



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Oct 29, 2019 – 02:51 PM EDT

PDB ID : 6J5K
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/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

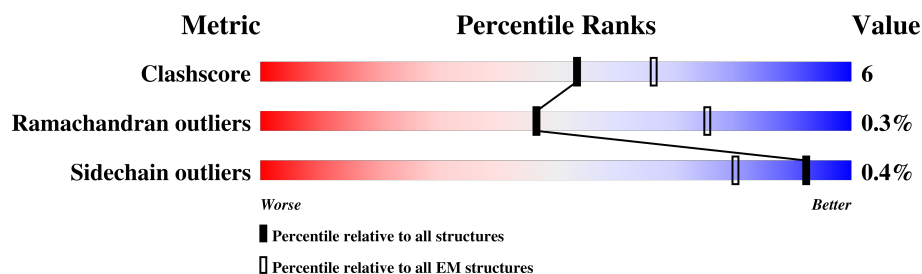
1 Overall quality at a glance

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.














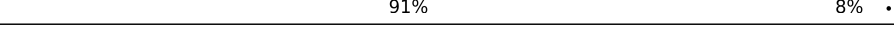
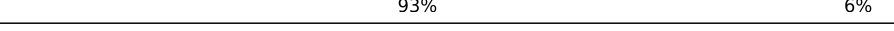






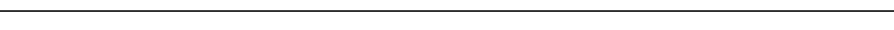

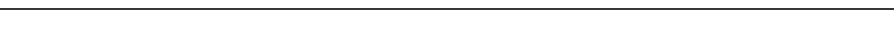
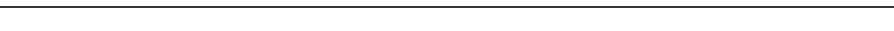


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	509	
1	AA	509	
1	AB	509	
1	AC	509	
1	B	509	
1	BA	509	
1	BB	509	
1	BC	509	
1	C	509	
















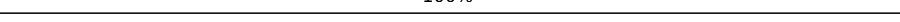
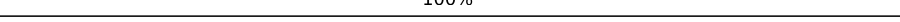
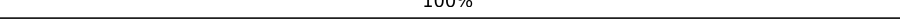
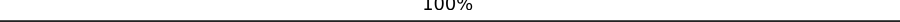
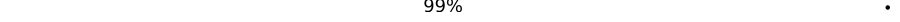
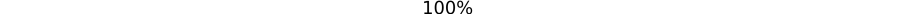
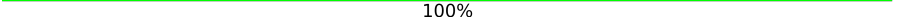
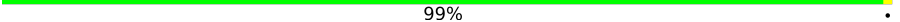

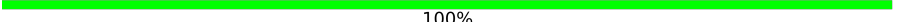
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Mol	Chain	Length	Quality of chain
1	CA	509	 89% 11%
1	CB	509	 81% 13% 6%
1	CC	509	 86% 12% ..
2	AD	469	 93% 7%
2	AE	469	 91% 8% .
2	AF	469	 90% 9% .
2	BD	469	 88% 12%
2	BE	469	 87% 12% .
2	BF	469	 90% 9% .
2	CD	469	 88% 12%
2	CE	469	 86% 13% .
2	CF	469	 91% 8% .
2	D	469	 93% 6%
2	E	469	 91% 8% .
2	F	469	 89% 10% .
3	AJ	83	 80% 14% 6%
3	BJ	83	 70% 20% 10%
3	CJ	83	 72% 18% 10%
3	J	83	 77% 17% 6%
4	AG	272	 93% 7%
4	BG	272	 83% 16%
4	CG	272	 84% 15%
4	G	272	 93% 7%
5	AH	132	 84% 14% .
5	BH	132	 80% 20%

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Mol	Chain	Length	Quality of chain
5	CH	132	 81% 19%
5	H	132	 83% 16% .
6	AI	48	 88% 13%
6	BI	48	 85% 15%
6	CI	48	 85% 15%
6	I	48	 85% 15%
7	AS	187	 83% 16% .
7	BS	187	 84% 16%
7	CS	187	 81% 19%
7	S	187	 84% 15% .
8	Ab	209	 100%
8	Bb	209	 100%
8	Cb	209	 100%
8	b	209	 100%
9	Ac	70	 100%
9	Bc	70	 100%
9	Cc	70	 100%
9	c	70	 100%
10	Ad	147	 99% .
10	Bd	147	 100%
10	Cd	147	 100%
10	d	147	 99% .
11	Ae	63	 100%
11	Be	63	 100%
11	Ce	63	 100%












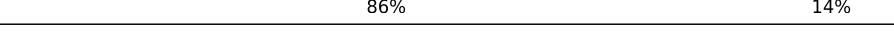


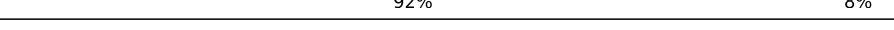




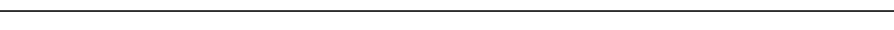

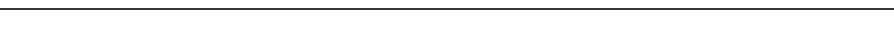
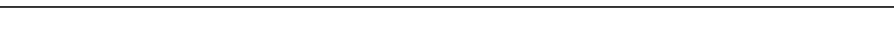


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Mol	Chain	Length	Quality of chain
11	e	63	100%
12	Af	87	95% 5%
12	Bf	87	87% 5% 8%
12	Cf	87	87% 5% 8%
12	f	87	95% 5%
13	Ag	84	100%
13	Bg	84	94% 6%
13	Cg	84	94% 5%
13	g	84	100%
14	Ai	42	100%
14	Bi	42	100%
14	Ci	42	100%
14	i	42	100%
15	Ak	29	100%
15	Bk	29	100%
15	Ck	29	100%
15	k	29	100%
16	8	67	66% 12% 16%
16	A8	67	67% 9% 6% 16%
16	B8	67	64% 12% 6% 16%
16	C8	67	63% 15% 16%
17	Aa	226	98%
17	Ba	226	98%
17	Ca	226	98%
17	a	226	98%

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Mol	Chain	Length	Quality of chain
18	AK	72	 85% 15%
18	AL	72	 92% 8%
18	AM	72	 81% 18%
18	AN	72	 83% 17%
18	AO	72	 85% 15%
18	AP	72	 90% 10%
18	AQ	72	 90% 10%
18	AR	72	 90% 10%
18	BK	72	 85% 15%
18	BL	72	 90% 10%
18	BM	72	 81% 18%
18	BN	72	 86% 14%
18	BO	72	 89% 11%
18	BP	72	 89% 11%
18	BQ	72	 92% 8%
18	BR	72	 86% 14%
18	CK	72	 85% 15%
18	CL	72	 90% 10%
18	CM	72	 83% 15%
18	CN	72	 82% 18%
18	CO	72	 88% 13%
18	CP	72	 89% 11%
18	CQ	72	 89% 11%
18	CR	72	 86% 14%
18	K	72	 83% 17%

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Mol	Chain	Length	Quality of chain
18	L	72	 89% 11%
18	M	72	 85% 14%
18	N	72	 85% 15%
18	O	72	 86% 14%
18	P	72	 90% 10%
18	Q	72	 90% 10%
18	R	72	 90% 10%
19	Au	42	 100%
19	Bu	42	 100%
19	Cu	42	 100%
19	u	42	 100%

2 Entry composition

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
18	CM	72	Total 513	C 340	N 80	O 89	S 4	0	0

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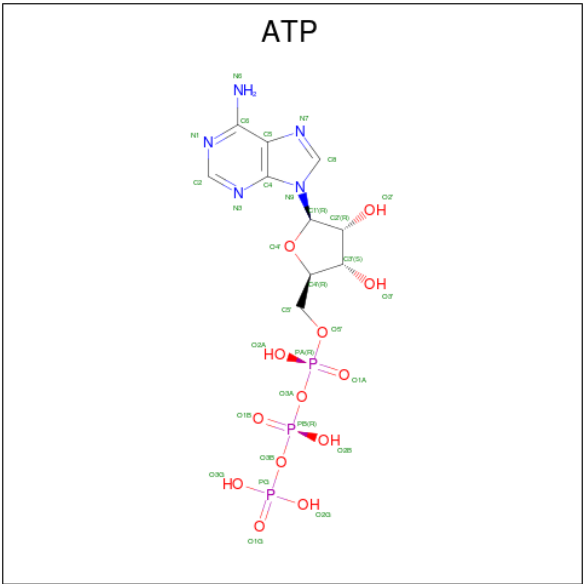
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Mol	Chain	Residues	Atoms					AltConf	Trace
18	CN	72	Total	C	N	O	S	0	0
			510	338	80	89	3		
18	CO	72	Total	C	N	O	S	0	0
			510	338	80	89	3		
18	CP	72	Total	C	N	O	S	0	0
			513	340	80	89	4		
18	CQ	72	Total	C	N	O	S	0	0
			513	340	80	89	4		
18	CR	72	Total	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 (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by author).



