3/2358 (0.1%)
17	Ca	0.44	0/1721	0.82	3/2358 (0.1%)
17	a	0.44	0/1736	0.82	3/2375 (0.1%)
18	AK	0.36	0/522	0.68	0/703
18	AL	0.30	0/522	0.75	0/703
18	AM	0.38	0/522	0.78	0/703

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
18	AN	0.37	0/519	0.67	0/700
18	AO	0.33	0/519	0.74	0/699
18	AP	0.28	0/522	0.67	0/703
18	AQ	0.29	0/522	0.62	0/703
18	AR	0.34	0/522	0.71	0/703
18	BK	0.36	0/522	0.67	0/703
18	BL	0.30	0/522	0.75	0/703
18	BM	0.38	0/522	0.78	0/703
18	BN	0.37	0/519	0.68	0/700
18	BO	0.34	0/519	0.74	0/700
18	BP	0.28	0/522	0.66	0/703
18	BQ	0.29	0/522	0.62	0/703
18	BR	0.34	0/519	0.71	0/699
18	CK	0.36	0/522	0.67	0/703
18	CL	0.30	0/522	0.75	0/703
18	CM	0.38	0/522	0.78	0/703
18	CN	0.37	0/519	0.67	0/700
18	CO	0.33	0/519	0.74	0/700
18	CP	0.28	0/522	0.66	0/703
18	CQ	0.29	0/522	0.62	0/703
18	CR	0.34	0/519	0.71	0/699
18	K	0.35	0/522	0.68	0/703
18	L	0.30	0/522	0.75	0/703
18	M	0.38	0/522	0.78	0/703
18	N	0.37	0/519	0.67	0/700
18	O	0.33	0/519	0.74	0/699
18	P	0.28	0/522	0.67	0/703
18	Q	0.29	0/522	0.62	0/703
18	R	0.34	0/522	0.71	0/703
All	All	0.32	0/150335	0.64	64/203395 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	BC	0	1
1	CC	0	1
2	AD	0	1
2	AE	0	1
2	AF	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	BD	0	1
2	BE	0	1
2	BF	0	1
2	CD	0	1
2	CE	0	1
2	CF	0	1
2	D	0	1
2	E	0	1
2	F	0	1
5	AH	0	2
5	BH	0	1
5	CH	0	1
5	H	0	2
7	AS	0	1
7	S	0	1
12	Af	0	2
12	Bf	0	1
12	Cf	0	1
12	f	0	2
13	Cg	0	1
16	8	0	4
16	A8	0	4
16	B8	0	4
16	C8	0	4
All	All	0	45

There are no bond length outliers.

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AJ	56	HIS	N-CA-C	-9.59	101.36	112.87
10	d	124	ILE	N-CA-C	7.93	118.71	110.62
10	Ad	124	ILE	N-CA-C	7.88	118.66	110.62
8	Bb	86	ASN	N-CA-C	-7.53	103.15	111.36
8	Cb	86	ASN	N-CA-C	-7.52	103.16	111.36

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	280	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	E	280	ALA	Peptide
2	F	280	ALA	Peptide
5	H	33	VAL	Peptide
5	H	68	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3837	0	3939	34	0
1	AA	3837	0	3939	37	0
1	AB	3814	0	3930	36	0
1	AC	3722	0	3826	32	0
1	B	3814	0	3930	32	0
1	BA	3873	0	3978	40	0
1	BB	3669	0	3781	49	0
1	BC	3821	0	3924	43	0
1	C	3722	0	3826	33	0
1	CA	3873	0	3978	33	0
1	CB	3669	0	3781	47	0
1	CC	3821	0	3924	45	0
2	AD	3555	0	3603	25	0
2	AE	3522	0	3580	26	0
2	AF	3527	0	3584	25	0
2	BD	3555	0	3603	36	0
2	BE	3522	0	3580	37	0
2	BF	3527	0	3585	30	0
2	CD	3555	0	3603	37	0
2	CE	3522	0	3580	37	0
2	CF	3527	0	3585	28	0
2	D	3552	0	3601	23	0
2	E	3522	0	3580	25	0
2	F	3527	0	3584	26	0
3	AJ	583	0	561	28	0
3	BJ	561	0	523	34	0
3	CJ	561	0	523	31	0
3	J	583	0	561	27	0
4	AG	2109	0	2187	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BG	2112	0	2189	30	0
4	CG	2109	0	2187	32	0
4	G	2109	0	2187	14	0
5	AH	970	0	962	14	0
5	BH	973	0	971	35	0
5	CH	973	0	971	33	0
5	H	970	0	962	15	0
6	AI	377	0	397	6	0
6	BI	377	0	397	5	0
6	CI	377	0	397	6	0
6	I	377	0	397	9	0
7	AS	1429	0	1535	19	0
7	BS	1435	0	1546	22	0
7	CS	1435	0	1546	25	0
7	S	1429	0	1535	20	0
8	Ab	1478	0	1340	27	0
8	Bb	1476	0	1340	31	0
8	Cb	1476	0	1340	32	0
8	b	1478	0	1340	27	0
9	Ac	428	0	305	3	0
9	Bc	428	0	305	3	0
9	Cc	428	0	305	4	0
9	c	428	0	305	2	0
10	Ad	741	0	348	3	0
10	Bd	741	0	348	5	0
10	Cd	741	0	348	5	0
10	d	741	0	348	4	0
11	Ae	315	0	65	5	0
11	Be	315	0	66	28	0
11	Ce	315	0	66	30	0
11	e	315	0	65	5	0
12	Af	530	0	385	4	0
12	Bf	495	0	371	14	0
12	Cf	486	0	351	13	0
12	f	530	0	385	4	0
13	Ag	420	0	88	4	0
13	Bg	395	0	83	16	0
13	Cg	400	0	84	5	0
13	g	420	0	88	3	0
14	Ai	306	0	293	4	0
14	Bi	303	0	284	21	0
14	Ci	303	0	284	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	i	306	0	293	4	0
15	Ak	145	0	32	2	0
15	Bk	145	0	31	16	0
15	Ck	145	0	31	16	0
15	k	145	0	32	2	0
16	8	374	0	299	13	0
16	A8	374	0	299	14	0
16	B8	374	0	299	48	0
16	C8	374	0	299	49	0
17	Aa	1699	0	1789	30	0
17	Ba	1684	0	1748	76	0
17	Ca	1684	0	1748	76	0
17	a	1699	0	1789	27	0
18	AK	513	0	530	8	0
18	AL	513	0	530	5	0
18	AM	513	0	530	12	0
18	AN	510	0	523	10	0
18	AO	510	0	526	16	0
18	AP	513	0	530	5	0
18	AQ	513	0	530	5	0
18	AR	513	0	530	8	0
18	BK	513	0	530	12	0
18	BL	513	0	530	6	0
18	BM	513	0	530	32	0
18	BN	510	0	523	16	0
18	BO	510	0	523	8	0
18	BP	513	0	530	23	0
18	BQ	513	0	530	17	0
18	BR	510	0	521	28	0
18	CK	513	0	530	13	0
18	CL	513	0	530	6	0
18	CM	513	0	530	29	0
18	CN	510	0	523	18	0
18	CO	510	0	523	10	0
18	CP	513	0	530	23	0
18	CQ	513	0	530	17	0
18	CR	510	0	521	26	0
18	K	513	0	530	10	0
18	L	513	0	530	7	0
18	M	513	0	530	11	0
18	N	510	0	523	10	0
18	O	510	0	526	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	P	513	0	530	7	0
18	Q	513	0	530	5	0
18	R	513	0	530	9	0
19	Au	210	0	45	4	0
19	Bu	210	0	45	32	0
19	Cu	210	0	45	31	0
19	u	210	0	45	5	0
20	A	31	0	12	0	0
20	AA	31	0	12	0	0
20	AB	31	0	12	0	0
20	AC	31	0	12	0	0
20	B	31	0	12	0	0
20	BA	31	0	12	1	0
20	BB	31	0	12	2	0
20	BC	31	0	12	1	0
20	C	31	0	12	0	0
20	CA	31	0	12	1	0
20	CB	31	0	12	2	0
20	CC	31	0	12	1	0
21	A	1	0	0	0	0
21	AA	1	0	0	0	0
21	AB	1	0	0	0	0
21	AC	1	0	0	0	0
21	AD	1	0	0	0	0
21	AF	1	0	0	0	0
21	B	1	0	0	0	0
21	BA	1	0	0	0	0
21	BB	1	0	0	0	0
21	BC	1	0	0	0	0
21	BD	1	0	0	0	0
21	BF	1	0	0	0	0
21	C	1	0	0	0	0
21	CA	1	0	0	0	0
21	CB	1	0	0	0	0
21	CC	1	0	0	0	0
21	CD	1	0	0	0	0
21	CF	1	0	0	0	0
21	D	1	0	0	0	0
21	F	1	0	0	0	0
22	AD	27	0	11	1	0
22	AF	27	0	12	0	0
22	BD	27	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	BF	27	0	12	1	0
22	CD	27	0	11	1	0
22	CF	27	0	12	1	0
22	D	27	0	11	1	0
22	F	27	0	12	0	0
All	All	153148	0	149285	1886	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 6.

The worst 5 of 1886 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)
5:BH:48:LEU:HD21	18:BR:41:SER:CB	1.23	1.65
5:CH:48:LEU:CD2	18:CR:41:SER:HB3	1.30	1.61
5:CH:48:LEU:HD21	18:CR:41:SER:CB	1.23	1.58
5:BH:48:LEU:CD2	18:BR:41:SER:HB3	1.30	1.55
16:C8:28:ILE:HA	16:C8:31:TYR:CE1	1.41	1.53

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/509 (99%)	479 (95%)	23 (5%)	0	100	100
1	AA	502/509 (99%)	479 (95%)	23 (5%)	0	100	100
1	AB	497/509 (98%)	476 (96%)	21 (4%)	0	100	100
1	AC	486/509 (96%)	459 (94%)	27 (6%)	0	100	100
1	B	497/509 (98%)	476 (96%)	21 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	507/509 (100%)	479 (94%)	28 (6%)	0	100	100
1	BB	477/509 (94%)	455 (95%)	22 (5%)	0	100	100
1	BC	500/509 (98%)	464 (93%)	36 (7%)	0	100	100
1	C	486/509 (96%)	459 (94%)	27 (6%)	0	100	100
1	CA	507/509 (100%)	479 (94%)	28 (6%)	0	100	100
1	CB	477/509 (94%)	455 (95%)	22 (5%)	0	100	100
1	CC	500/509 (98%)	464 (93%)	36 (7%)	0	100	100
2	AD	467/469 (100%)	433 (93%)	33 (7%)	1 (0%)	43	78
2	AE	463/469 (99%)	442 (96%)	18 (4%)	3 (1%)	21	59
2	AF	464/469 (99%)	432 (93%)	30 (6%)	2 (0%)	30	67
2	BD	467/469 (100%)	421 (90%)	45 (10%)	1 (0%)	43	78
2	BE	463/469 (99%)	423 (91%)	39 (8%)	1 (0%)	43	78
2	BF	464/469 (99%)	422 (91%)	41 (9%)	1 (0%)	43	78
2	CD	467/469 (100%)	421 (90%)	45 (10%)	1 (0%)	43	78
2	CE	463/469 (99%)	423 (91%)	39 (8%)	1 (0%)	43	78
2	CF	464/469 (99%)	422 (91%)	41 (9%)	1 (0%)	43	78
2	D	467/469 (100%)	434 (93%)	32 (7%)	1 (0%)	43	78
2	E	463/469 (99%)	442 (96%)	18 (4%)	3 (1%)	21	59
2	F	464/469 (99%)	431 (93%)	31 (7%)	2 (0%)	30	67
3	AJ	76/83 (92%)	73 (96%)	3 (4%)	0	100	100
3	BJ	73/83 (88%)	71 (97%)	2 (3%)	0	100	100
3	CJ	73/83 (88%)	71 (97%)	2 (3%)	0	100	100
3	J	76/83 (92%)	73 (96%)	3 (4%)	0	100	100
4	AG	270/272 (99%)	257 (95%)	12 (4%)	1 (0%)	30	67
4	BG	270/272 (99%)	254 (94%)	14 (5%)	2 (1%)	18	56
4	CG	270/272 (99%)	253 (94%)	14 (5%)	3 (1%)	11	46
4	G	270/272 (99%)	258 (96%)	11 (4%)	1 (0%)	30	67
5	AH	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	8	39
5	BH	130/132 (98%)	117 (90%)	12 (9%)	1 (1%)	16	54
5	CH	130/132 (98%)	117 (90%)	12 (9%)	1 (1%)	16	54
5	H	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	8	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AI	46/48 (96%)	38 (83%)	8 (17%)	0	100	100
6	BI	46/48 (96%)	39 (85%)	7 (15%)	0	100	100
6	CI	46/48 (96%)	39 (85%)	7 (15%)	0	100	100
6	I	46/48 (96%)	38 (83%)	8 (17%)	0	100	100
7	AS	185/187 (99%)	163 (88%)	22 (12%)	0	100	100
7	BS	185/187 (99%)	163 (88%)	22 (12%)	0	100	100
7	CS	185/187 (99%)	163 (88%)	22 (12%)	0	100	100
7	S	185/187 (99%)	162 (88%)	23 (12%)	0	100	100
8	Ab	207/209 (99%)	195 (94%)	12 (6%)	0	100	100
8	Bb	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
8	Cb	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
8	b	207/209 (99%)	195 (94%)	12 (6%)	0	100	100
9	Ac	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
9	Bc	68/70 (97%)	61 (90%)	7 (10%)	0	100	100
9	Cc	68/70 (97%)	61 (90%)	7 (10%)	0	100	100
9	c	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
10	Ad	145/147 (99%)	132 (91%)	12 (8%)	1 (1%)	18	56
10	Bd	145/147 (99%)	126 (87%)	19 (13%)	0	100	100
10	Cd	145/147 (99%)	126 (87%)	19 (13%)	0	100	100
10	d	145/147 (99%)	132 (91%)	12 (8%)	1 (1%)	18	56
12	Af	85/87 (98%)	63 (74%)	22 (26%)	0	100	100
12	Bf	76/87 (87%)	63 (83%)	12 (16%)	1 (1%)	9	42
12	Cf	76/87 (87%)	62 (82%)	12 (16%)	2 (3%)	4	25
12	f	85/87 (98%)	63 (74%)	22 (26%)	0	100	100
14	Ai	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
14	Bi	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
14	Ci	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
14	i	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
16	8	54/67 (81%)	46 (85%)	4 (7%)	4 (7%)	1	10
16	A8	54/67 (81%)	46 (85%)	4 (7%)	4 (7%)	1	10
16	B8	54/67 (81%)	46 (85%)	4 (7%)	4 (7%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	C8	54/67 (81%)	46 (85%)	4 (7%)	4 (7%)	1	10
17	Aa	221/226 (98%)	195 (88%)	26 (12%)	0	100	100
17	Ba	221/226 (98%)	194 (88%)	27 (12%)	0	100	100
17	Ca	221/226 (98%)	194 (88%)	27 (12%)	0	100	100
17	a	221/226 (98%)	195 (88%)	26 (12%)	0	100	100
18	AK	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
18	AL	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
18	AM	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
18	AN	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
18	AO	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
18	AP	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
18	AQ	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
18	AR	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
18	BK	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
18	BL	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
18	BM	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
18	BN	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
18	BO	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
18	BP	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
18	BQ	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
18	BR	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
18	CK	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
18	CL	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
18	CM	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
18	CN	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
18	CO	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
18	CP	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
18	CQ	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
18	CR	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
18	K	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
18	L	70/72 (97%)	66 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	M	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
18	N	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
18	O	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
18	P	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
18	Q	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
18	R	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
All	All	19838/20320 (98%)	18401 (93%)	1385 (7%)	52 (0%)	37	72