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 (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

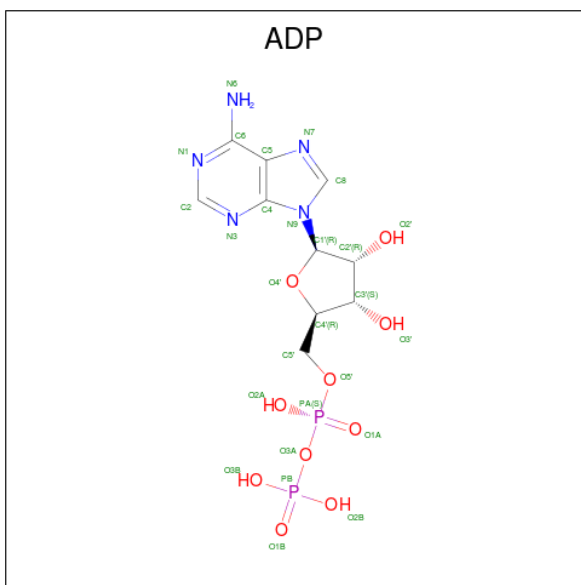
Mol	Chain	Residues	Atoms		AltConf
21	BB	1	Total	Mg	0
			1	1	
21	D	1	Total	Mg	0
			1	1	
21	BF	1	Total	Mg	0
			1	1	
21	BA	1	Total	Mg	0
			1	1	
21	CB	1	Total	Mg	0
			1	1	
21	BD	1	Total	Mg	0
			1	1	
21	B	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
21	CC	1	Total 1	Mg 1	0
21	C	1	Total 1	Mg 1	0
21	AC	1	Total 1	Mg 1	0
21	A	1	Total 1	Mg 1	0
21	AA	1	Total 1	Mg 1	0
21	AF	1	Total 1	Mg 1	0
21	CD	1	Total 1	Mg 1	0
21	AD	1	Total 1	Mg 1	0
21	BC	1	Total 1	Mg 1	0
21	CF	1	Total 1	Mg 1	0
21	AB	1	Total 1	Mg 1	0
21	F	1	Total 1	Mg 1	0
21	CA	1	Total 1	Mg 1	0

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

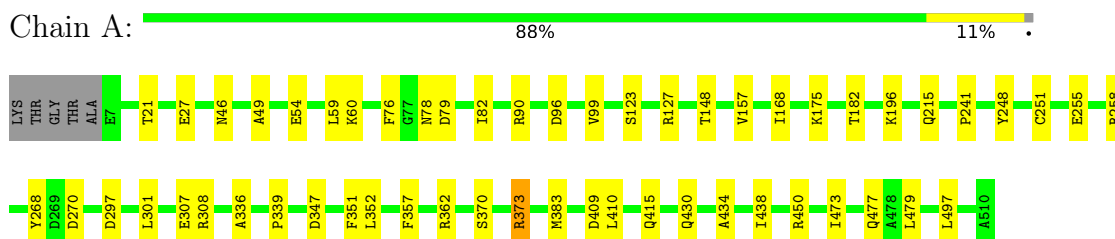


Mol	Chain	Residues	Atoms					AltConf
22	D	1	Total 27	C 10	N 5	O 10	P 2	0
22	F	1	Total 27	C 10	N 5	O 10	P 2	0
22	AD	1	Total 27	C 10	N 5	O 10	P 2	0
22	AF	1	Total 27	C 10	N 5	O 10	P 2	0
22	BD	1	Total 27	C 10	N 5	O 10	P 2	0
22	BF	1	Total 27	C 10	N 5	O 10	P 2	0
22	CD	1	Total 27	C 10	N 5	O 10	P 2	0
22	CF	1	Total 27	C 10	N 5	O 10	P 2	0

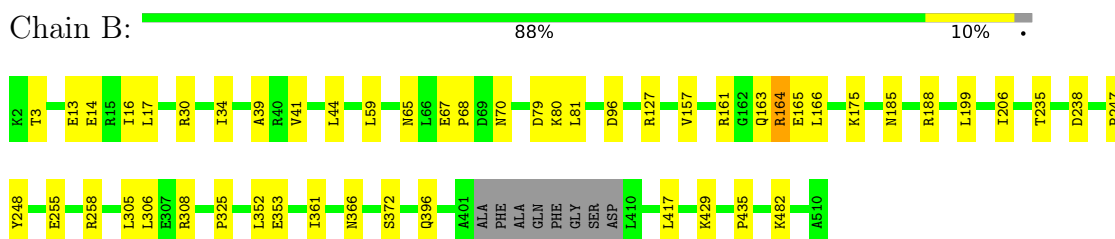
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

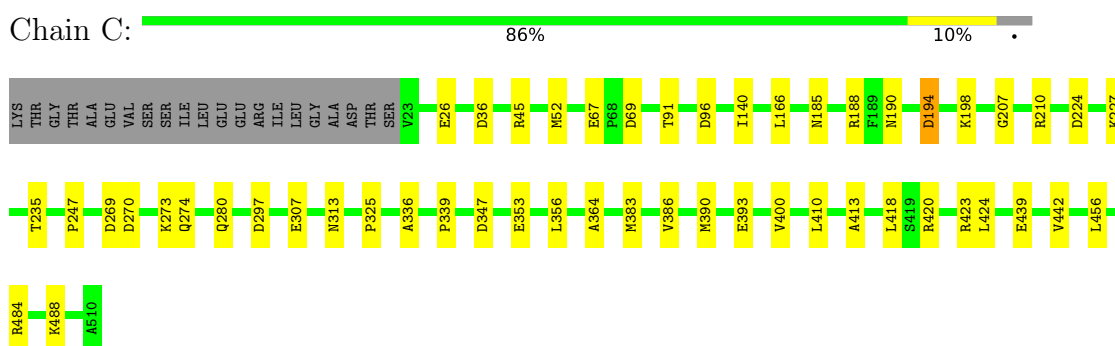
- Molecule 1: ATP synthase F1 subunit alpha



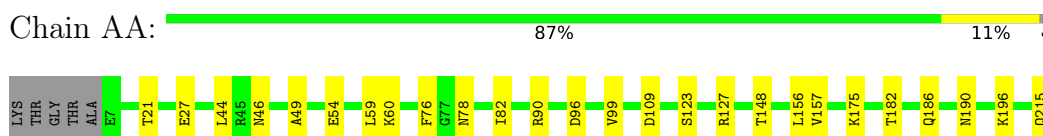
- Molecule 1: ATP synthase F1 subunit alpha



- Molecule 1: ATP synthase F1 subunit alpha



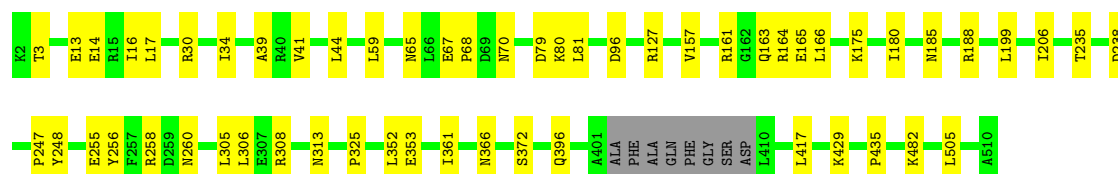
- Molecule 1: ATP synthase F1 subunit alpha





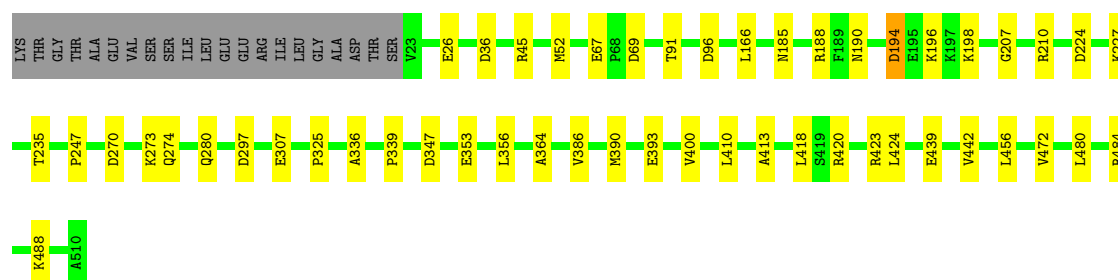
- Molecule 1: ATP synthase F1 subunit alpha

Chain AB: 87% 11%



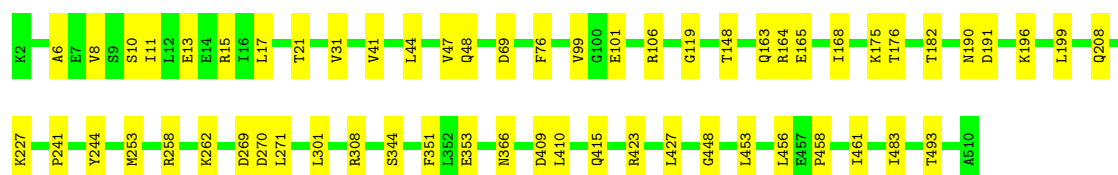
- Molecule 1: ATP synthase F1 subunit alpha

Chain AC: 86% 10%



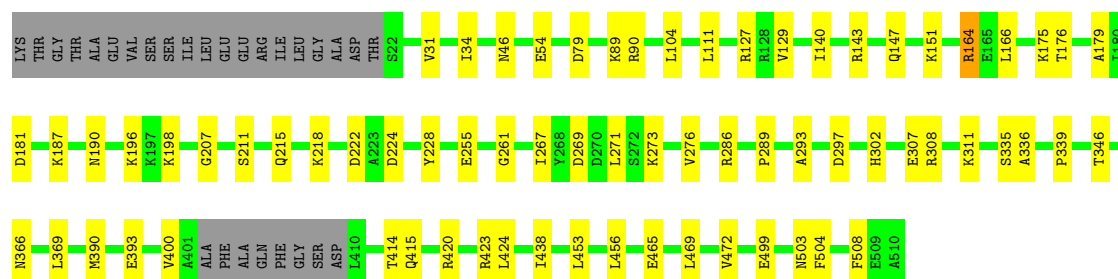
- Molecule 1: ATP synthase F1 subunit alpha

Chain BA: 88% 12%

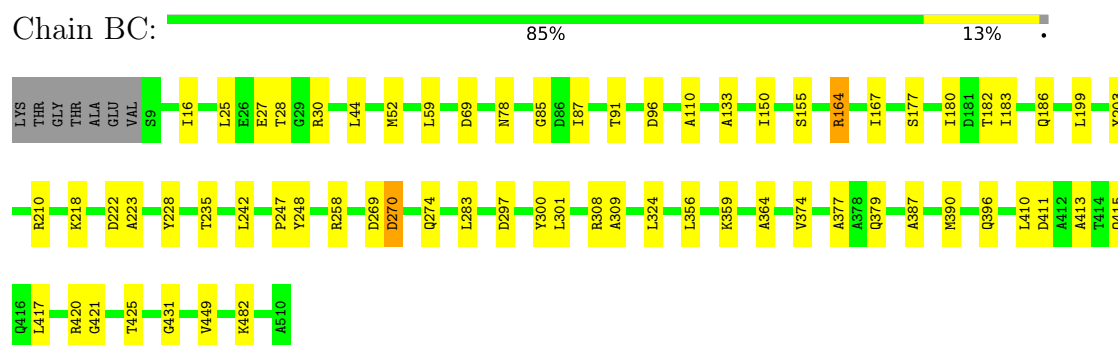


- Molecule 1: ATP synthase F1 subunit alpha

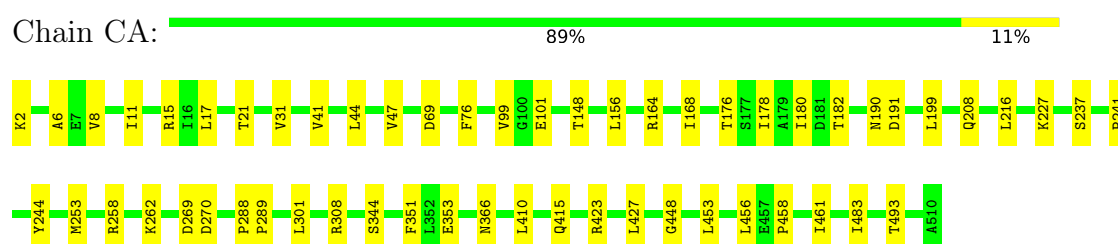
Chain BB: 81% 14% 6%



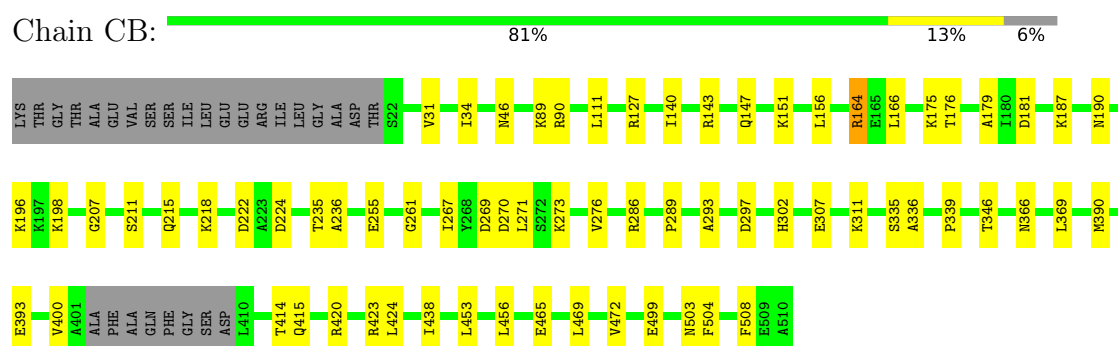
- Molecule 1: ATP synthase F1 subunit alpha



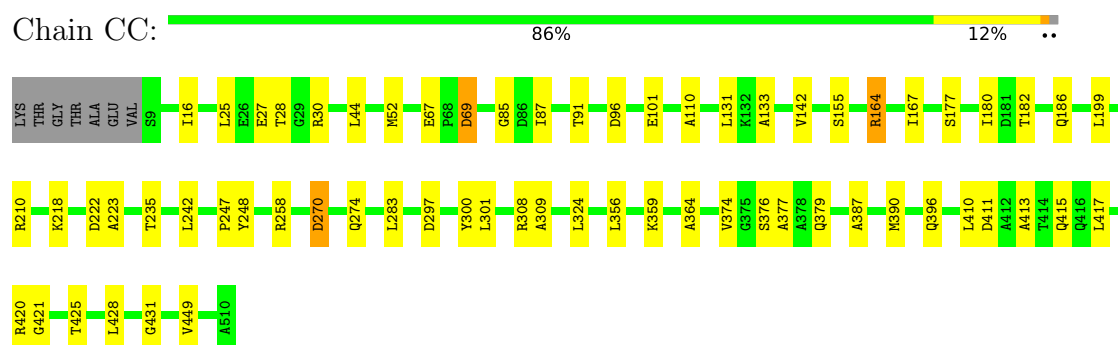
- Molecule 1: ATP synthase F1 subunit alpha