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	281	VAL
2	E	281	VAL
2	F	281	VAL
5	H	69	ASP
10	d	126	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/410 (99%)	404 (100%)	2 (0%)	81	83
1	AA	406/410 (99%)	404 (100%)	2 (0%)	81	83
1	AB	405/410 (99%)	404 (100%)	1 (0%)	87	87
1	AC	393/410 (96%)	391 (100%)	2 (0%)	81	83
1	B	405/410 (99%)	404 (100%)	1 (0%)	87	87
1	BA	410/410 (100%)	405 (99%)	5 (1%)	63	75
1	BB	389/410 (95%)	388 (100%)	1 (0%)	86	85
1	BC	404/410 (98%)	399 (99%)	5 (1%)	63	75
1	C	393/410 (96%)	391 (100%)	2 (0%)	81	83
1	CA	410/410 (100%)	405 (99%)	5 (1%)	63	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CB	389/410 (95%)	388 (100%)	1 (0%)	86	85
1	CC	404/410 (98%)	399 (99%)	5 (1%)	63	75
2	AD	378/378 (100%)	376 (100%)	2 (0%)	81	83
2	AE	375/378 (99%)	373 (100%)	2 (0%)	81	83
2	AF	375/378 (99%)	375 (100%)	0	100	100
2	BD	378/378 (100%)	375 (99%)	3 (1%)	73	80
2	BE	375/378 (99%)	373 (100%)	2 (0%)	81	83
2	BF	375/378 (99%)	374 (100%)	1 (0%)	86	85
2	CD	378/378 (100%)	375 (99%)	3 (1%)	73	80
2	CE	375/378 (99%)	373 (100%)	2 (0%)	81	83
2	CF	375/378 (99%)	374 (100%)	1 (0%)	86	85
2	D	377/378 (100%)	375 (100%)	2 (0%)	81	83
2	E	375/378 (99%)	373 (100%)	2 (0%)	81	83
2	F	375/378 (99%)	375 (100%)	0	100	100
3	AJ	52/68 (76%)	52 (100%)	0	100	100
3	BJ	50/68 (74%)	50 (100%)	0	100	100
3	CJ	50/68 (74%)	50 (100%)	0	100	100
3	J	52/68 (76%)	52 (100%)	0	100	100
4	AG	229/230 (100%)	229 (100%)	0	100	100
4	BG	230/230 (100%)	229 (100%)	1 (0%)	84	84
4	CG	229/230 (100%)	228 (100%)	1 (0%)	84	84
4	G	229/230 (100%)	229 (100%)	0	100	100
5	AH	104/105 (99%)	104 (100%)	0	100	100
5	BH	105/105 (100%)	104 (99%)	1 (1%)	68	78
5	CH	105/105 (100%)	104 (99%)	1 (1%)	68	78
5	H	104/105 (99%)	104 (100%)	0	100	100
6	AI	38/38 (100%)	38 (100%)	0	100	100
6	BI	38/38 (100%)	38 (100%)	0	100	100
6	CI	38/38 (100%)	38 (100%)	0	100	100
6	I	38/38 (100%)	38 (100%)	0	100	100
7	AS	162/163 (99%)	162 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	BS	163/163 (100%)	163 (100%)	0	100	100
7	CS	163/163 (100%)	163 (100%)	0	100	100
7	S	162/163 (99%)	162 (100%)	0	100	100
8	Ab	124/182 (68%)	124 (100%)	0	100	100
8	Bb	123/182 (68%)	121 (98%)	2 (2%)	55	70
8	Cb	123/182 (68%)	121 (98%)	2 (2%)	55	70
8	b	124/182 (68%)	124 (100%)	0	100	100
9	Ac	22/63 (35%)	22 (100%)	0	100	100
9	Bc	22/63 (35%)	22 (100%)	0	100	100
9	Cc	22/63 (35%)	22 (100%)	0	100	100
9	c	22/63 (35%)	22 (100%)	0	100	100
10	Ad	1/127 (1%)	1 (100%)	0	100	100
10	Bd	1/127 (1%)	1 (100%)	0	100	100
10	Cd	1/127 (1%)	1 (100%)	0	100	100
10	d	1/127 (1%)	1 (100%)	0	100	100
12	Af	27/75 (36%)	27 (100%)	0	100	100
12	Bf	27/75 (36%)	27 (100%)	0	100	100
12	Cf	25/75 (33%)	25 (100%)	0	100	100
12	f	27/75 (36%)	27 (100%)	0	100	100
14	Ai	29/36 (81%)	29 (100%)	0	100	100
14	Bi	28/36 (78%)	28 (100%)	0	100	100
14	Ci	28/36 (78%)	28 (100%)	0	100	100
14	i	29/36 (81%)	29 (100%)	0	100	100
16	8	29/66 (44%)	28 (97%)	1 (3%)	32	54
16	A8	29/66 (44%)	28 (97%)	1 (3%)	32	54
16	B8	29/66 (44%)	28 (97%)	1 (3%)	32	54
16	C8	29/66 (44%)	28 (97%)	1 (3%)	32	54
17	Aa	187/199 (94%)	184 (98%)	3 (2%)	55	70
17	Ba	183/199 (92%)	180 (98%)	3 (2%)	55	70
17	Ca	183/199 (92%)	180 (98%)	3 (2%)	55	70
17	a	187/199 (94%)	184 (98%)	3 (2%)	55	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AK	49/49 (100%)	49 (100%)	0	100	100
18	AL	49/49 (100%)	48 (98%)	1 (2%)	48	66
18	AM	49/49 (100%)	48 (98%)	1 (2%)	48	66
18	AN	48/49 (98%)	47 (98%)	1 (2%)	47	65
18	AO	48/49 (98%)	48 (100%)	0	100	100
18	AP	49/49 (100%)	48 (98%)	1 (2%)	48	66
18	AQ	49/49 (100%)	49 (100%)	0	100	100
18	AR	49/49 (100%)	49 (100%)	0	100	100
18	BK	49/49 (100%)	49 (100%)	0	100	100
18	BL	49/49 (100%)	48 (98%)	1 (2%)	48	66
18	BM	49/49 (100%)	48 (98%)	1 (2%)	48	66
18	BN	48/49 (98%)	47 (98%)	1 (2%)	47	65
18	BO	48/49 (98%)	48 (100%)	0	100	100
18	BP	49/49 (100%)	48 (98%)	1 (2%)	48	66
18	BQ	49/49 (100%)	49 (100%)	0	100	100
18	BR	48/49 (98%)	48 (100%)	0	100	100
18	CK	49/49 (100%)	49 (100%)	0	100	100
18	CL	49/49 (100%)	48 (98%)	1 (2%)	48	66
18	CM	49/49 (100%)	48 (98%)	1 (2%)	48	66
18	CN	48/49 (98%)	47 (98%)	1 (2%)	47	65
18	CO	48/49 (98%)	48 (100%)	0	100	100
18	CP	49/49 (100%)	48 (98%)	1 (2%)	48	66
18	CQ	49/49 (100%)	49 (100%)	0	100	100
18	CR	48/49 (98%)	48 (100%)	0	100	100
18	K	49/49 (100%)	49 (100%)	0	100	100
18	L	49/49 (100%)	48 (98%)	1 (2%)	48	66
18	M	49/49 (100%)	48 (98%)	1 (2%)	48	66
18	N	48/49 (98%)	47 (98%)	1 (2%)	47	65
18	O	48/49 (98%)	48 (100%)	0	100	100
18	P	49/49 (100%)	48 (98%)	1 (2%)	48	66
18	Q	49/49 (100%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	49/49 (100%)	49 (100%)	0	100	100
All	All	14886/16432 (91%)	14794 (99%)	92 (1%)	76	83

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Ba	142	VAL
1	CC	229	THR
18	BL	42	LEU
1	CA	176	THR
2	CD	130	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 196 such sidechains are listed below:

Mol	Chain	Res	Type
1	BB	466	ASN
17	Ba	47	GLN
1	BC	330	GLN
2	BF	295	GLN
1	CA	42	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 20 are monoatomic - leaving 20 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
20	ATP	CC	601	21	32,33,33	1.33	4 (12%)	48,52,52	1.79	7 (14%)
22	ADP	AF	501	21	28,29,29	1.41	4 (14%)	43,45,45	1.83	8 (18%)
20	ATP	AB	601	21	32,33,33	1.34	5 (15%)	48,52,52	1.77	8 (16%)
22	ADP	D	501	21	28,29,29	1.44	7 (25%)	43,45,45	2.11	11 (25%)
20	ATP	BB	601	21	32,33,33	1.28	4 (12%)	48,52,52	1.82	10 (20%)
20	ATP	BC	601	21	32,33,33	1.33	4 (12%)	48,52,52	1.80	7 (14%)
22	ADP	AD	501	21	28,29,29	1.44	7 (25%)	43,45,45	2.11	11 (25%)
22	ADP	BF	501	21	28,29,29	1.38	4 (14%)	43,45,45	1.80	8 (18%)
20	ATP	C	601	21	32,33,33	1.33	4 (12%)	48,52,52	1.76	8 (16%)
22	ADP	F	501	21	28,29,29	1.40	4 (14%)	43,45,45	1.84	8 (18%)
20	ATP	AA	601	21	32,33,33	1.34	5 (15%)	48,52,52	1.80	8 (16%)
20	ATP	CA	601	21	32,33,33	1.39	6 (18%)	48,52,52	1.80	7 (14%)
22	ADP	CD	501	21	28,29,29	1.49	6 (21%)	43,45,45	2.24	9 (20%)
22	ADP	CF	501	21	28,29,29	1.38	4 (14%)	43,45,45	1.80	8 (18%)
20	ATP	AC	601	21	32,33,33	1.33	4 (12%)	48,52,52	1.77	8 (16%)
20	ATP	A	601	21	32,33,33	1.35	5 (15%)	48,52,52	1.80	8 (16%)
20	ATP	B	601	21	32,33,33	1.34	5 (15%)	48,52,52	1.76	8 (16%)
20	ATP	BA	601	21	32,33,33	1.40	5 (15%)	48,52,52	1.79	7 (14%)
22	ADP	BD	501	21	28,29,29	1.48	6 (21%)	43,45,45	2.23	9 (20%)
20	ATP	CB	601	21	32,33,33	1.28	4 (12%)	48,52,52	1.82	10 (20%)

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
20	ATP	CC	601	21	-	0/22/38/38	0/3/3/3
22	ADP	AF	501	21	-	4/16/32/32	0/3/3/3
20	ATP	AB	601	21	-	4/22/38/38	0/3/3/3
22	ADP	D	501	21	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	ATP	BB	601	21	-	8/22/38/38	0/3/3/3
20	ATP	BC	601	21	-	0/22/38/38	0/3/3/3
22	ADP	AD	501	21	-	3/16/32/32	0/3/3/3
22	ADP	BF	501	21	-	4/16/32/32	0/3/3/3
20	ATP	C	601	21	-	3/22/38/38	0/3/3/3
22	ADP	F	501	21	-	4/16/32/32	0/3/3/3
20	ATP	AA	601	21	-	1/22/38/38	0/3/3/3
20	ATP	CA	601	21	-	5/22/38/38	0/3/3/3
22	ADP	CD	501	21	-	9/16/32/32	0/3/3/3
22	ADP	CF	501	21	-	4/16/32/32	0/3/3/3
20	ATP	AC	601	21	-	3/22/38/38	0/3/3/3
20	ATP	A	601	21	-	1/22/38/38	0/3/3/3
20	ATP	B	601	21	-	4/22/38/38	0/3/3/3
20	ATP	BA	601	21	-	5/22/38/38	0/3/3/3
22	ADP	BD	501	21	-	9/16/32/32	0/3/3/3
20	ATP	CB	601	21	-	8/22/38/38	0/3/3/3

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	501	ADP	C5-C4	4.56	1.47	1.39
22	AF	501	ADP	C5-C4	4.56	1.47	1.39
20	AC	601	ATP	C5-C4	4.54	1.47	1.39
20	C	601	ATP	C5-C4	4.52	1.47	1.39
20	AB	601	ATP	C5-C4	4.45	1.47	1.39

The worst 5 of 168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CD	501	ADP	N3-C2-N1	-7.92	116.60	128.58
22	BD	501	ADP	N3-C2-N1	-7.89	116.63	128.58
22	AD	501	ADP	N3-C2-N1	-6.83	118.24	128.58
22	D	501	ADP	N3-C2-N1	-6.81	118.27	128.58
20	CA	601	ATP	C5-C4-N3	-6.18	118.21	126.72

There are no chirality outliers.

5 of 83 torsion outliers are listed below:

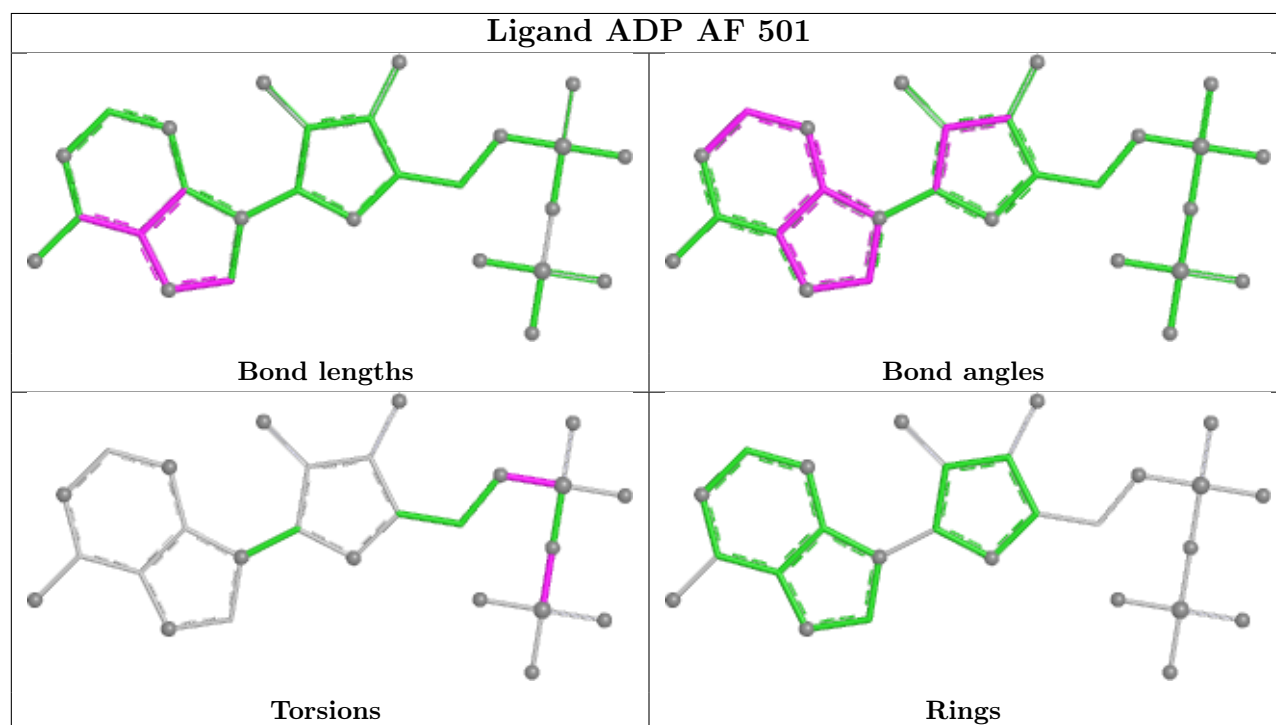
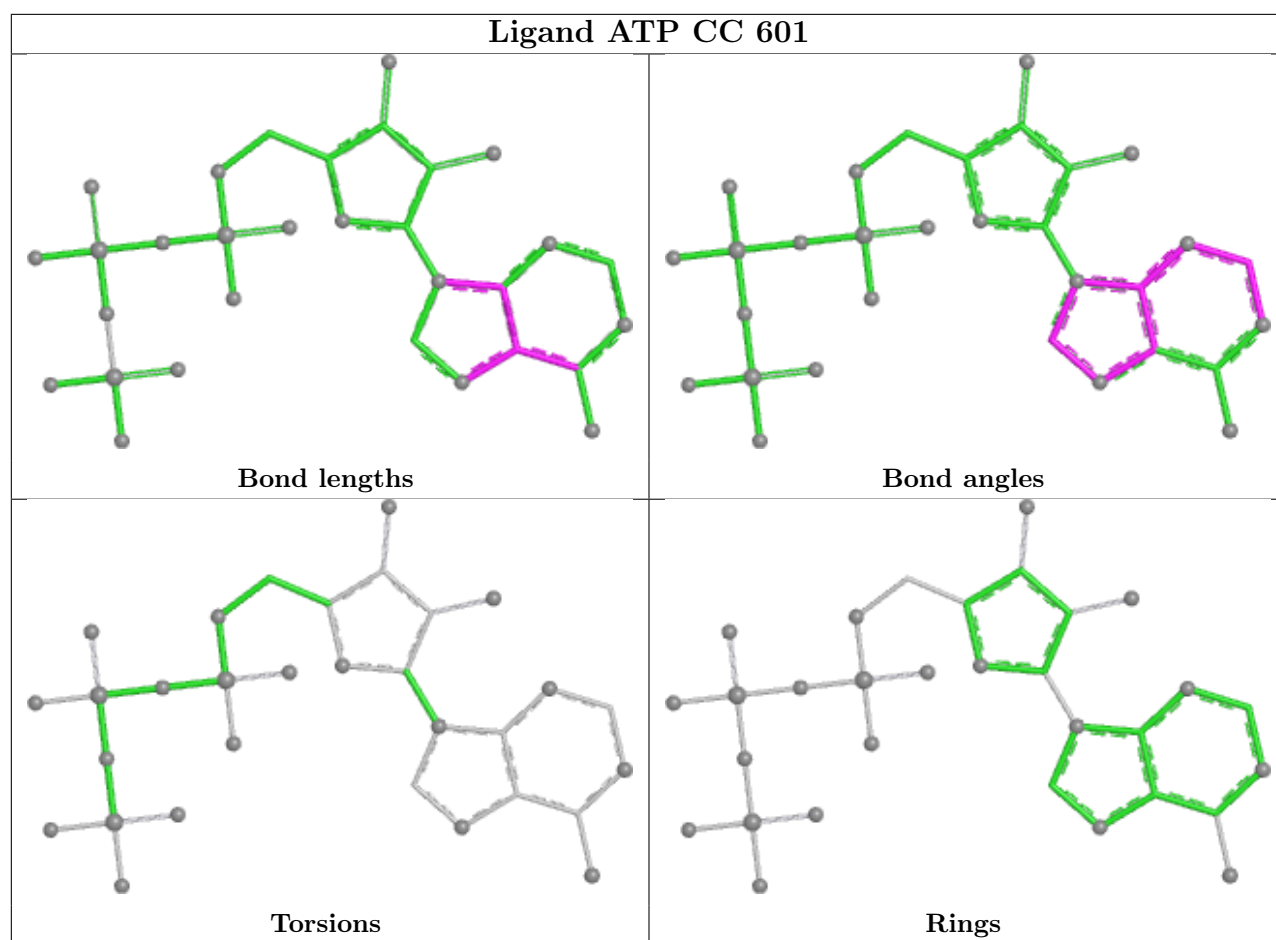
Mol	Chain	Res	Type	Atoms
20	B	601	ATP	PB-O3B-PG-O3G
20	C	601	ATP	C5'-O5'-PA-O2A
20	C	601	ATP	C5'-O5'-PA-O3A
20	AB	601	ATP	PB-O3B-PG-O3G
20	AC	601	ATP	C5'-O5'-PA-O2A

There are no ring outliers.