- Molecule 1: ATP synthase F1 subunit alpha



- Molecule 1: ATP synthase F1 subunit alpha



- Molecule 2: ATP synthase subunit beta

Chain D:  93% 6%



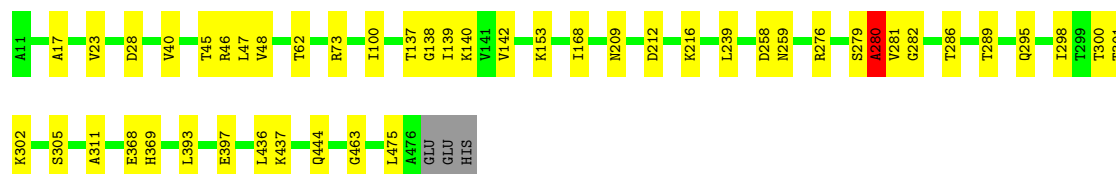
- Molecule 2: ATP synthase subunit beta

Chain E:  91% 8%



- Molecule 2: ATP synthase subunit beta

Chain F:  89% 10%



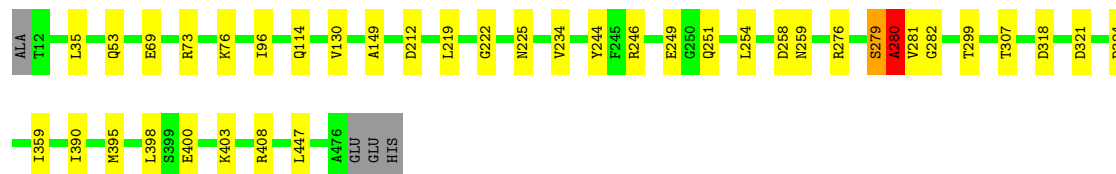
- Molecule 2: ATP synthase subunit beta

Chain AD:  93% 7%



- Molecule 2: ATP synthase subunit beta

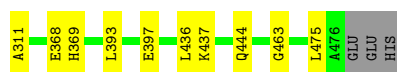
Chain AE:  91% 8%



- Molecule 2: ATP synthase subunit beta

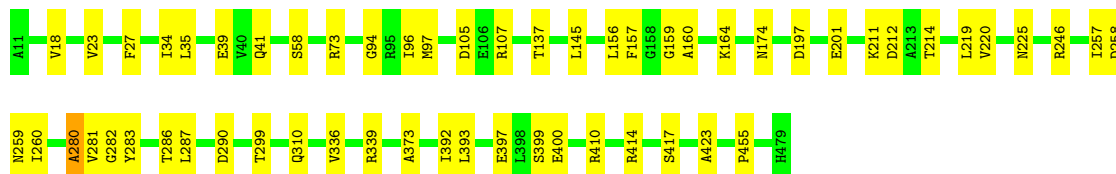
Chain AF:  90% 9%





• Molecule 2: ATP synthase subunit beta

Chain BD: 88% 12%



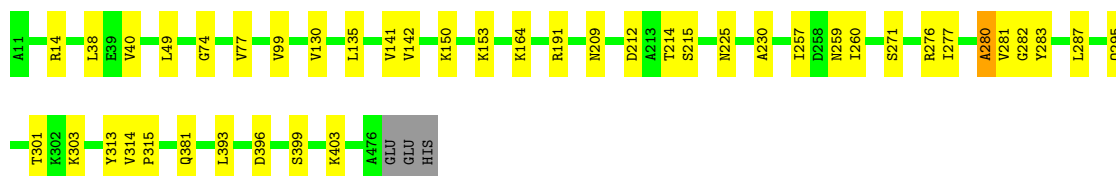
• Molecule 2: ATP synthase subunit beta

Chain BE: 87% 12%



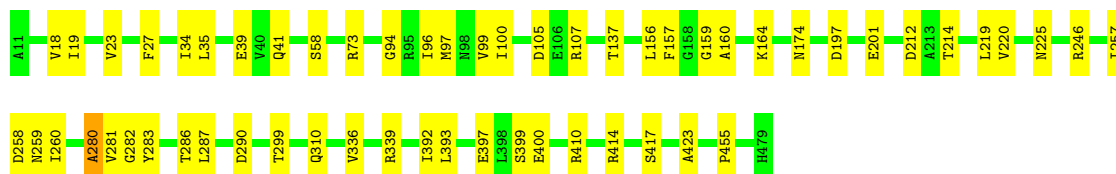
• Molecule 2: ATP synthase subunit beta

Chain BF: 90% 9%



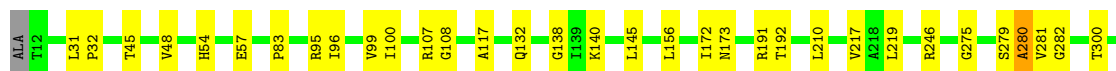
• Molecule 2: ATP synthase subunit beta

Chain CD: 88% 12%



• Molecule 2: ATP synthase subunit beta

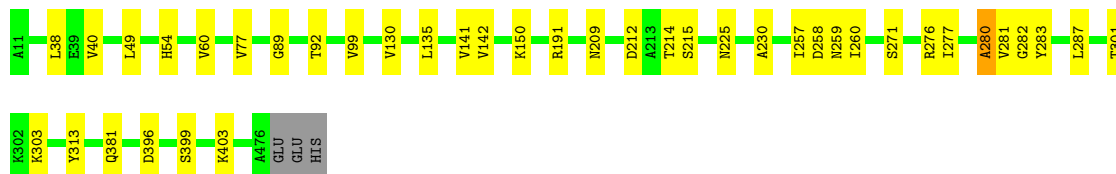
Chain CE: 86% 13%





- Molecule 2: ATP synthase subunit beta

Chain CF: 91% 8%



- Molecule 3: ATPase inhibitor, mitochondrial

Chain J: 77% 17% 6%



- Molecule 3: ATPase inhibitor, mitochondrial

Chain AJ: 80% 14% 6%



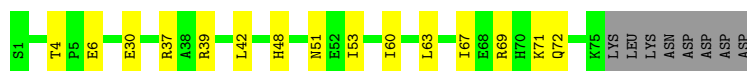
- Molecule 3: ATPase inhibitor, mitochondrial

Chain BJ: 70% 20% 10%



- Molecule 3: ATPase inhibitor, mitochondrial

Chain CJ: 72% 18% 10%



- Molecule 4: ATP synthase subunit gamma

Chain G: 93% 7%



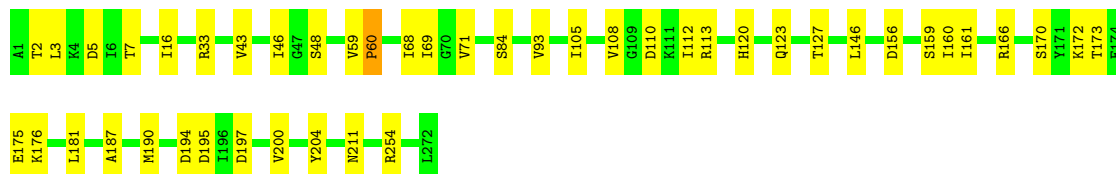
- Molecule 4: ATP synthase subunit gamma

Chain AG: 93% 7%



- Molecule 4: ATP synthase subunit gamma

Chain BG: 83% 16%



- Molecule 4: ATP synthase subunit gamma

Chain CG: 84% 15%



- Molecule 5: ATP synthase subunit delta, mitochondrial

Chain H: 83% 16%



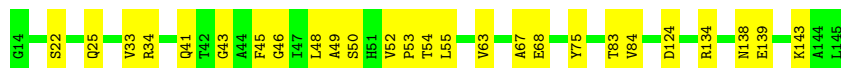
- Molecule 5: ATP synthase subunit delta, mitochondrial

Chain AH: 84% 14%



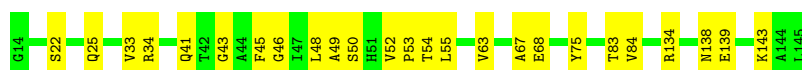
- Molecule 5: ATP synthase subunit delta, mitochondrial

Chain BH: 80% 20%

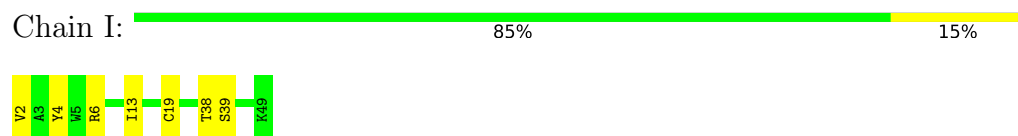


- Molecule 5: ATP synthase subunit delta, mitochondrial

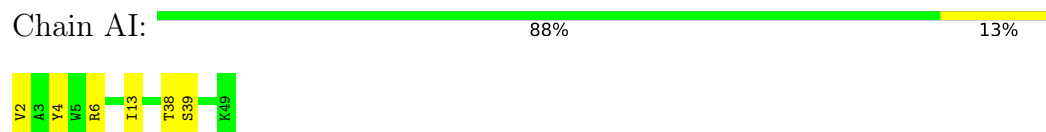
Chain CH: 81% 19%



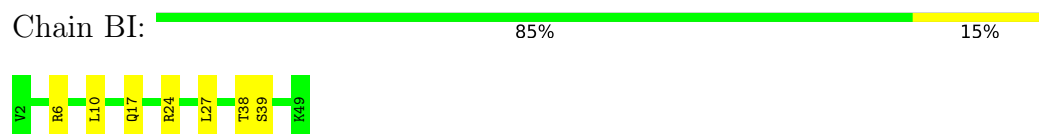
- Molecule 6: ATP synthase F1 subunit epsilon



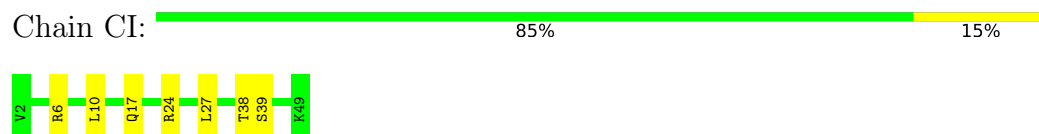
- Molecule 6: ATP synthase F1 subunit epsilon



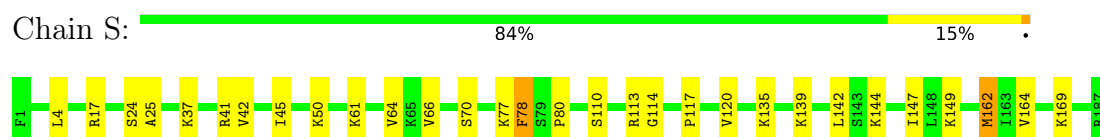
- Molecule 6: ATP synthase F1 subunit epsilon



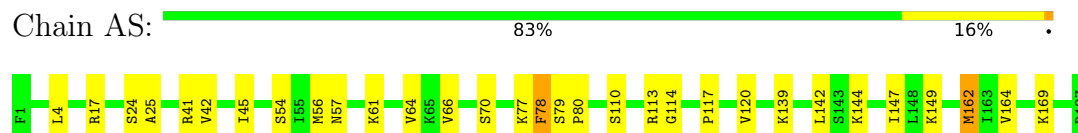
- Molecule 6: ATP synthase F1 subunit epsilon



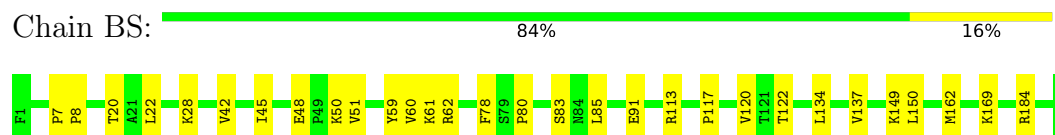
- Molecule 7: ATP synthase subunit O, mitochondrial



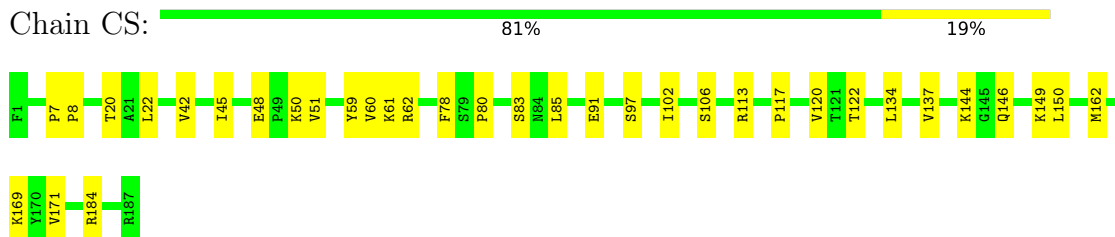
- Molecule 7: ATP synthase subunit O, mitochondrial



- Molecule 7: ATP synthase subunit O, mitochondrial



- Molecule 7: ATP synthase subunit O, mitochondrial



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



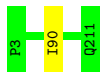
There are no outlier residues recorded for this chain.