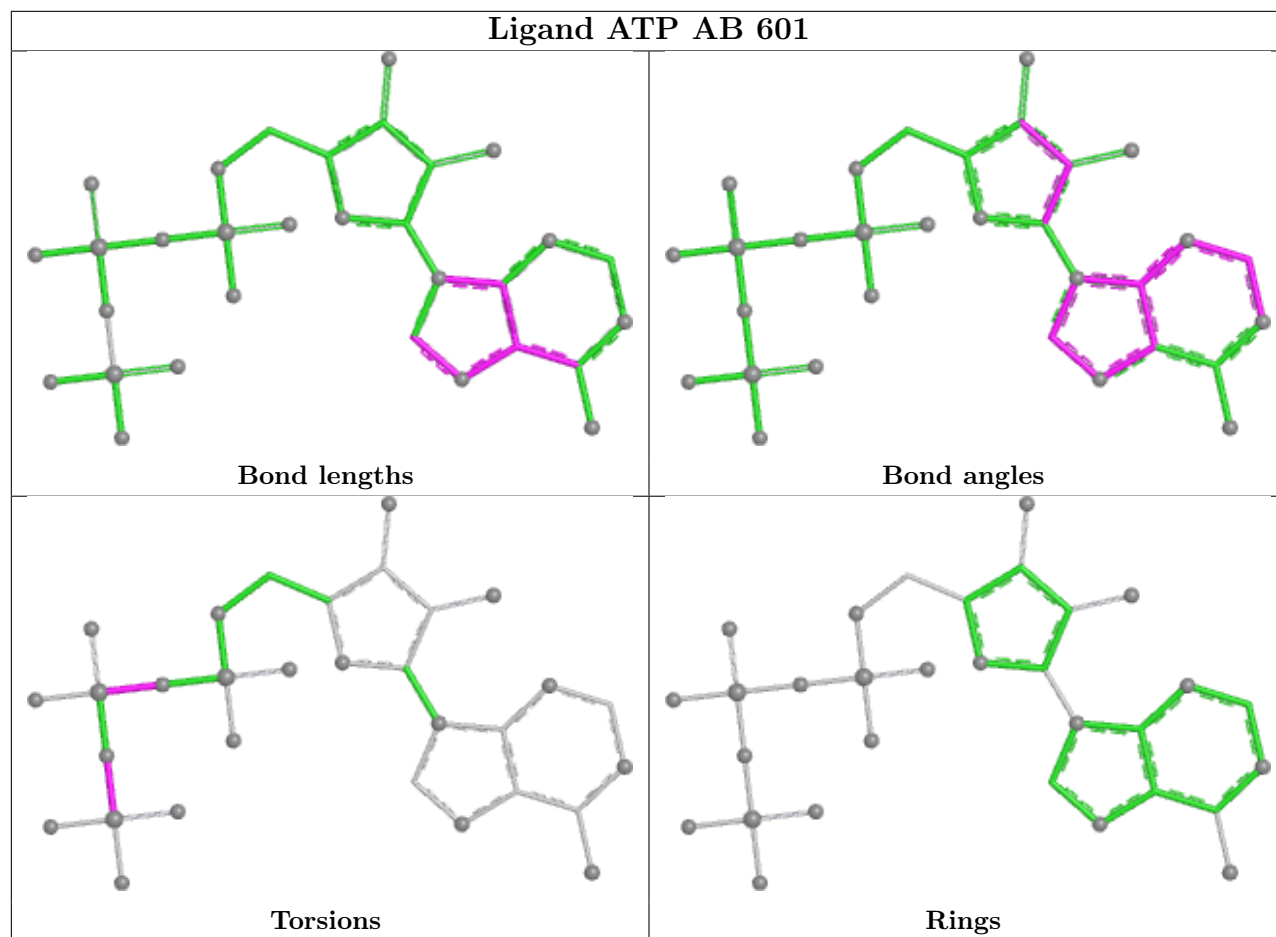
12 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	CC	601	ATP	1	0
22	D	501	ADP	1	0
20	BB	601	ATP	2	0
20	BC	601	ATP	1	0
22	AD	501	ADP	1	0
22	BF	501	ADP	1	0
20	CA	601	ATP	1	0
22	CD	501	ADP	1	0
22	CF	501	ADP	1	0
20	BA	601	ATP	1	0
22	BD	501	ADP	1	0
20	CB	601	ATP	2	0

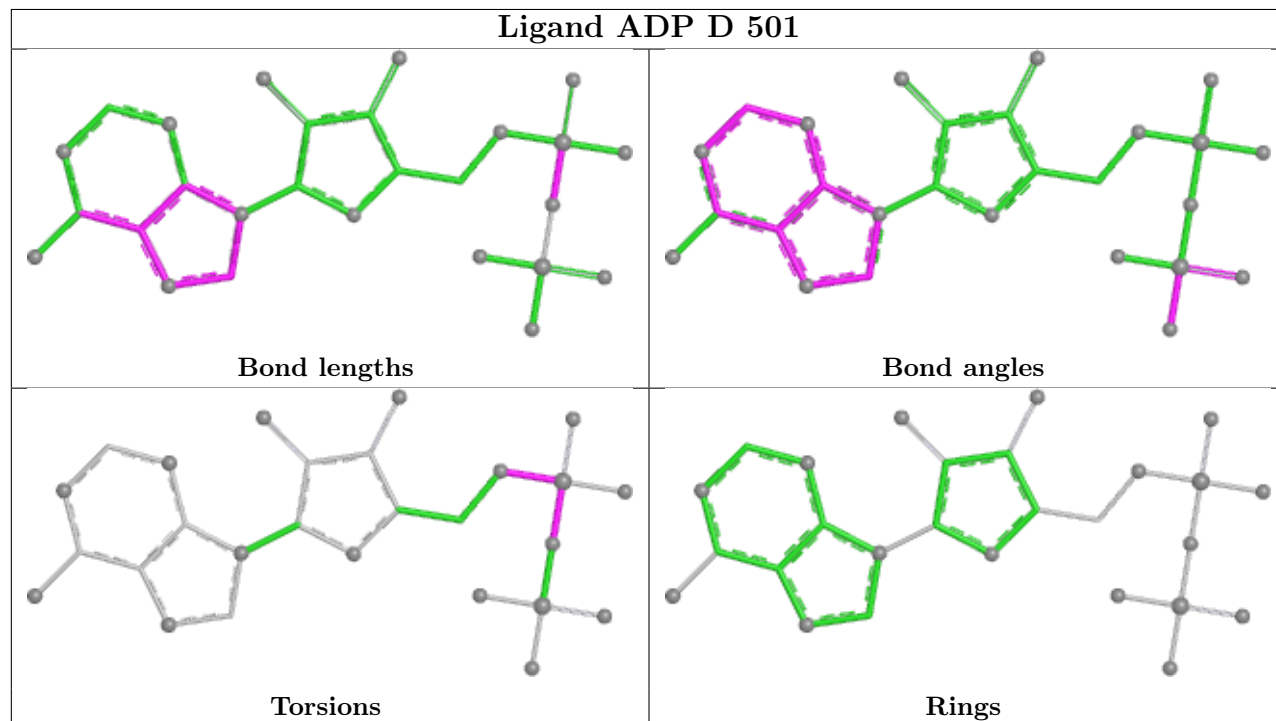
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

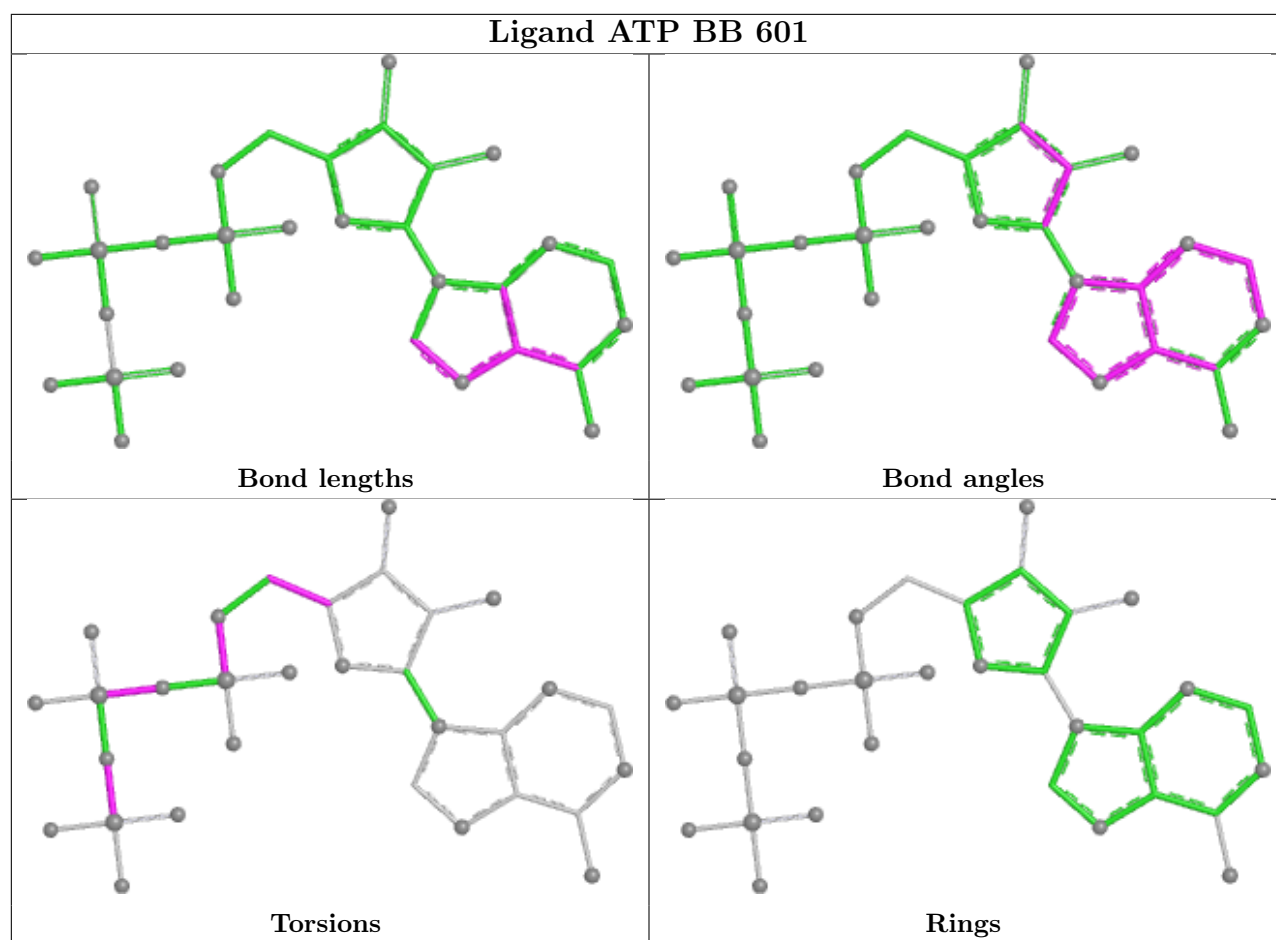


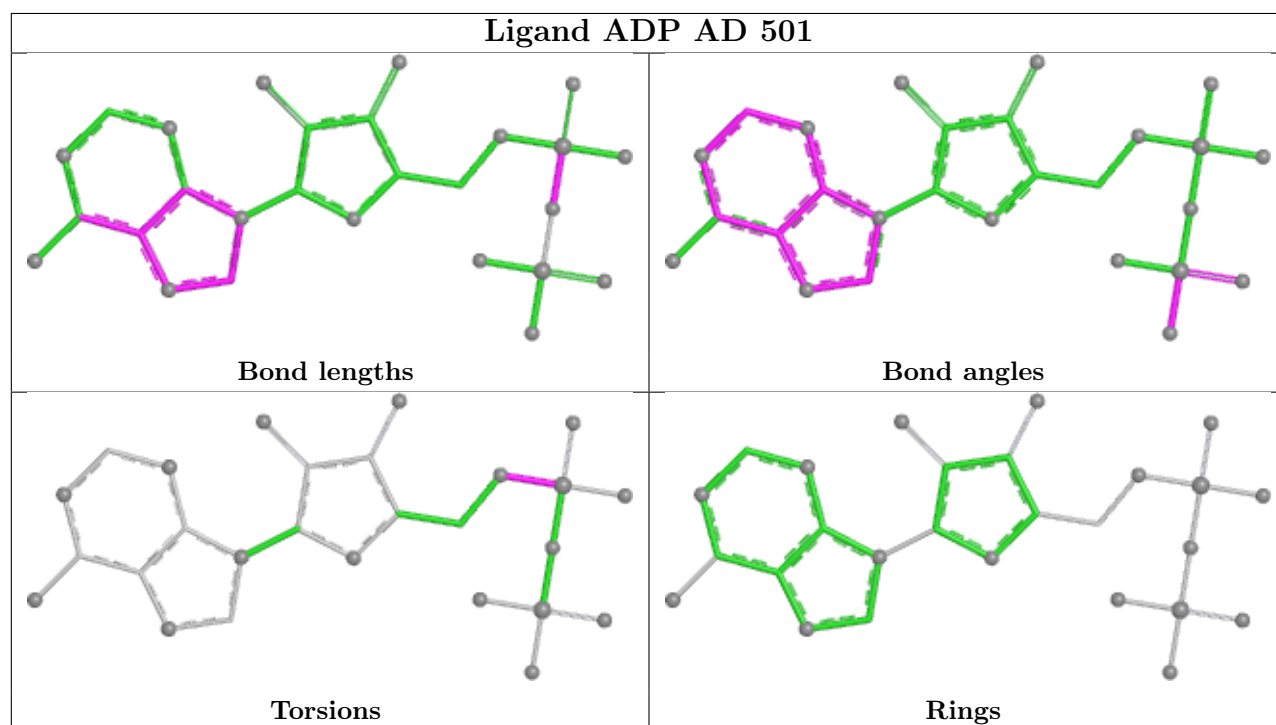
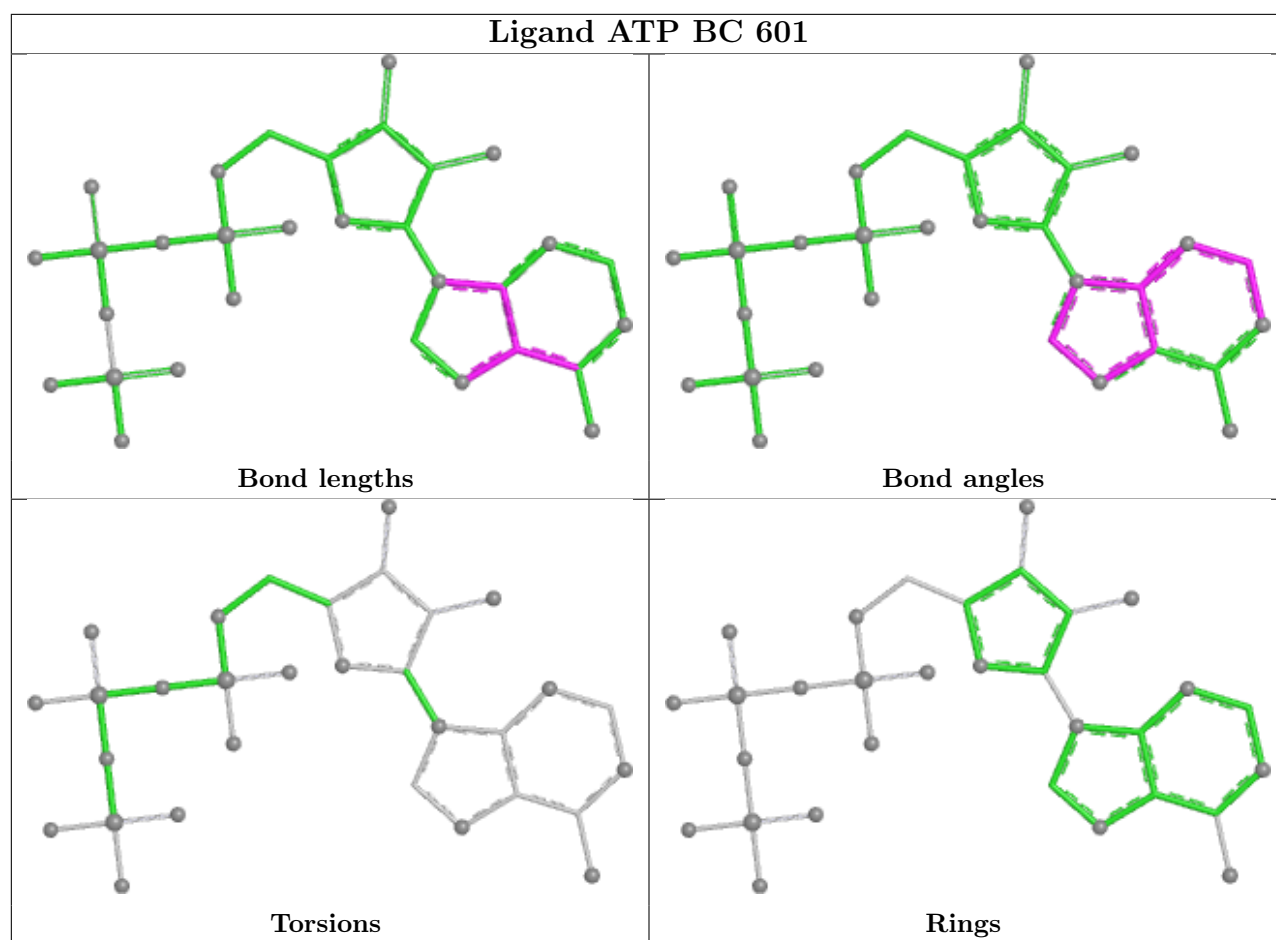
Ligand ATP AB 601

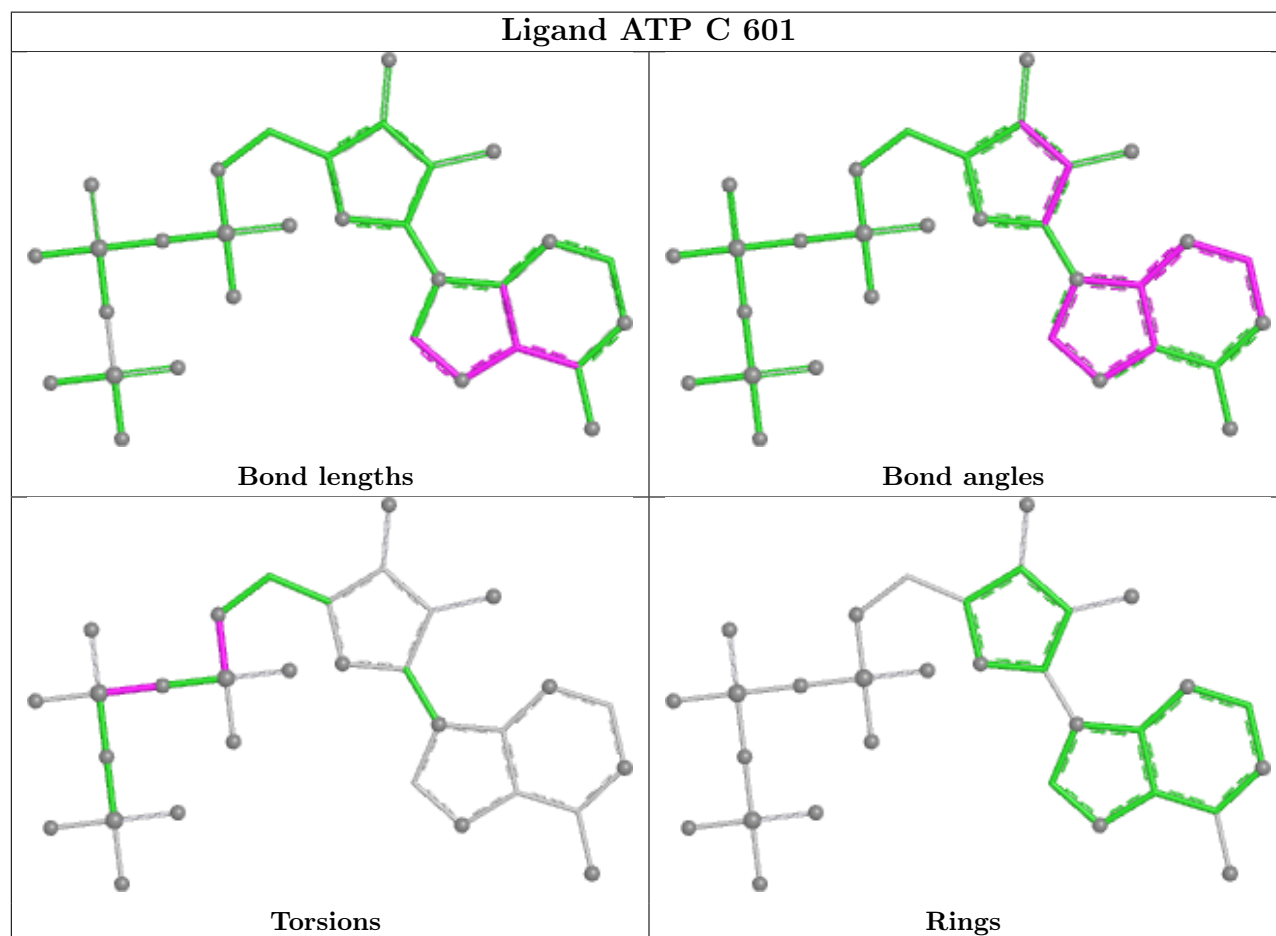
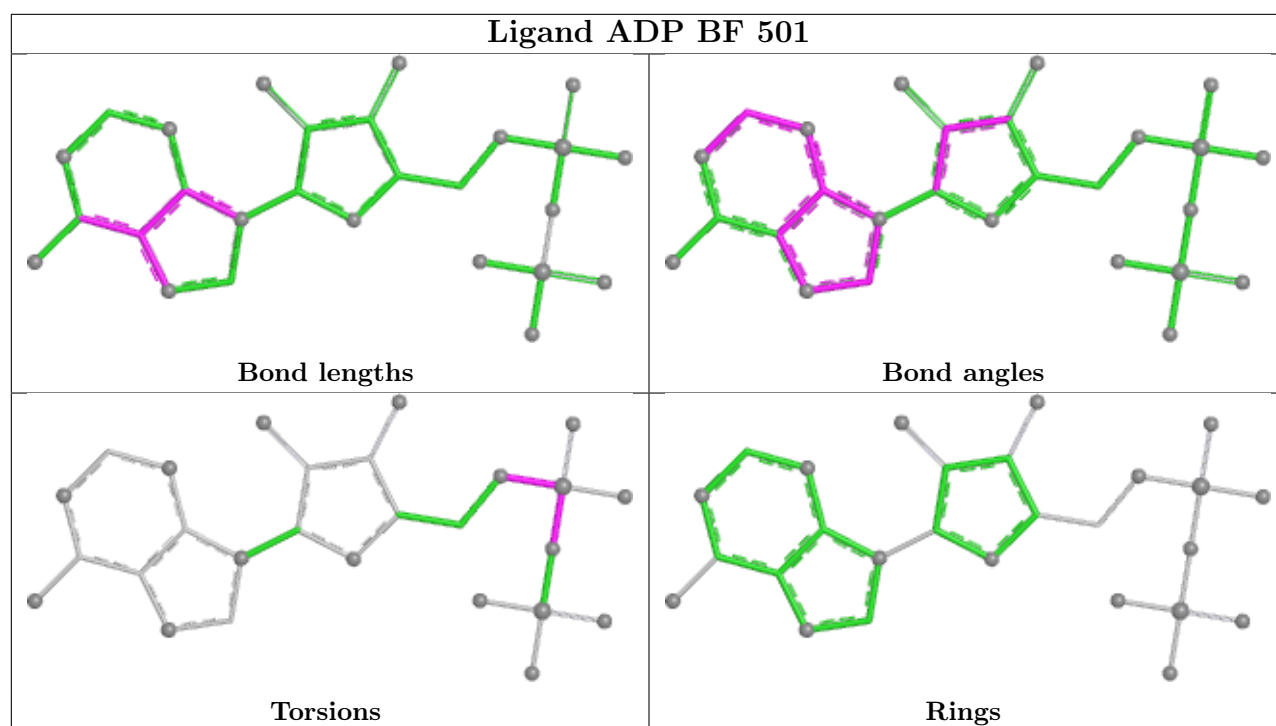


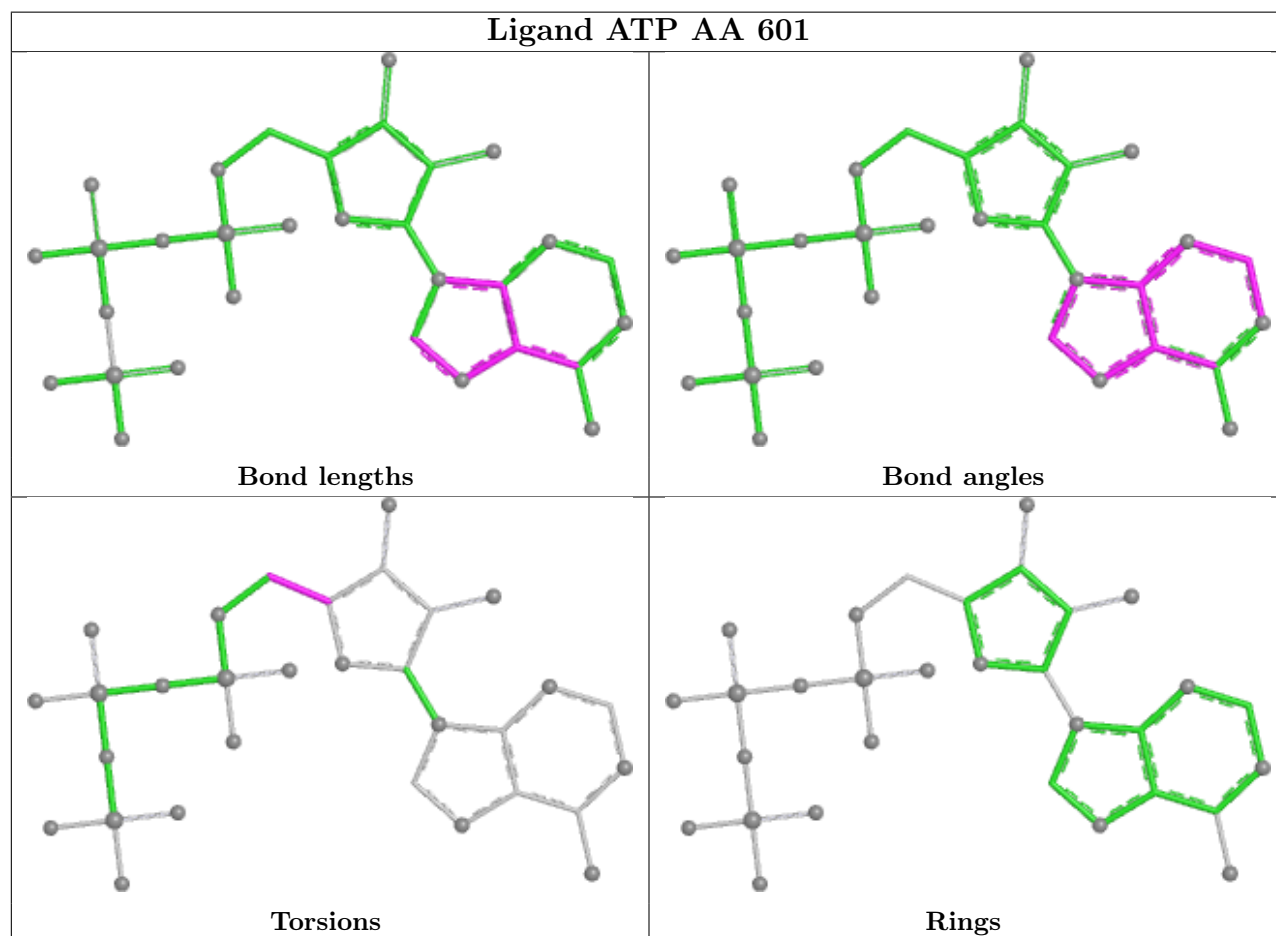
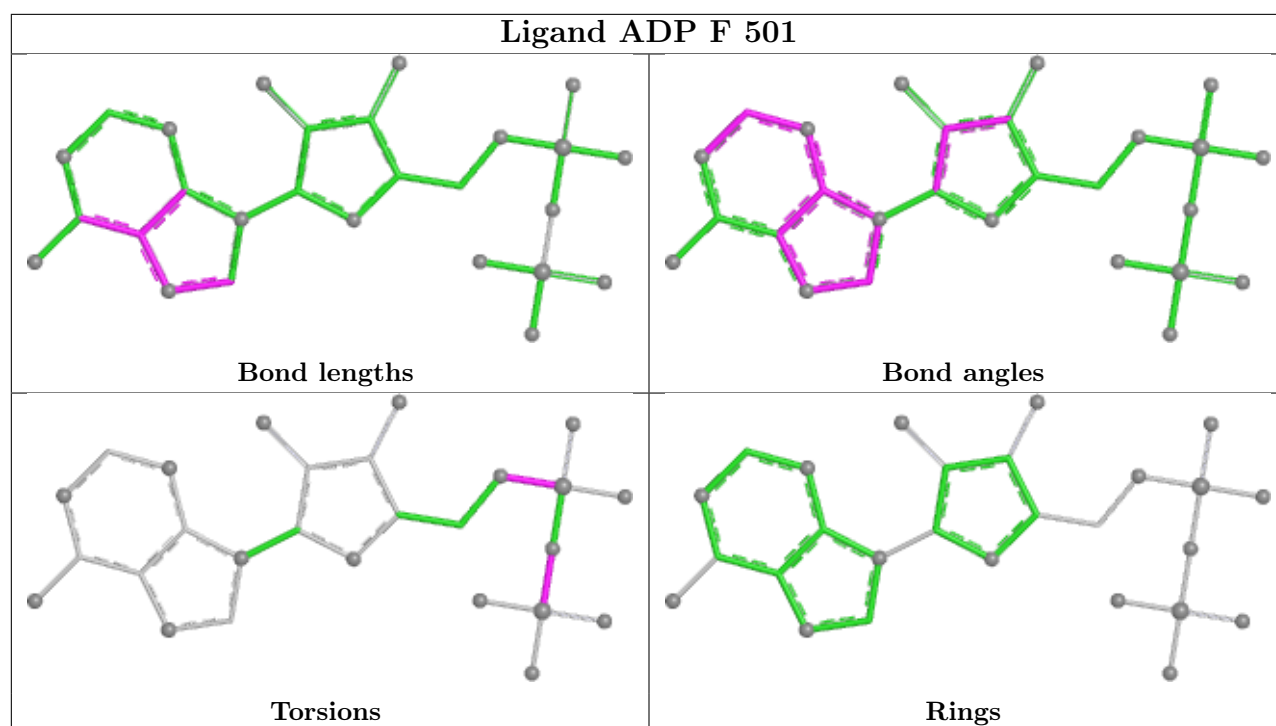
Ligand ADP D 501