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



There are no outlier residues recorded for this chain.

- 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



There are no outlier residues recorded for this chain.

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



There are no outlier residues recorded for this chain.

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



There are no outlier residues recorded for this chain.

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

Chain Cc:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: ATP synthase subunit d, mitochondrial

Chain d:  99%



- Molecule 10: ATP synthase subunit d, mitochondrial

Chain Ad:  99%



- Molecule 10: ATP synthase subunit d, mitochondrial

Chain Bd:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: ATP synthase subunit d, mitochondrial

Chain Cd:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: ATP synthase subunit e

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: ATP synthase subunit e

Chain Ae:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: ATP synthase subunit e

Chain Be:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: ATP synthase subunit e

Chain Ce:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: ATP synthase subunit f, mitochondrial

Chain f:  95% 5%




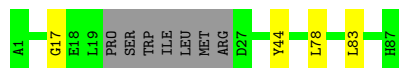
- Molecule 12: ATP synthase subunit f, mitochondrial

Chain Af:  95% 5%




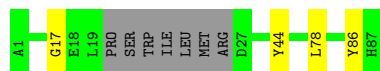
- Molecule 12: ATP synthase subunit f, mitochondrial

Chain Bf:  87% 5% 8%



- Molecule 12: ATP synthase subunit f, mitochondrial

Chain Cf:  87% 5% 8%



- Molecule 13: ATP synthase subunit g

Chain g:  100%

There are no outlier residues recorded for this chain.

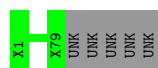
- Molecule 13: ATP synthase subunit g

Chain Ag:  100%

There are no outlier residues recorded for this chain.

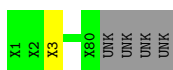
- Molecule 13: ATP synthase subunit g

Chain Bg:  94% 6%



- Molecule 13: ATP synthase subunit g

Chain Cg:  94% 5%



- Molecule 14: ATP synthase membrane subunit DAPIT

Chain i: 100%

There are no outlier residues recorded for this chain.

- Molecule 14: ATP synthase membrane subunit DAPIT

Chain Ai: 100%

There are no outlier residues recorded for this chain.

- Molecule 14: ATP synthase membrane subunit DAPIT

Chain Bi: 100%

There are no outlier residues recorded for this chain.

- Molecule 14: ATP synthase membrane subunit DAPIT

Chain Ci: 100%

There are no outlier residues recorded for this chain.

- Molecule 15: subunit k analog

Chain k: 100%

There are no outlier residues recorded for this chain.

- Molecule 15: subunit k analog

Chain Ak: 100%

There are no outlier residues recorded for this chain.

- Molecule 15: subunit k analog

Chain Bk: 100%

There are no outlier residues recorded for this chain.

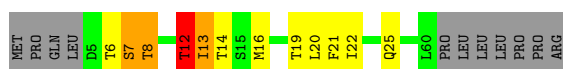
- Molecule 15: subunit k analog

Chain Ck: 100%

There are no outlier residues recorded for this chain.

- Molecule 16: ATP synthase protein 8

Chain 8: 66% 12% 16%



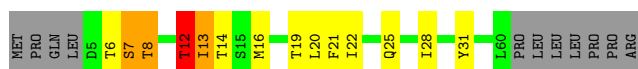
- Molecule 16: ATP synthase protein 8



- Molecule 16: ATP synthase protein 8



- Molecule 16: ATP synthase protein 8



- Molecule 17: ATP synthase subunit a



- Molecule 17: ATP synthase subunit a




- Molecule 17: ATP synthase subunit a



- Molecule 17: ATP synthase subunit a




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

Chain K:  83% 17%




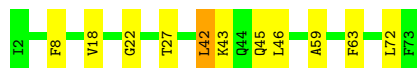
- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1

Chain L:  89% 11%



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

Chain M:  85% 14%



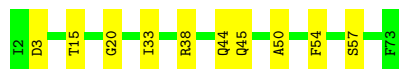
- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1

Chain N:  85% 15%




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

Chain O:  86% 14%



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

Chain P:  90% 10%




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

Chain Q:  90% 10%




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

Chain R:  90% 10%



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

Chain AK:  85% 15%




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

Chain AL:  92% 8%




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

Chain AM:  81% 18%




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

Chain AN:  83% 17%



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

Chain AO:  85% 15%



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

Chain AP:  90% 10%



- 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: 90% 10%



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

Chain BM: 81% 18%



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

Chain BN: 86% 14%



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

Chain BO: 89% 11%



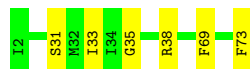
- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1

Chain BP: 89% 11%




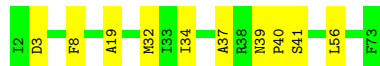
- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1

Chain BQ:  92% 8%




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

Chain BR:  86% 14%



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

Chain CK:  85% 15%




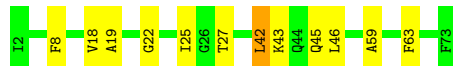
- Molecule 18: Mitochondrial H⁺ transporting ATP synthase subunit c isoform 1

Chain CL:  90% 10%




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

Chain CM:  83% 15%




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

Chain CN:  82% 18%



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

Chain CO:  88% 13%



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

Chain CP:  89% 11%



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

Chain CQ:  89% 11%



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

Chain CR:  86% 14%



- Molecule 19: ATP synthase membrane subunit 6.8PL

Chain u:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: ATP synthase membrane subunit 6.8PL

Chain Au:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: ATP synthase membrane subunit 6.8PL

Chain Bu:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: ATP synthase membrane subunit 6.8PL

Chain Cu:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
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	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	0.32	0/3888	0.52	0/5247
1	AA	0.32	0/3888	0.52	0/5247
1	AB	0.30	0/3862	0.52	0/5210
1	AC	0.30	0/3773	0.53	0/5091
1	B	0.29	0/3862	0.52	0/5210
1	BA	0.43	0/3924	0.59	0/5295
1	BB	0.42	0/3717	0.59	0/5014
1	BC	0.47	0/3872	0.64	0/5225
1	C	0.30	0/3773	0.53	0/5091
1	CA	0.43	0/3924	0.58	0/5295
1	CB	0.42	0/3717	0.59	0/5014
1	CC	0.47	0/3872	0.64	0/5225
10	Ad	0.25	0/742	0.42	0/1036
10	Bd	0.25	0/742	0.42	0/1036
10	Cd	0.25	0/742	0.42	0/1036
10	d	0.25	0/742	0.42	0/1036
12	Af	0.34	0/535	0.66	2/730 (0.3%)
12	Bf	0.34	0/499	0.63	2/678 (0.3%)
12	Cf	0.34	0/490	0.62	1/667 (0.1%)
12	f	0.34	0/535	0.66	2/730 (0.3%)
14	Ai	0.34	0/311	0.51	0/421
14	Bi	0.34	0/308	0.49	0/417
14	Ci	0.33	0/308	0.49	0/417
14	i	0.34	0/311	0.51	0/421
16	8	0.44	0/380	0.76	0/522
16	A8	0.44	0/380	0.76	0/522
16	B8	0.42	0/380	0.76	0/522
16	C8	0.42	0/380	0.75	0/522
17	Aa	0.43	0/1736	0.68	0/2375
17	Ba	0.43	0/1721	0.67	0/2358
17	Ca	0.43	0/1721	0.67	0/2358
17	a	0.43	0/1736	0.68	0/2375

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
18	AK	0.41	0/522	0.55	0/703
18	AL	0.39	0/522	0.56	0/703
18	AM	0.42	0/522	0.59	0/703
18	AN	0.44	0/519	0.50	0/700
18	AO	0.40	0/519	0.59	0/699
18	AP	0.34	0/522	0.53	0/703
18	AQ	0.34	0/522	0.47	0/703
18	AR	0.40	0/522	0.57	0/703
18	BK	0.41	0/522	0.55	0/703
18	BL	0.39	0/522	0.56	0/703
18	BM	0.43	0/522	0.59	0/703
18	BN	0.44	0/519	0.50	0/700
18	BO	0.40	0/519	0.59	0/700
18	BP	0.35	0/522	0.53	0/703
18	BQ	0.34	0/522	0.47	0/703
18	BR	0.40	0/519	0.57	0/699
18	CK	0.41	0/522	0.54	0/703
18	CL	0.39	0/522	0.56	0/703
18	CM	0.43	0/522	0.59	0/703
18	CN	0.44	0/519	0.50	0/700
18	CO	0.41	0/519	0.59	0/700
18	CP	0.35	0/522	0.53	0/703
18	CQ	0.34	0/522	0.47	0/703
18	CR	0.40	0/519	0.57	0/699
18	K	0.41	0/522	0.54	0/703
18	L	0.39	0/522	0.56	0/703
18	M	0.43	0/522	0.59	0/703
18	N	0.44	0/519	0.51	0/700
18	O	0.40	0/519	0.59	0/699
18	P	0.35	0/522	0.53	0/703
18	Q	0.34	0/522	0.47	0/703
18	R	0.40	0/522	0.57	0/703
2	AD	0.33	0/3613	0.52	0/4900
2	AE	0.29	0/3579	0.51	0/4854
2	AF	0.30	0/3584	0.51	1/4861 (0.0%)
2	BD	0.46	0/3613	0.60	1/4900 (0.0%)
2	BE	0.40	0/3579	0.58	0/4854
2	BF	0.48	0/3584	0.61	0/4861
2	CD	0.46	0/3613	0.60	1/4900 (0.0%)
2	CE	0.40	0/3579	0.58	0/4854
2	CF	0.48	0/3584	0.61	0/4861
2	D	0.33	0/3610	0.52	0/4896
2	E	0.29	0/3579	0.51	0/4854