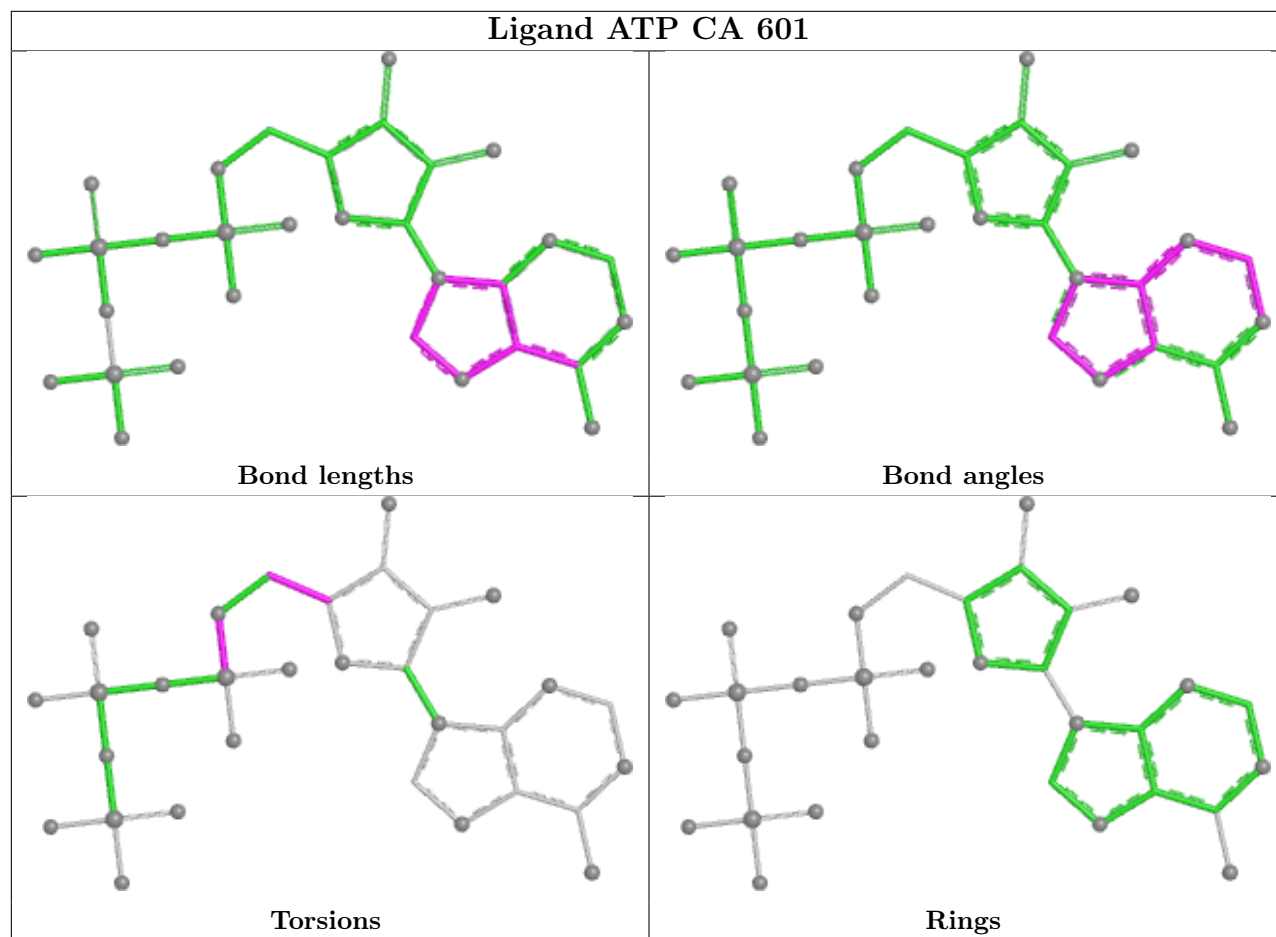




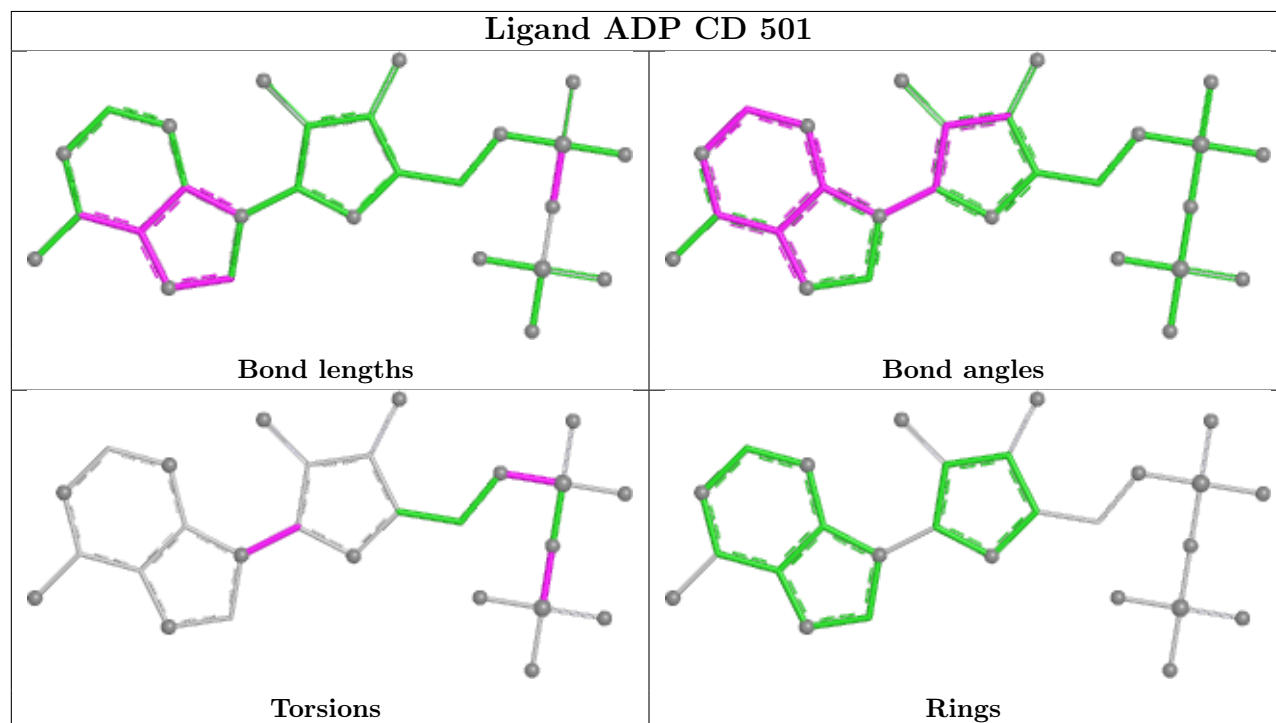


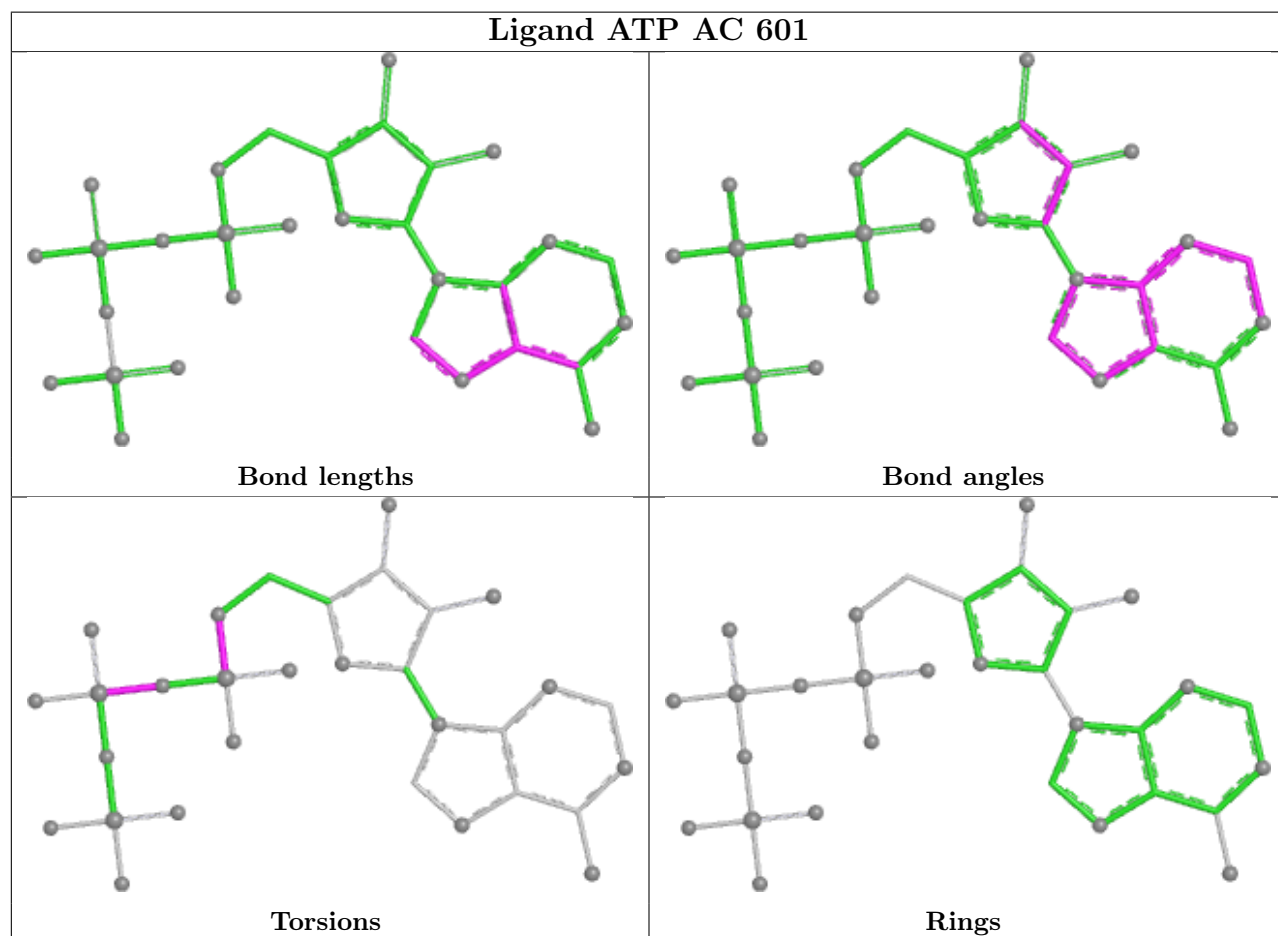
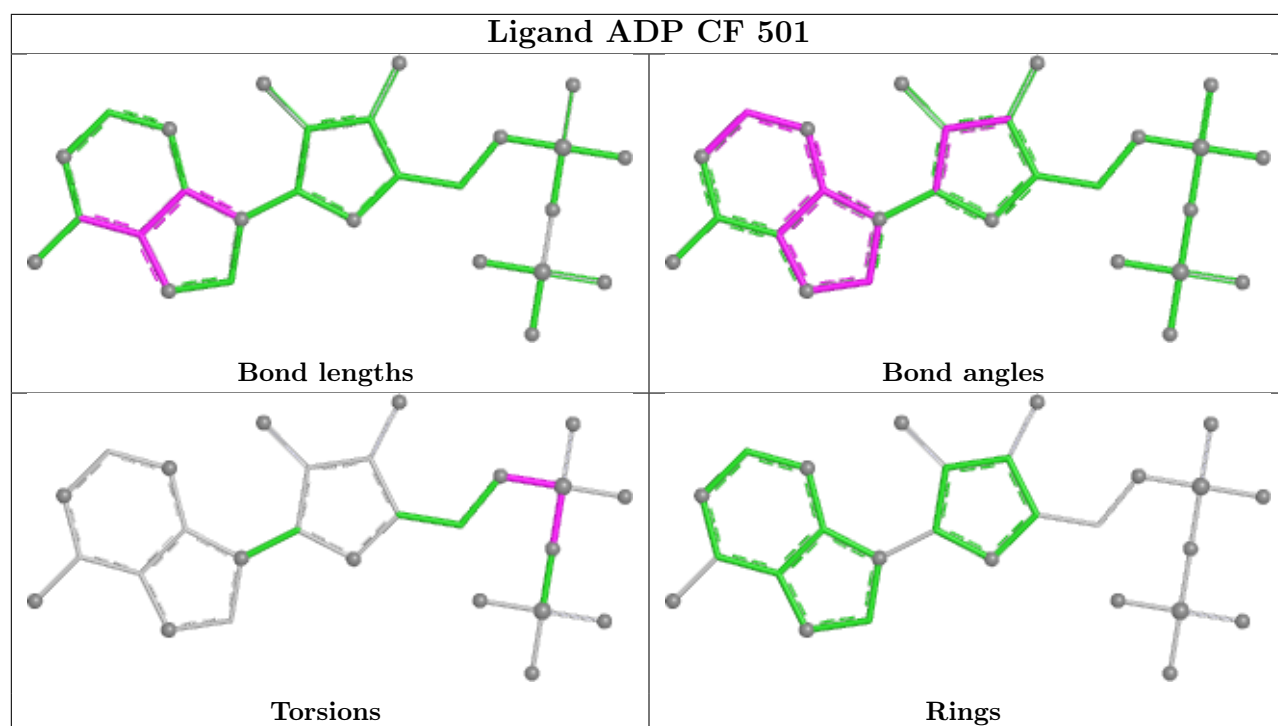


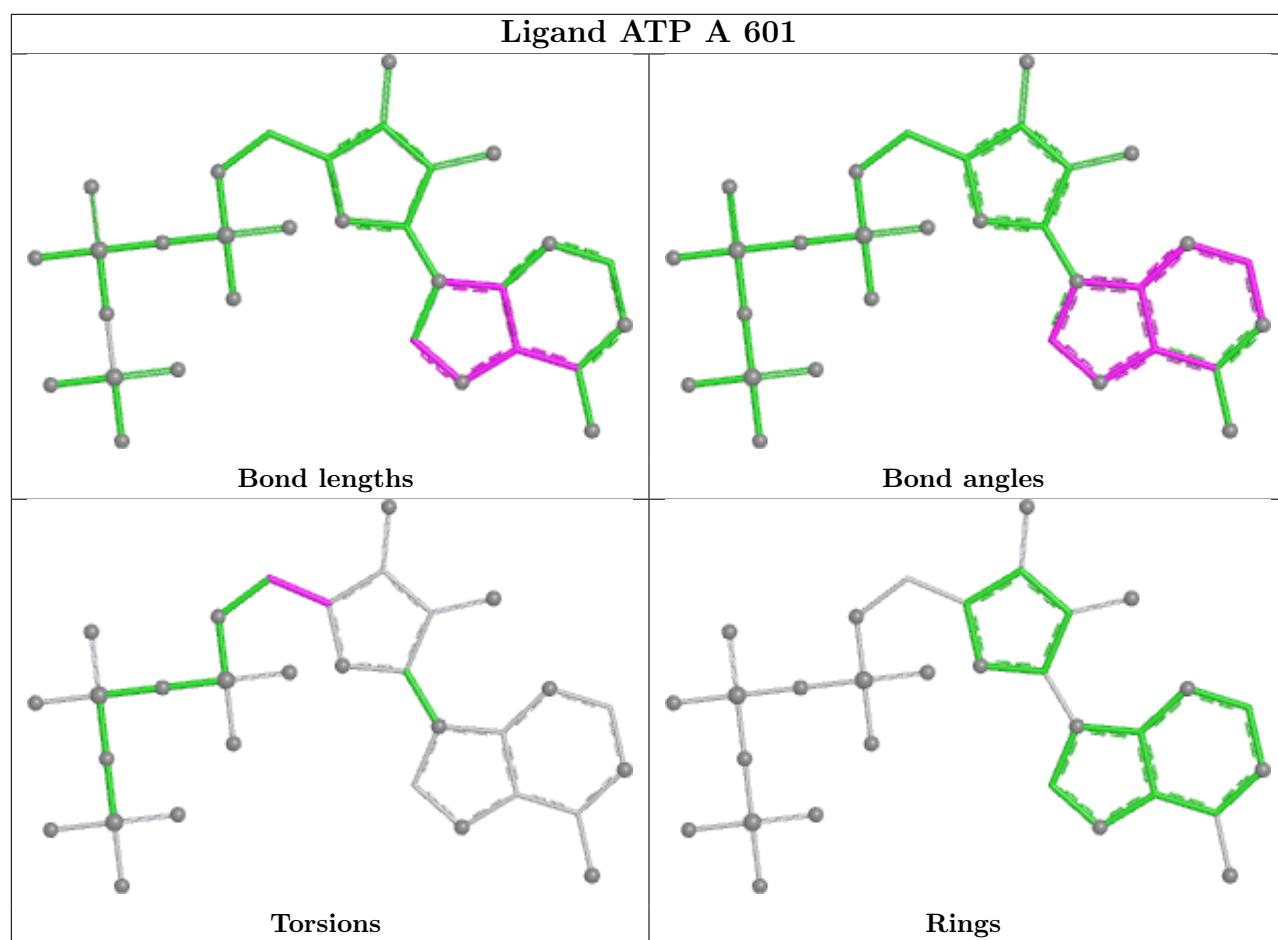
Ligand ATP CA 601

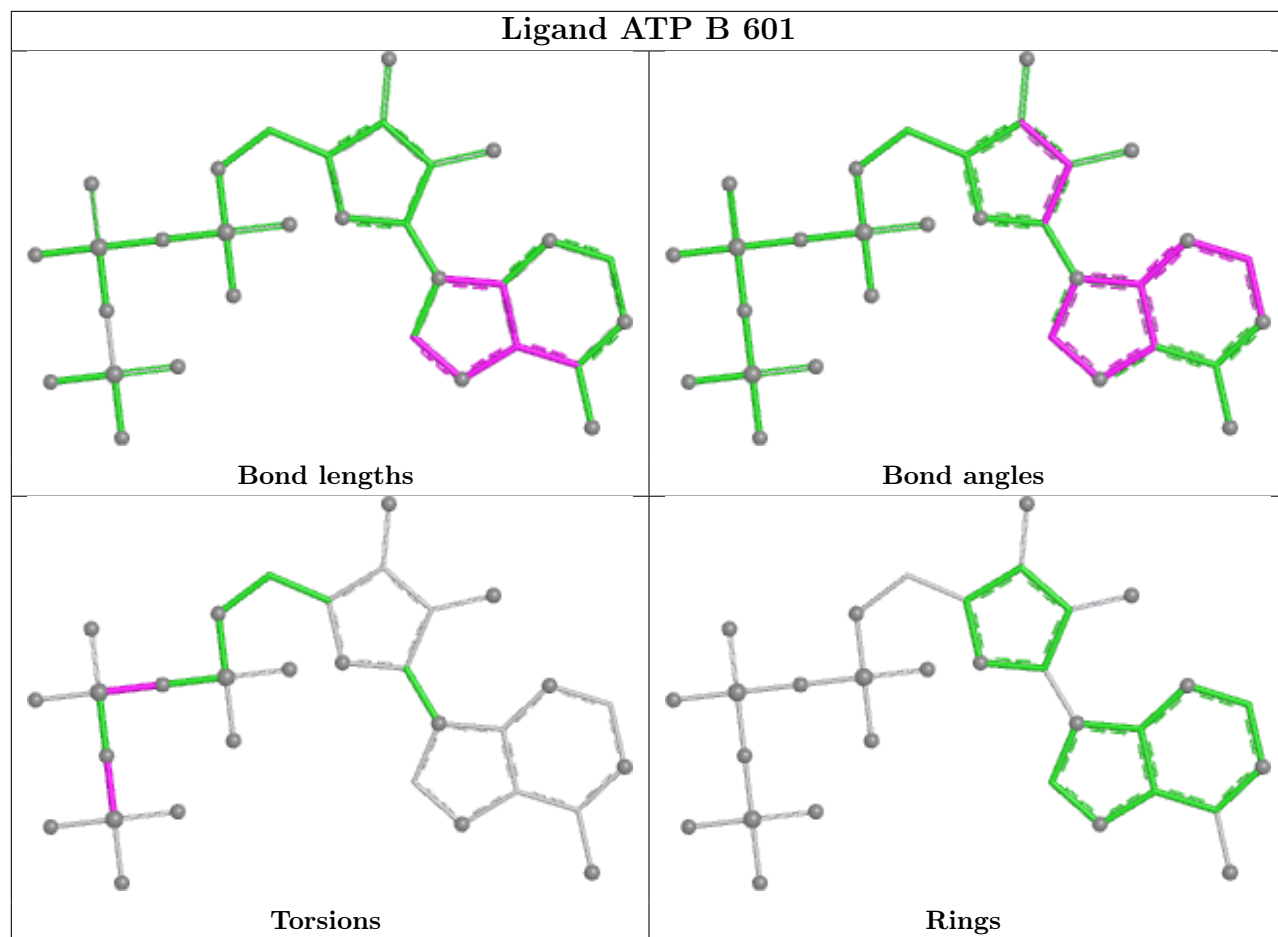


Ligand ADP CD 501

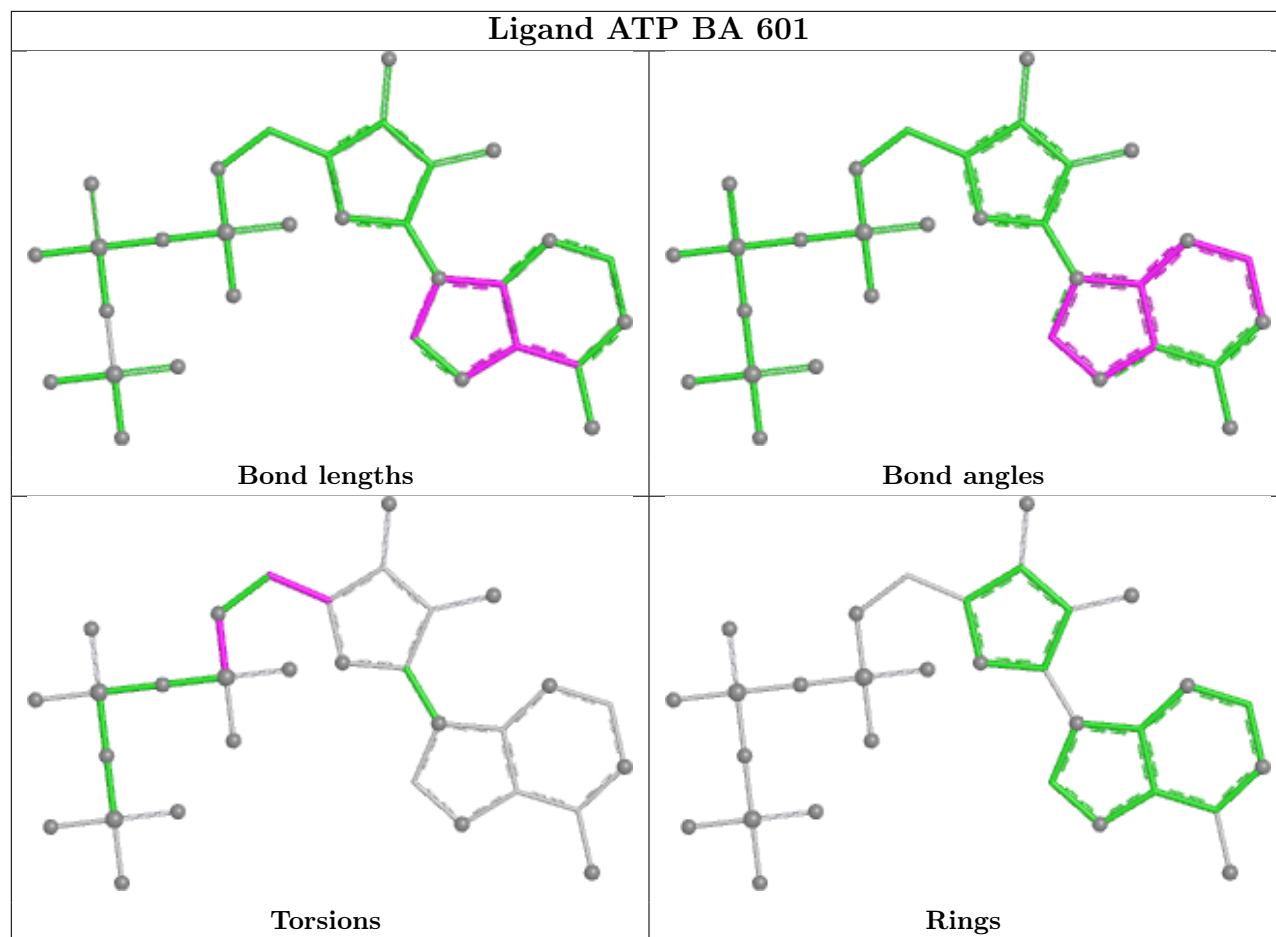




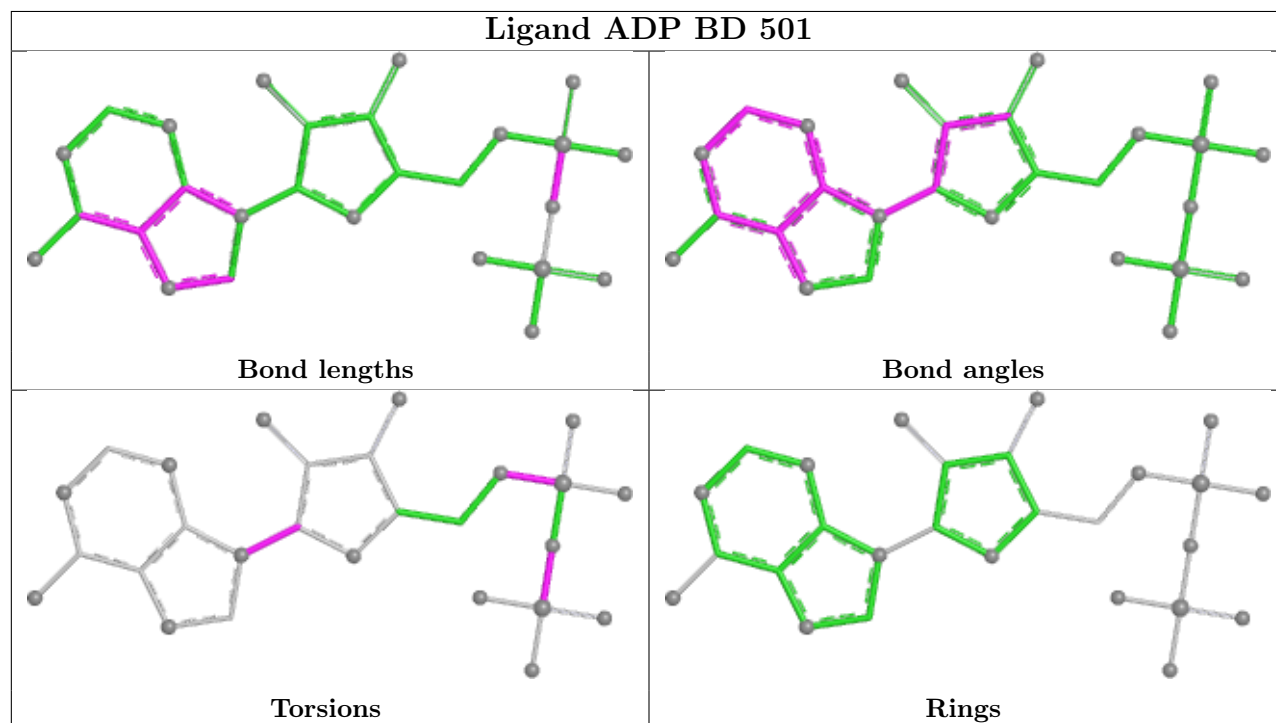


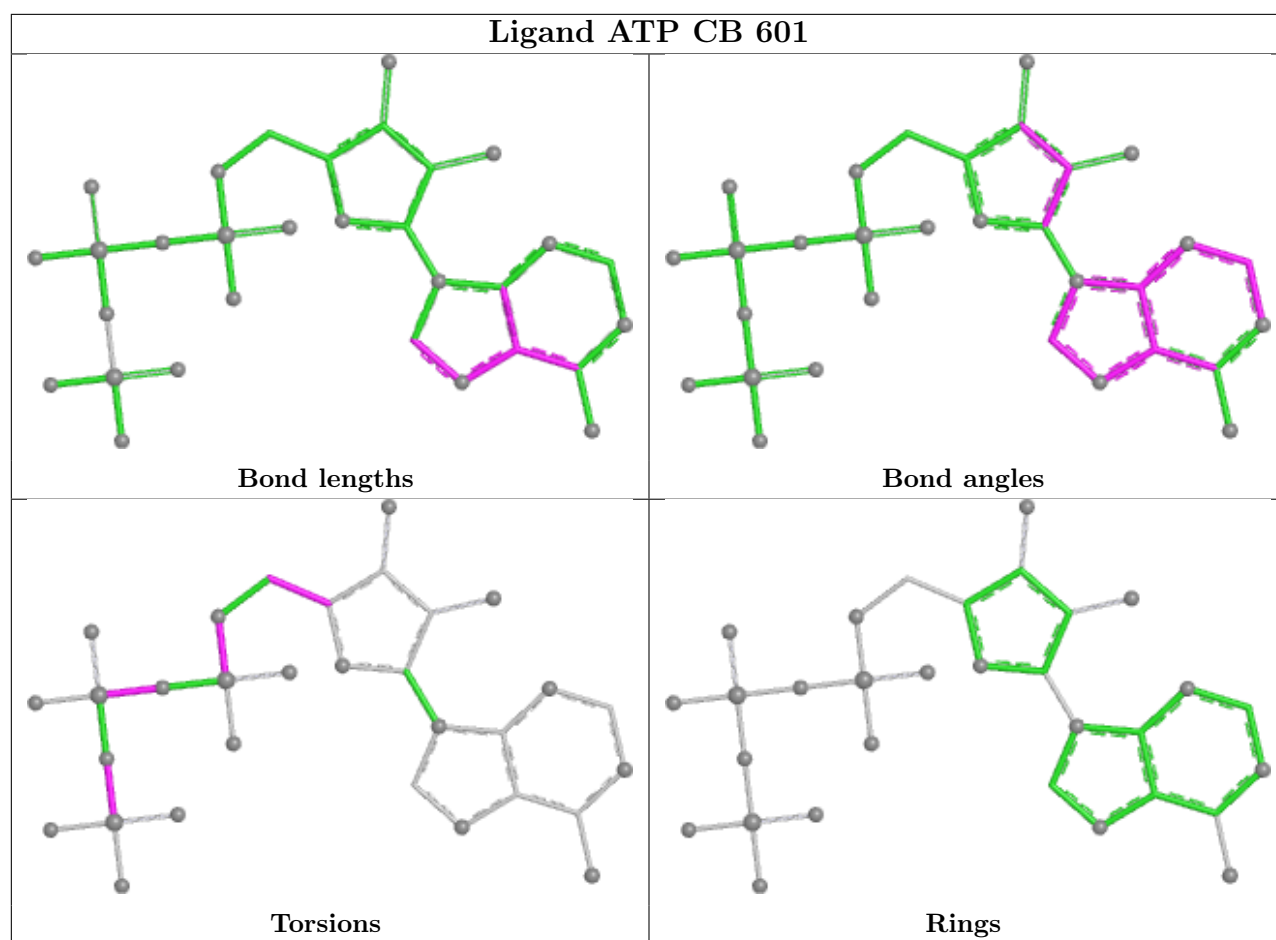


Ligand ATP BA 601



Ligand ADP BD 501





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.

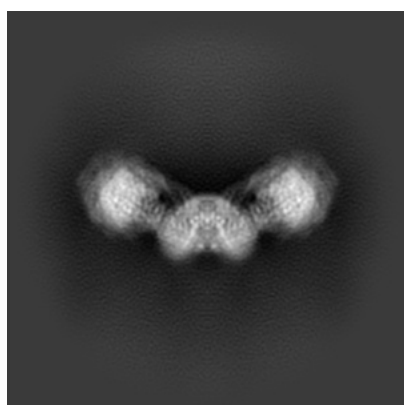
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0667. These allow visual inspection of the internal detail of the map and identification of artifacts.