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
2	F	0.30	0/3584	0.51	1/4861 (0.0%)
3	AJ	0.32	0/587	0.48	0/780
3	BJ	0.42	0/565	0.50	0/752
3	CJ	0.42	0/565	0.50	0/752
3	J	0.32	0/587	0.49	0/780
4	AG	0.28	0/2135	0.49	0/2870
4	BG	0.35	0/2138	0.56	0/2874
4	CG	0.35	0/2135	0.56	0/2870
4	G	0.28	0/2135	0.49	0/2870
5	AH	0.30	0/983	0.62	1/1338 (0.1%)
5	BH	0.31	0/986	0.61	0/1342
5	CH	0.31	0/986	0.61	0/1342
5	H	0.30	0/983	0.62	1/1338 (0.1%)
6	AI	0.28	0/382	0.50	0/511
6	BI	0.33	0/382	0.52	0/511
6	CI	0.33	0/382	0.53	0/511
6	I	0.28	0/382	0.50	0/511
7	AS	0.27	0/1447	0.57	0/1947
7	BS	0.33	0/1453	0.62	0/1954
7	CS	0.33	0/1453	0.62	0/1954
7	S	0.27	0/1447	0.57	0/1947
8	Ab	0.25	0/1489	0.48	0/2010
8	Bb	0.28	0/1487	0.54	0/2006
8	Cb	0.28	0/1487	0.53	0/2006
8	b	0.25	0/1489	0.48	0/2010
9	Ac	0.26	0/431	0.43	0/587
9	Bc	0.28	0/431	0.49	0/587
9	Cc	0.28	0/431	0.49	0/587
9	c	0.26	0/431	0.43	0/587
All	All	0.37	0/150335	0.56	13/203395 (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
12	Af	0	2
12	Bf	0	1
12	Cf	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	f	0	2
13	Cg	0	1
16	8	0	4
16	A8	0	4
16	B8	0	4
16	C8	0	4
2	AD	0	1
2	AE	0	1
2	AF	0	1
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
All	All	0	45

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CD	156	LEU	CA-CB-CG	5.58	128.13	115.30
2	BD	156	LEU	CA-CB-CG	5.56	128.09	115.30
2	F	475	LEU	CA-CB-CG	5.35	127.61	115.30
2	AF	475	LEU	CA-CB-CG	5.33	127.55	115.30
5	H	55	LEU	CA-CB-CG	5.21	127.27	115.30

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	33	0
1	AA	3837	0	3939	36	0
1	AB	3814	0	3930	35	0
1	AC	3722	0	3826	32	0
1	B	3814	0	3930	32	0
1	BA	3873	0	3978	38	0
1	BB	3669	0	3781	49	0
1	BC	3821	0	3924	40	0
1	C	3722	0	3826	33	0
1	CA	3873	0	3978	35	0
1	CB	3669	0	3781	46	0
1	CC	3821	0	3924	42	0
2	AD	3555	0	3603	23	0
2	AE	3522	0	3580	25	0
2	AF	3527	0	3584	25	0
2	BD	3555	0	3603	34	0
2	BE	3522	0	3580	34	0
2	BF	3527	0	3585	28	0
2	CD	3555	0	3603	36	0
2	CE	3522	0	3580	35	0
2	CF	3527	0	3585	26	0
2	D	3552	0	3601	21	0
2	E	3522	0	3580	24	0
2	F	3527	0	3584	27	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	31	0
4	CG	2109	0	2187	31	0
4	G	2109	0	2187	14	0
5	AH	970	0	962	13	0
5	BH	973	0	971	36	0
5	CH	973	0	971	34	0
5	H	970	0	962	15	0
6	AI	377	0	397	5	0
6	BI	377	0	397	4	0
6	CI	377	0	397	5	0
6	I	377	0	397	8	0
7	AS	1429	0	1535	18	0
7	BS	1435	0	1546	20	0
7	CS	1435	0	1546	23	0
7	S	1429	0	1535	18	0
8	Ab	1478	0	1340	0	0
8	Bb	1476	0	1340	0	0
8	Cb	1476	0	1340	0	0
8	b	1478	0	1340	0	0
9	Ac	428	0	305	0	0
9	Bc	428	0	305	0	0
9	Cc	428	0	305	0	0
9	c	428	0	305	0	0
10	Ad	741	0	348	0	0
10	Bd	741	0	348	0	0
10	Cd	741	0	348	0	0
10	d	741	0	348	0	0
11	Ae	315	0	65	0	0
11	Be	315	0	66	0	0
11	Ce	315	0	66	0	0
11	e	315	0	65	0	0
12	Af	530	0	385	0	0
12	Bf	495	0	371	0	0
12	Cf	486	0	351	0	0
12	f	530	0	385	0	0
13	Ag	420	0	88	0	0
13	Bg	395	0	83	0	0
13	Cg	400	0	84	0	0
13	g	420	0	88	0	0
14	Ai	306	0	293	0	0
14	Bi	303	0	284	0	0
14	Ci	303	0	284	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	i	306	0	293	0	0
15	Ak	145	0	32	0	0
15	Bk	145	0	31	0	0
15	Ck	145	0	31	0	0
15	k	145	0	32	0	0
16	8	374	0	299	6	0
16	A8	374	0	299	7	0
16	B8	374	0	299	19	0
16	C8	374	0	299	19	0
17	Aa	1699	0	1789	0	0
17	Ba	1684	0	1748	0	0
17	Ca	1684	0	1748	0	0
17	a	1699	0	1789	0	0
18	AK	513	0	530	9	0
18	AL	513	0	530	5	0
18	AM	513	0	530	12	0
18	AN	510	0	523	9	0
18	AO	510	0	526	14	0
18	AP	513	0	530	5	0
18	AQ	513	0	530	5	0
18	AR	513	0	530	7	0
18	BK	513	0	530	12	0
18	BL	513	0	530	6	0
18	BM	513	0	530	12	0
18	BN	510	0	523	7	0
18	BO	510	0	523	6	0
18	BP	513	0	530	8	0
18	BQ	513	0	530	6	0
18	BR	510	0	521	25	0
18	CK	513	0	530	13	0
18	CL	513	0	530	6	0
18	CM	513	0	530	11	0
18	CN	510	0	523	10	0
18	CO	510	0	523	8	0
18	CP	513	0	530	8	0
18	CQ	513	0	530	7	0
18	CR	510	0	521	24	0
18	K	513	0	530	10	0
18	L	513	0	530	7	0
18	M	513	0	530	9	0
18	N	510	0	523	8	0
18	O	510	0	526	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	P	513	0	530	6	0
18	Q	513	0	530	5	0
18	R	513	0	530	7	0
19	Au	210	0	45	0	0
19	Bu	210	0	45	0	0
19	Cu	210	0	45	0	0
19	u	210	0	45	0	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	0	0
22	D	27	0	11	1	0
22	F	27	0	12	0	0
All	All	153148	0	149285	1279	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 1279 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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	49	84
2	AE	463/469 (99%)	442 (96%)	18 (4%)	3 (1%)	27	70
2	AF	464/469 (99%)	432 (93%)	30 (6%)	2 (0%)	36	77
2	BD	467/469 (100%)	421 (90%)	45 (10%)	1 (0%)	49	84
2	BE	463/469 (99%)	423 (91%)	39 (8%)	1 (0%)	49	84
2	BF	464/469 (99%)	422 (91%)	41 (9%)	1 (0%)	49	84
2	CD	467/469 (100%)	421 (90%)	45 (10%)	1 (0%)	49	84
2	CE	463/469 (99%)	423 (91%)	39 (8%)	1 (0%)	49	84
2	CF	464/469 (99%)	422 (91%)	41 (9%)	1 (0%)	49	84
2	D	467/469 (100%)	434 (93%)	32 (7%)	1 (0%)	49	84
2	E	463/469 (99%)	442 (96%)	18 (4%)	3 (1%)	27	70
2	F	464/469 (99%)	431 (93%)	31 (7%)	2 (0%)	36	77
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%)	36	77
4	BG	270/272 (99%)	254 (94%)	14 (5%)	2 (1%)	24	67
4	CG	270/272 (99%)	253 (94%)	14 (5%)	3 (1%)	16	58
4	G	270/272 (99%)	258 (96%)	11 (4%)	1 (0%)	36	77
5	AH	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	11	51
5	BH	130/132 (98%)	117 (90%)	12 (9%)	1 (1%)	21	65
5	CH	130/132 (98%)	117 (90%)	12 (9%)	1 (1%)	21	65
5	H	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	11	51

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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%)	24	67
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%)	24	67
12	Af	85/87 (98%)	63 (74%)	22 (26%)	0	100	100
12	Bf	76/87 (87%)	63 (83%)	12 (16%)	1 (1%)	13	54
12	Cf	76/87 (87%)	62 (82%)	12 (16%)	2 (3%)	6	38
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	17
16	A8	54/67 (81%)	46 (85%)	4 (7%)	4 (7%)	1	17
16	B8	54/67 (81%)	46 (85%)	4 (7%)	4 (7%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	C8	54/67 (81%)	46 (85%)	4 (7%)	4 (7%)	1	17
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%)	47	81

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%)	90	95
1	AA	406/410 (99%)	404 (100%)	2 (0%)	90	95
1	AB	405/410 (99%)	403 (100%)	2 (0%)	90	95
1	AC	393/410 (96%)	392 (100%)	1 (0%)	93	96
1	B	405/410 (99%)	403 (100%)	2 (0%)	90	95
1	BA	410/410 (100%)	409 (100%)	1 (0%)	94	96
1	BB	389/410 (95%)	388 (100%)	1 (0%)	93	96
1	BC	404/410 (98%)	401 (99%)	3 (1%)	85	93
1	C	393/410 (96%)	392 (100%)	1 (0%)	93	96
1	CA	410/410 (100%)	409 (100%)	1 (0%)	94	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CB	389/410 (95%)	388 (100%)	1 (0%)	93	96
1	CC	404/410 (98%)	401 (99%)	3 (1%)	85	93
2	AD	378/378 (100%)	377 (100%)	1 (0%)	93	96
2	AE	375/378 (99%)	374 (100%)	1 (0%)	93	96
2	AF	375/378 (99%)	374 (100%)	1 (0%)	93	96
2	BD	378/378 (100%)	378 (100%)	0	100	100
2	BE	375/378 (99%)	373 (100%)	2 (0%)	90	95
2	BF	375/378 (99%)	374 (100%)	1 (0%)	93	96
2	CD	378/378 (100%)	378 (100%)	0	100	100
2	CE	375/378 (99%)	373 (100%)	2 (0%)	90	95
2	CF	375/378 (99%)	374 (100%)	1 (0%)	93	96
2	D	377/378 (100%)	376 (100%)	1 (0%)	93	96
2	E	375/378 (99%)	374 (100%)	1 (0%)	93	96
2	F	375/378 (99%)	374 (100%)	1 (0%)	93	96
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%)	230 (100%)	0	100	100
4	CG	229/230 (100%)	229 (100%)	0	100	100
4	G	229/230 (100%)	229 (100%)	0	100	100
5	AH	104/105 (99%)	103 (99%)	1 (1%)	78	89
5	BH	105/105 (100%)	105 (100%)	0	100	100
5	CH	105/105 (100%)	105 (100%)	0	100	100
5	H	104/105 (99%)	103 (99%)	1 (1%)	78	89
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%)	160 (99%)	2 (1%)	74	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	BS	163/163 (100%)	162 (99%)	1 (1%)	87	93
7	CS	163/163 (100%)	162 (99%)	1 (1%)	87	93
7	S	162/163 (99%)	160 (99%)	2 (1%)	74	87
8	Ab	124/182 (68%)	124 (100%)	0	100	100
8	Bb	123/182 (68%)	122 (99%)	1 (1%)	83	92
8	Cb	123/182 (68%)	122 (99%)	1 (1%)	83	92
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%)	29 (100%)	0	100	100
16	A8	29/66 (44%)	29 (100%)	0	100	100
16	B8	29/66 (44%)	29 (100%)	0	100	100
16	C8	29/66 (44%)	29 (100%)	0	100	100
17	Aa	187/199 (94%)	186 (100%)	1 (0%)	90	95
17	Ba	183/199 (92%)	182 (100%)	1 (0%)	90	95
17	Ca	183/199 (92%)	182 (100%)	1 (0%)	90	95
17	a	187/199 (94%)	186 (100%)	1 (0%)	90	95

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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%)	49 (100%)	0	100	100
18	AM	49/49 (100%)	48 (98%)	1 (2%)	58	79
18	AN	48/49 (98%)	48 (100%)	0	100	100
18	AO	48/49 (98%)	48 (100%)	0	100	100
18	AP	49/49 (100%)	48 (98%)	1 (2%)	58	79
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%)	49 (100%)	0	100	100
18	BM	49/49 (100%)	48 (98%)	1 (2%)	58	79
18	BN	48/49 (98%)	48 (100%)	0	100	100
18	BO	48/49 (98%)	48 (100%)	0	100	100
18	BP	49/49 (100%)	48 (98%)	1 (2%)	58	79
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%)	49 (100%)	0	100	100
18	CM	49/49 (100%)	48 (98%)	1 (2%)	58	79
18	CN	48/49 (98%)	48 (100%)	0	100	100
18	CO	48/49 (98%)	48 (100%)	0	100	100
18	CP	49/49 (100%)	48 (98%)	1 (2%)	58	79
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%)	49 (100%)	0	100	100
18	M	49/49 (100%)	48 (98%)	1 (2%)	58	79
18	N	48/49 (98%)	48 (100%)	0	100	100
18	O	48/49 (98%)	48 (100%)	0	100	100
18	P	49/49 (100%)	48 (98%)	1 (2%)	58	79
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%)	14832 (100%)	54 (0%)	92	96

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	AS	162	MET
1	BC	69	ASP
7	CS	113	ARG
17	Aa	185	ASN
18	AP	43	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 127 such sidechains are listed below:

Mol	Chain	Res	Type
17	Aa	39	ASN
1	BC	330	GLN
5	CH	85	ASN
17	Aa	63	GLN
1	BA	415	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	A	601	21	26,33,33	0.93	1 (3%)	27,52,52	1.51	4 (14%)
20	ATP	AA	601	21	26,33,33	0.92	1 (3%)	27,52,52	1.51	4 (14%)
20	ATP	AB	601	21	26,33,33	0.96	1 (3%)	27,52,52	1.60	4 (14%)
20	ATP	AC	601	21	26,33,33	0.95	1 (3%)	27,52,52	1.65	4 (14%)
22	ADP	AD	501	21	24,29,29	1.00	1 (4%)	25,45,45	1.86	4 (16%)
22	ADP	AF	501	21	24,29,29	1.00	1 (4%)	25,45,45	1.35	3 (12%)
20	ATP	B	601	21	26,33,33	0.96	1 (3%)	27,52,52	1.60	4 (14%)
20	ATP	BA	601	21	26,33,33	0.92	1 (3%)	27,52,52	1.52	4 (14%)
20	ATP	BB	601	21	26,33,33	0.95	1 (3%)	27,52,52	1.56	4 (14%)
20	ATP	BC	601	21	26,33,33	0.92	1 (3%)	27,52,52	1.55	4 (14%)
22	ADP	BD	501	21	24,29,29	1.15	2 (8%)	25,45,45	1.97	3 (12%)
22	ADP	BF	501	21	24,29,29	0.97	1 (4%)	25,45,45	1.44	4 (16%)
20	ATP	C	601	21	26,33,33	0.95	1 (3%)	27,52,52	1.65	4 (14%)
20	ATP	CA	601	21	26,33,33	0.92	1 (3%)	27,52,52	1.52	4 (14%)
20	ATP	CB	601	21	26,33,33	0.94	1 (3%)	27,52,52	1.57	4 (14%)
20	ATP	CC	601	21	26,33,33	0.92	1 (3%)	27,52,52	1.55	4 (14%)
22	ADP	CD	501	21	24,29,29	1.16	2 (8%)	25,45,45	1.98	3 (12%)
22	ADP	CF	501	21	24,29,29	0.97	1 (4%)	25,45,45	1.44	4 (16%)
22	ADP	D	501	21	24,29,29	1.00	1 (4%)	25,45,45	1.86	4 (16%)
22	ADP	F	501	21	24,29,29	0.99	1 (4%)	25,45,45	1.35	3 (12%)

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	A	601	21	-	2/18/38/38	0/3/3/3
20	ATP	AA	601	21	-	2/18/38/38	0/3/3/3
20	ATP	AB	601	21	-	4/18/38/38	0/3/3/3
20	ATP	AC	601	21	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	ADP	AD	501	21	-	3/12/32/32	0/3/3/3
22	ADP	AF	501	21	-	5/12/32/32	0/3/3/3
20	ATP	B	601	21	-	4/18/38/38	0/3/3/3
20	ATP	BA	601	21	-	5/18/38/38	0/3/3/3
20	ATP	BB	601	21	-	8/18/38/38	0/3/3/3
20	ATP	BC	601	21	-	0/18/38/38	0/3/3/3
22	ADP	BD	501	21	-	6/12/32/32	0/3/3/3
22	ADP	BF	501	21	-	5/12/32/32	0/3/3/3
20	ATP	C	601	21	-	2/18/38/38	0/3/3/3
20	ATP	CA	601	21	-	5/18/38/38	0/3/3/3
20	ATP	CB	601	21	-	8/18/38/38	0/3/3/3
20	ATP	CC	601	21	-	0/18/38/38	0/3/3/3
22	ADP	CD	501	21	-	7/12/32/32	0/3/3/3
22	ADP	CF	501	21	-	5/12/32/32	0/3/3/3
22	ADP	D	501	21	-	3/12/32/32	0/3/3/3
22	ADP	F	501	21	-	5/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CD	501	ADP	C2-N3	3.09	1.37	1.32
22	BD	501	ADP	C2-N3	3.04	1.37	1.32
22	F	501	ADP	C5-C4	2.98	1.47	1.40
22	AF	501	ADP	C5-C4	2.98	1.47	1.40
20	AC	601	ATP	C5-C4	2.96	1.47	1.40