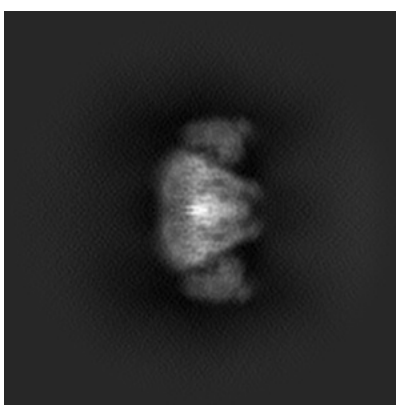
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

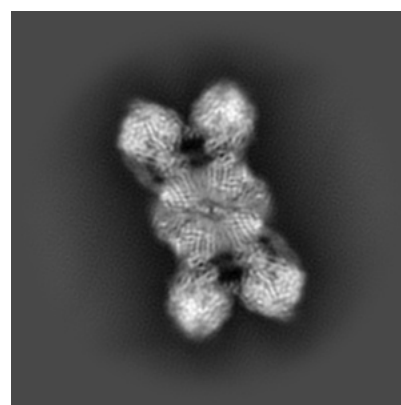
6.1.1 Primary map



X



Y

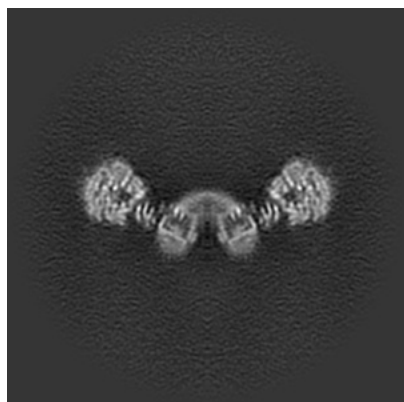


Z

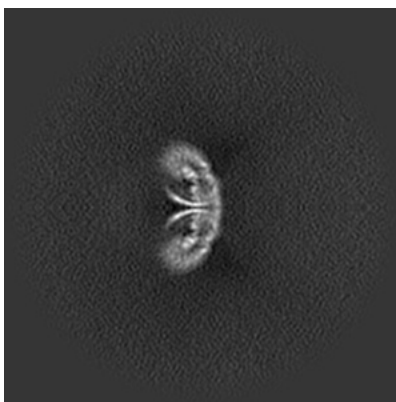
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

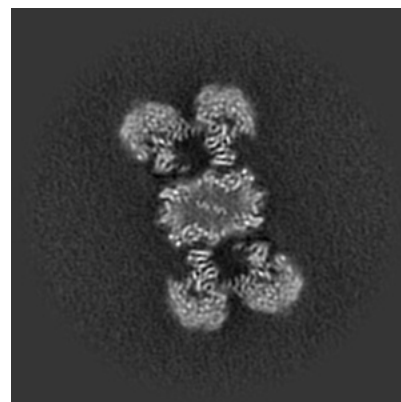
6.2.1 Primary map



X Index: 240



Y Index: 240

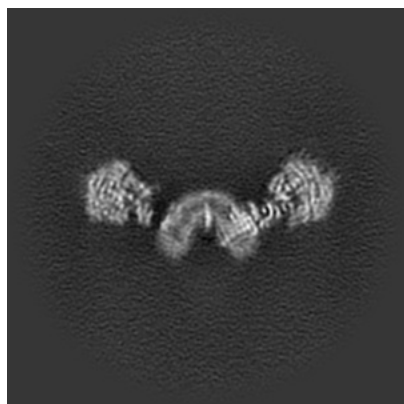


Z Index: 240

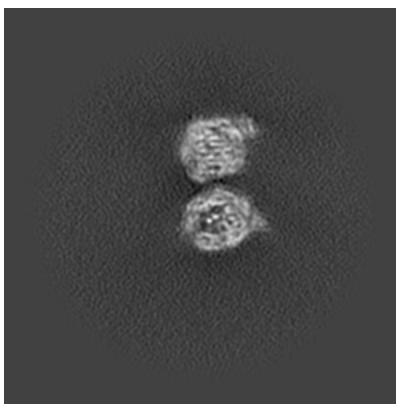
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

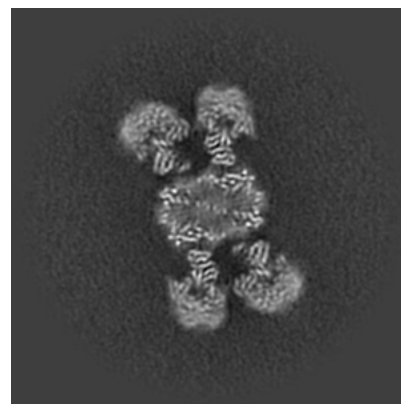
6.3.1 Primary map



X Index: 244



Y Index: 137

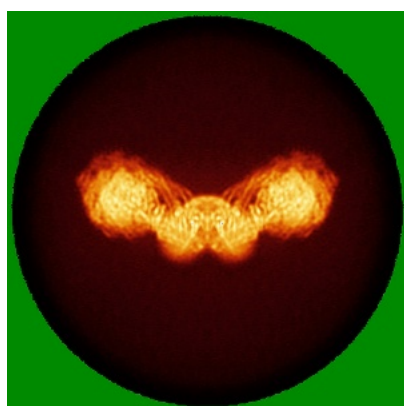


Z Index: 237

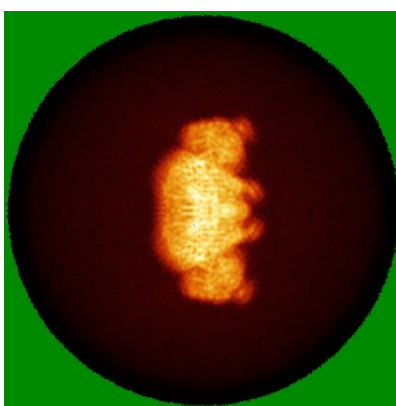
The images above show the largest variance slices of the map in three orthogonal directions.

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

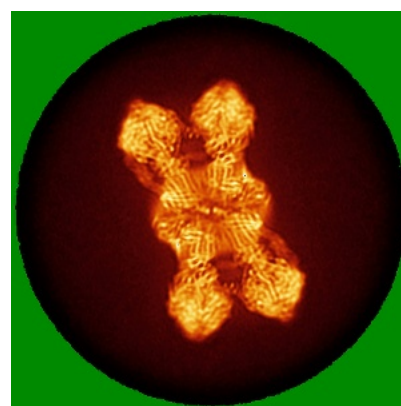
6.4.1 Primary map



X



Y

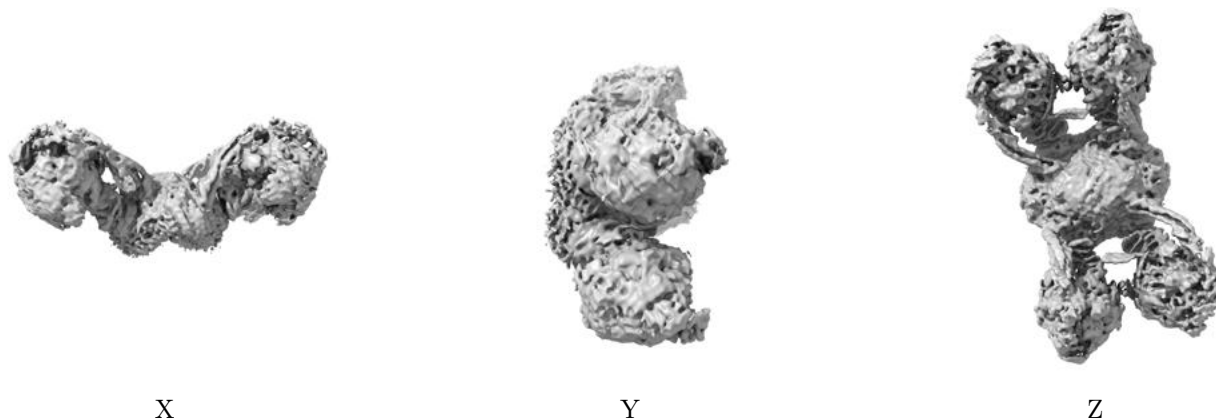


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.315. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

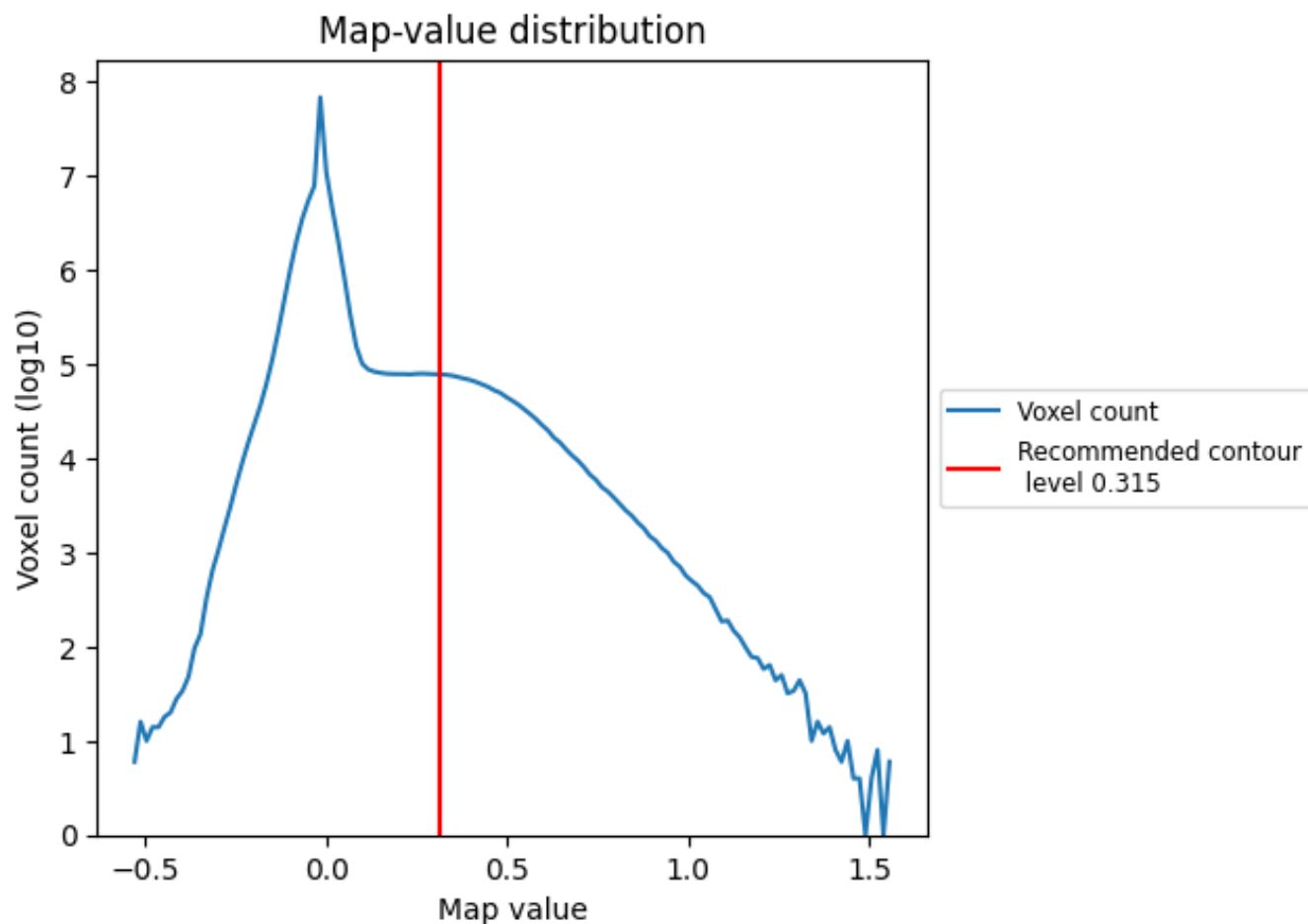
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

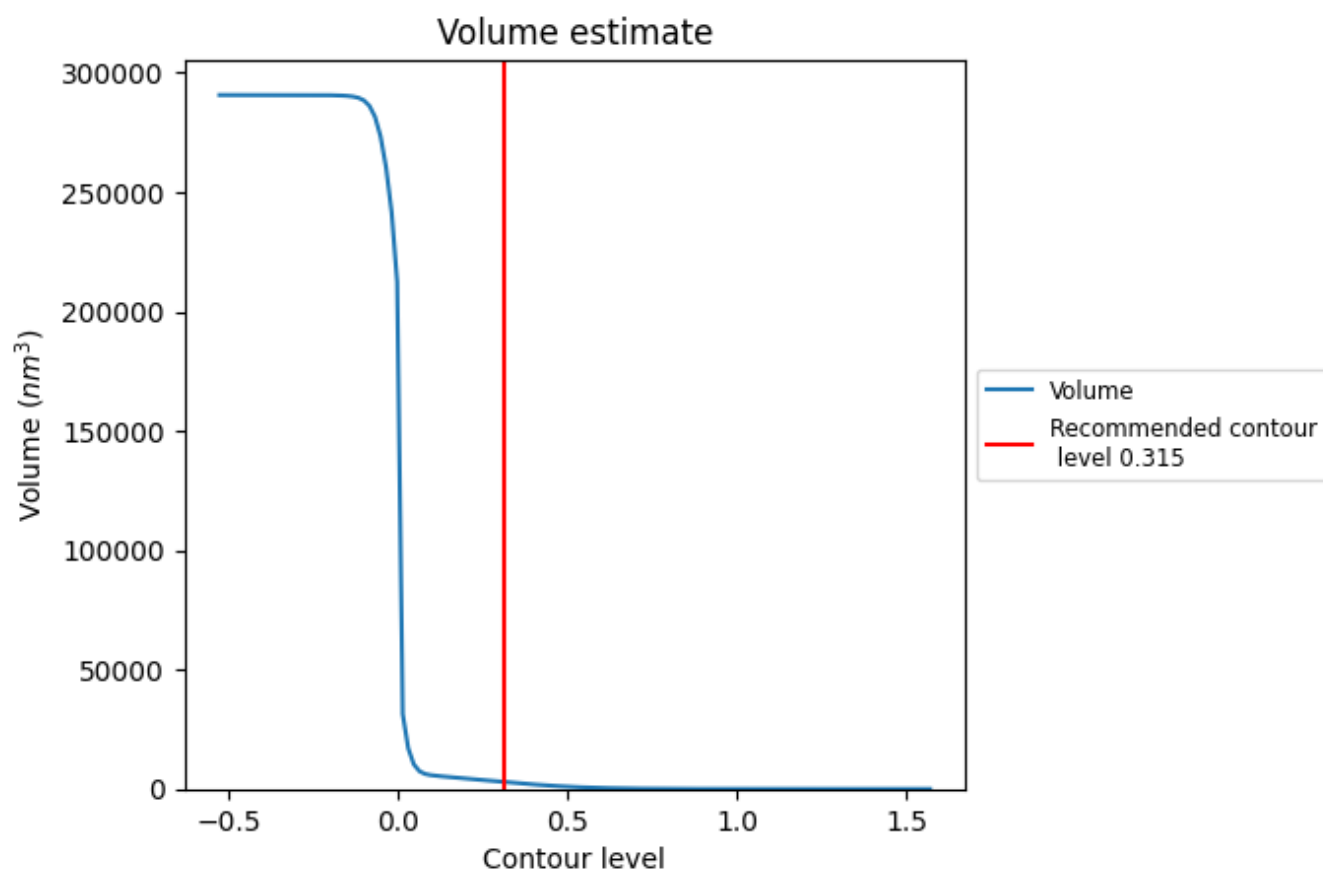
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

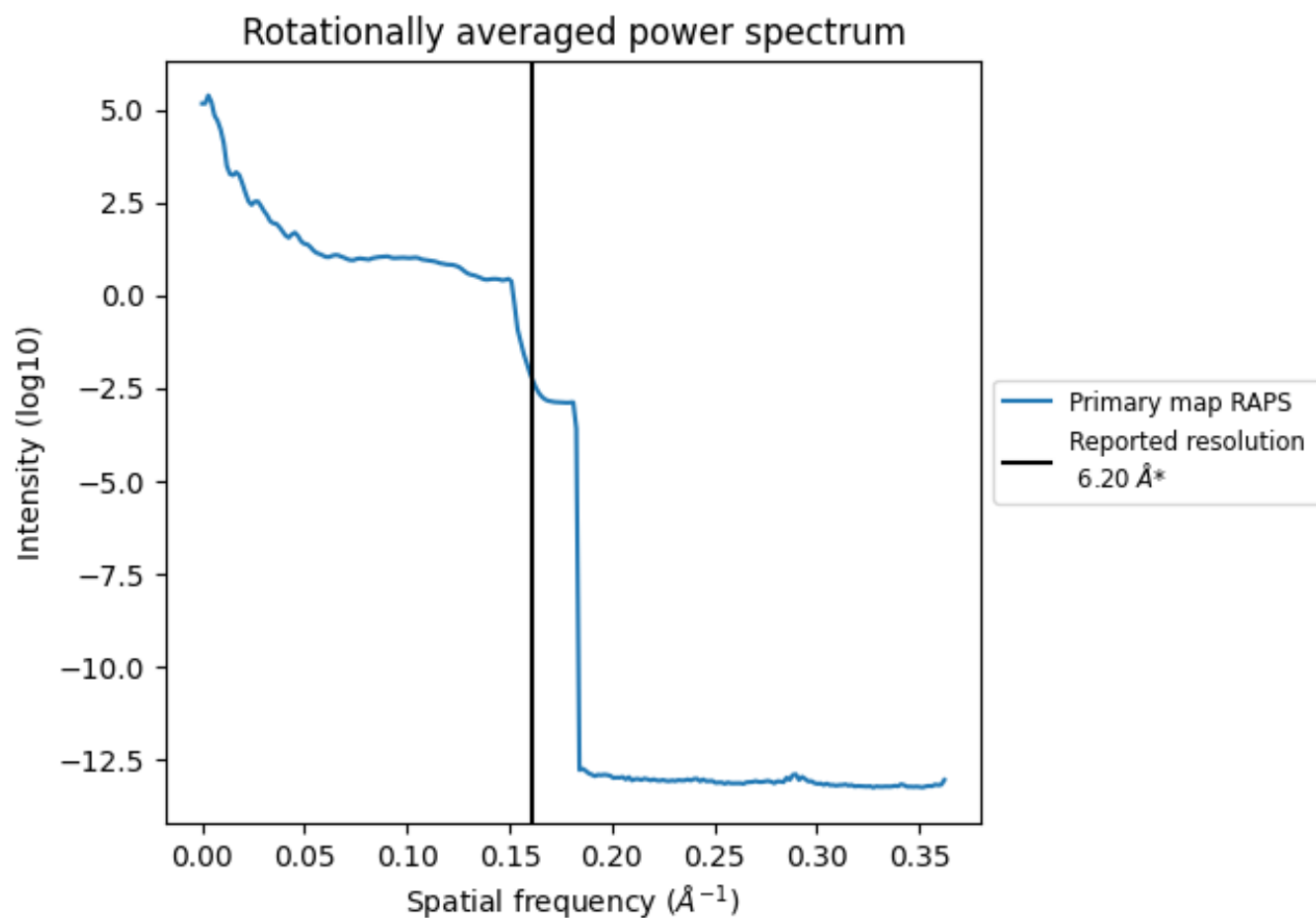
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2912 nm³; this corresponds to an approximate mass of 2630 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 0.161 Å⁻¹

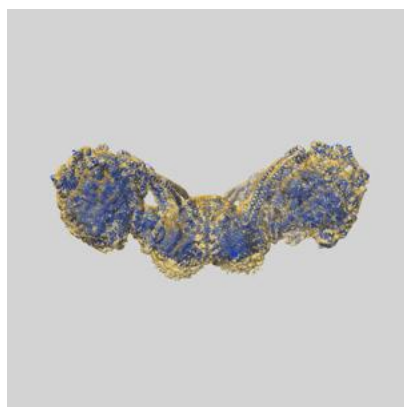
8 Fourier-Shell correlation

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

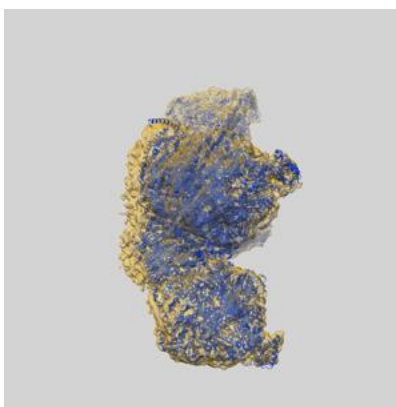
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0667 and PDB model 6J5K. Per-residue inclusion information can be found in section [3](#) on page [19](#).

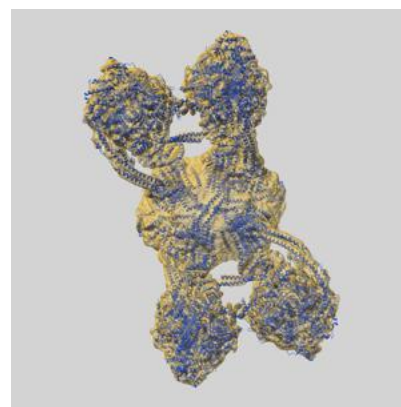
9.1 Map-model overlay [i](#)



X



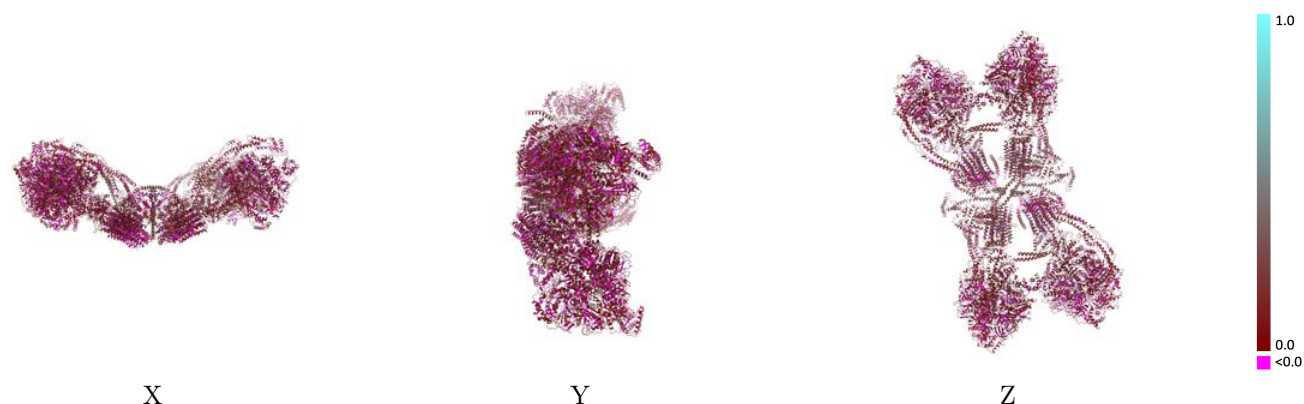
Y



Z

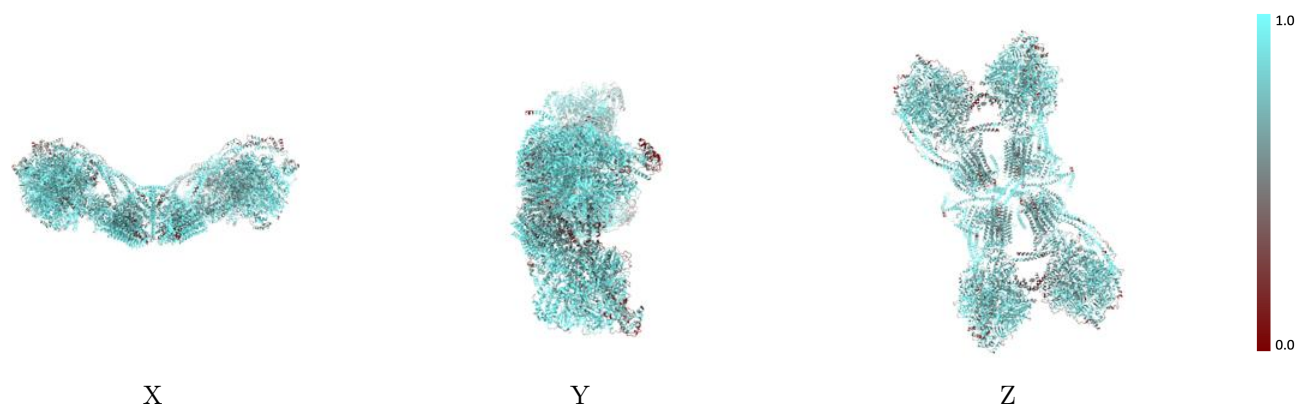
The images above show the 3D surface view of the map at the recommended contour level 0.315 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



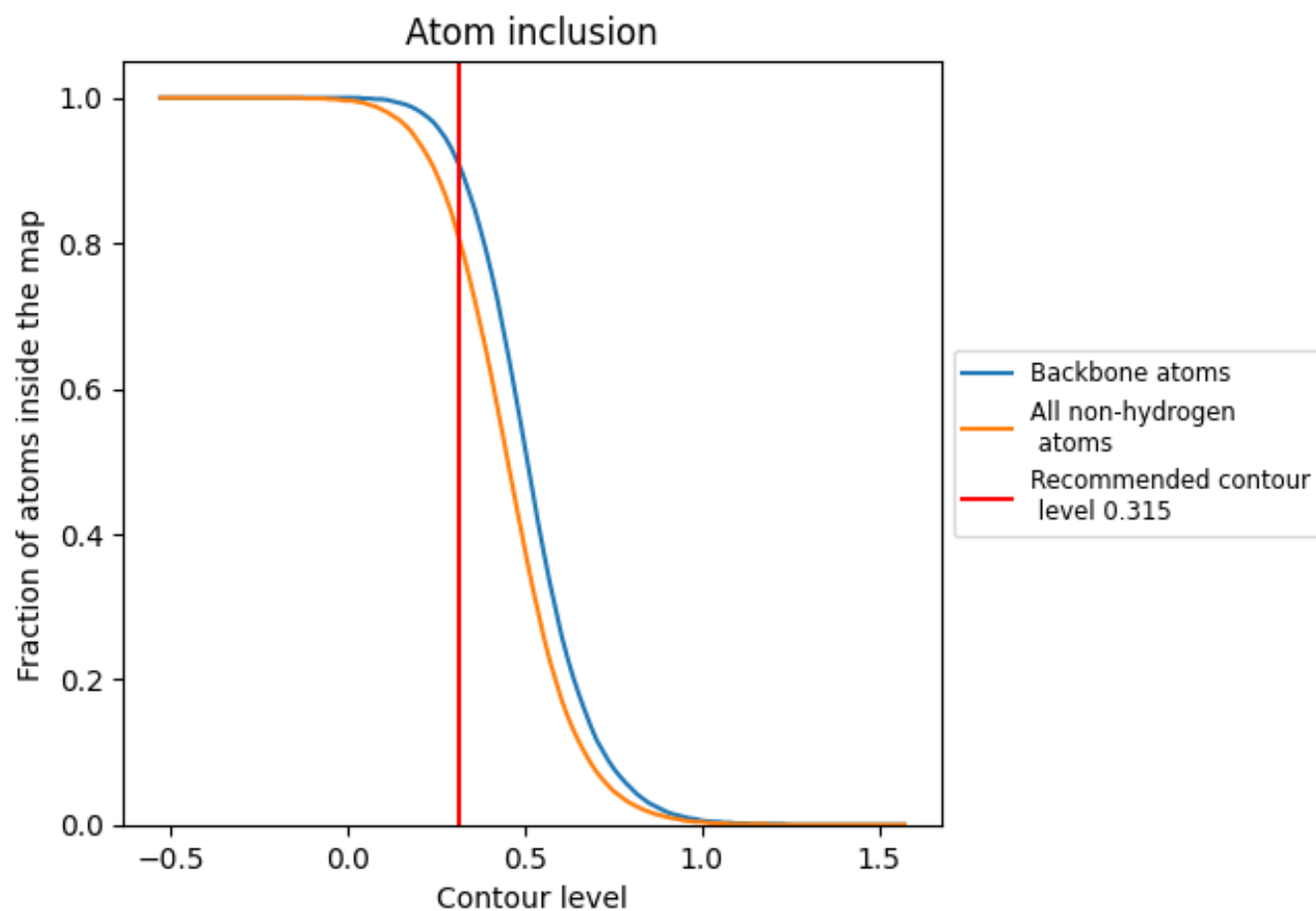
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.315).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 80% 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 (0.315) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8050	 0.1260
8	 0.8040	 0.1780
A	 0.8400	 0.1280
A8	 0.8010	 0.1720
AA	 0.8400	 0.1270
AB	 0.8810	 0.1090
AC	 0.7760	 0.1240
AD	 0.8340	 0.1250
AE	 0.8850	 0.1240
AF	 0.8660	 0.1200
AG	 0.7940	 0.1510
AH	 0.8390	 0.1730
AI	 0.7740	 0.1460
AJ	 0.6660	 0.1580
AK	 0.7920	 0.1570
AL	 0.7310	 0.1220
AM	 0.7450	 0.1280
AN	 0.8340	 0.1510
AO	 0.8910	 0.1140
AP	 0.9290	 0.1220
AQ	 0.9230	 0.1460
AR	 0.8530	 0.1540
AS	 0.6360	 0.1040
Aa	 0.8090	 0.1540
Ab	 0.7900	 0.1600
Ac	 0.6760	 0.1380
Ad	 0.8000	 0.1850
Ae	 0.9210	 0.2320
Af	 0.9210	 0.1680
Ag	 0.8980	 0.2230
Ai	 0.8610	 0.1700
Ak	 0.8690	 0.1730
Au	 0.1910	 0.0700
B	 0.8820	 0.1080
B8	 0.7710	 0.1040



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Chain	Atom inclusion	Q-score
BA	 0.6910	 0.1020
BB	 0.8940	 0.1070
BC	 0.7810	 0.1180
BD	 0.7180	 0.0930
BE	 0.8460	 0.1020
BF	 0.8820	 0.1160
BG	 0.8410	 0.1560
BH	 0.8190	 0.1550
BI	 0.6100	 0.1370
BJ	 0.6030	 0.1440
BK	 0.9470	 0.1010
BL	 0.8430	 0.0790
BM	 0.7920	 0.1360
BN	 0.7530	 0.1320
BO	 0.7190	 0.1060
BP	 0.7880	 0.1210
BQ	 0.8680	 0.1400
BR	 0.9250	 0.1260
BS	 0.6330	 0.1110
Ba	 0.7600	 0.1200
Bb	 0.7330	 0.1410
Bc	 0.6910	 0.1280
Bd	 0.7450	 0.1780
Be	 0.9620	 0.2920
Bf	 0.7860	 0.1110
Bg	 0.9920	 0.2600
Bi	 0.7760	 0.1220
Bk	 0.7450	 0.0980
Bu	 0.2620	 0.1040
C	 0.7760	 0.1260
C8	 0.7740	 0.1050
CA	 0.6920	 0.1000
CB	 0.8940	 0.1050
CC	 0.7810	 0.1160
CD	 0.7180	 0.0940
CE	 0.8460	 0.1010
CF	 0.8810	 0.1150
CG	 0.8430	 0.1550
CH	 0.8190	 0.1490
CI	 0.6100	 0.1320
CJ	 0.6030	 0.1400
CK	 0.9470	 0.1090

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Chain	Atom inclusion	Q-score
CL	 0.8430	 0.0770
CM	 0.7900	 0.1410
CN	 0.7510	 0.1290
CO	 0.7210	 0.1080
CP	 0.7880	 0.1150
CQ	 0.8680	 0.1340
CR	 0.9270	 0.1280
CS	 0.6320	 0.1080
Ca	 0.7600	 0.1190
Cb	 0.7310	 0.1370
Cc	 0.6910	 0.1310
Cd	 0.7450	 0.1730
Ce	 0.9400	 0.2790
Cf	 0.7830	 0.1160
Cg	 0.9880	 0.2460
Ci	 0.7760	 0.1160
Ck	 0.7450	 0.0990
Cu	 0.2620	 0.0990
D	 0.8330	 0.1240
E	 0.8850	 0.1240
F	 0.8660	 0.1220
G	 0.7940	 0.1510
H	 0.8370	 0.1740
I	 0.7710	 0.1490
J	 0.6660	 0.1550
K	 0.7940	 0.1580
L	 0.7330	 0.1290
M	 0.7450	 0.1300
N	 0.8300	 0.1530
O	 0.8890	 0.1110
P	 0.9290	 0.1230
Q	 0.9230	 0.1440
R	 0.8550	 0.1550
S	 0.6370	 0.1030
a	 0.8070	 0.1550
b	 0.7890	 0.1600
c	 0.6790	 0.1410
d	 0.7990	 0.1850
e	 0.9240	 0.2280
f	 0.9210	 0.1690
g	 0.8980	 0.2210
i	 0.8640	 0.1660

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Chain	Atom inclusion	Q-score
k	 0.8690	 0.1760
u	 0.1860	 0.0780