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CD	501	ADP	N3-C2-N1	-7.50	116.60	128.68
22	BD	501	ADP	N3-C2-N1	-7.47	116.63	128.68
22	AD	501	ADP	N3-C2-N1	-6.48	118.24	128.68
22	D	501	ADP	N3-C2-N1	-6.46	118.27	128.68
20	C	601	ATP	PA-O3A-PB	-4.27	119.00	132.57

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

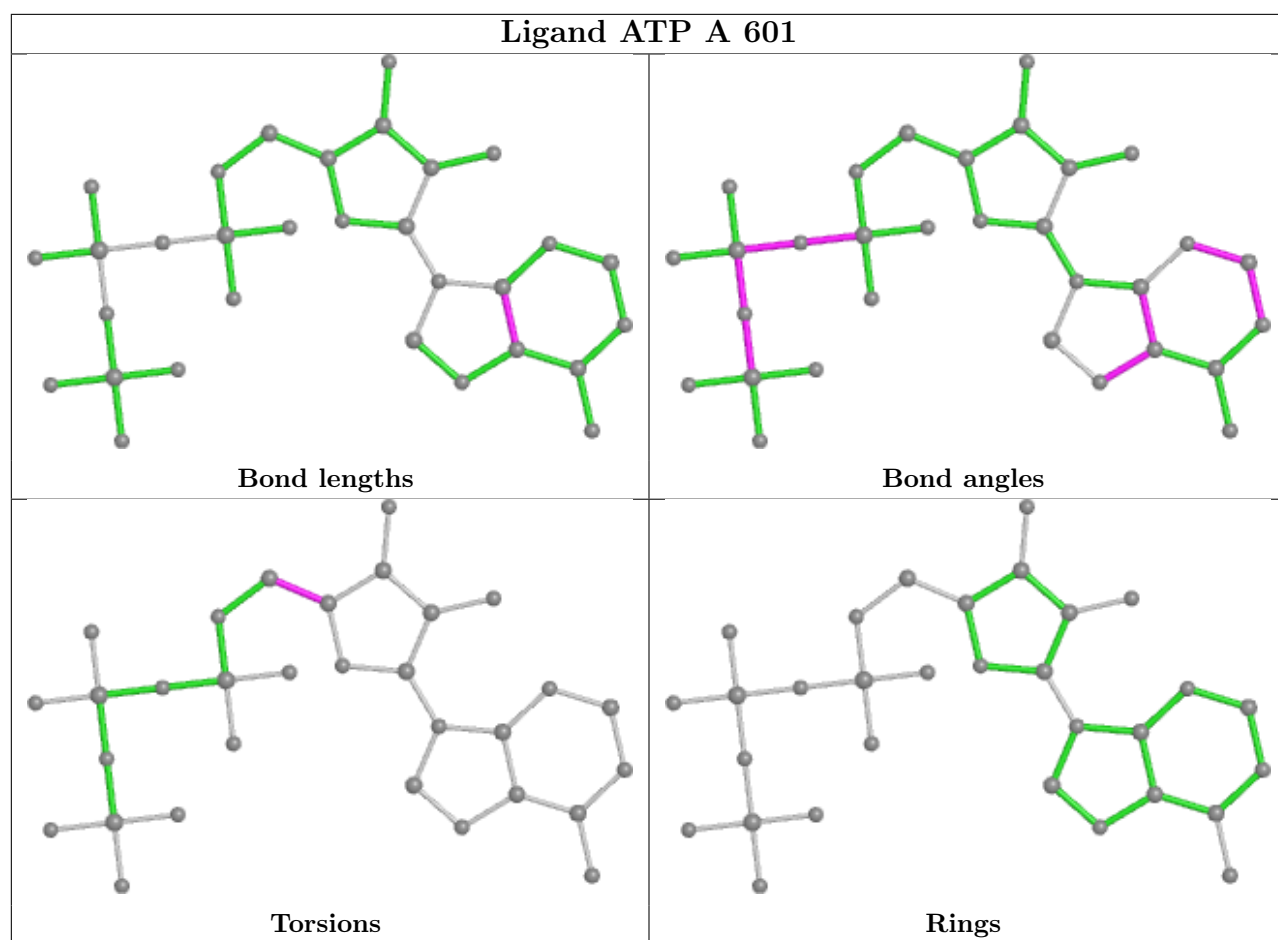
Mol	Chain	Res	Type	Atoms
22	D	501	ADP	C5'-O5'-PA-O1A
22	D	501	ADP	C5'-O5'-PA-O2A
22	D	501	ADP	C5'-O5'-PA-O3A
22	AD	501	ADP	C5'-O5'-PA-O1A
22	AD	501	ADP	C5'-O5'-PA-O2A

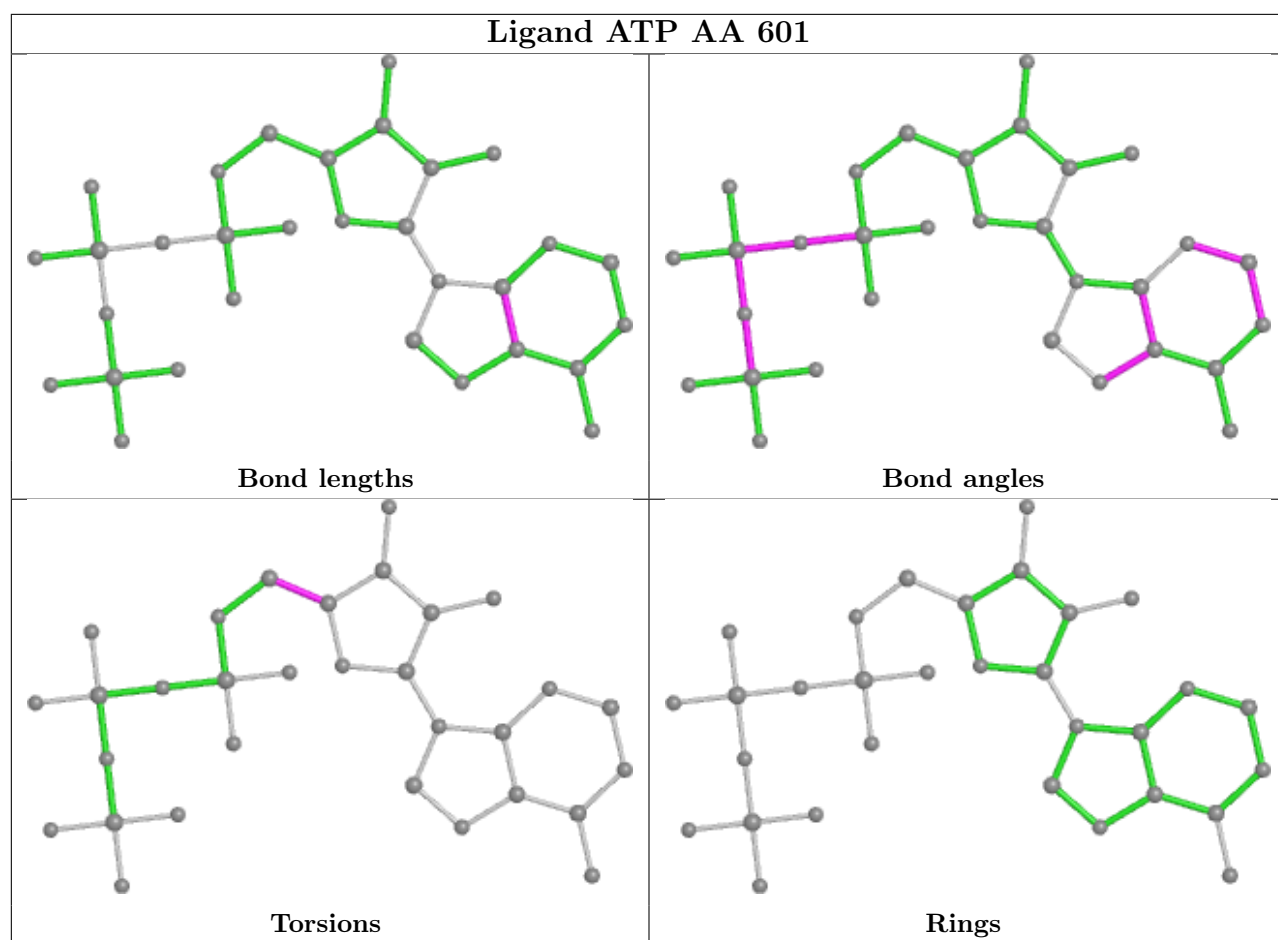
There are no ring outliers.

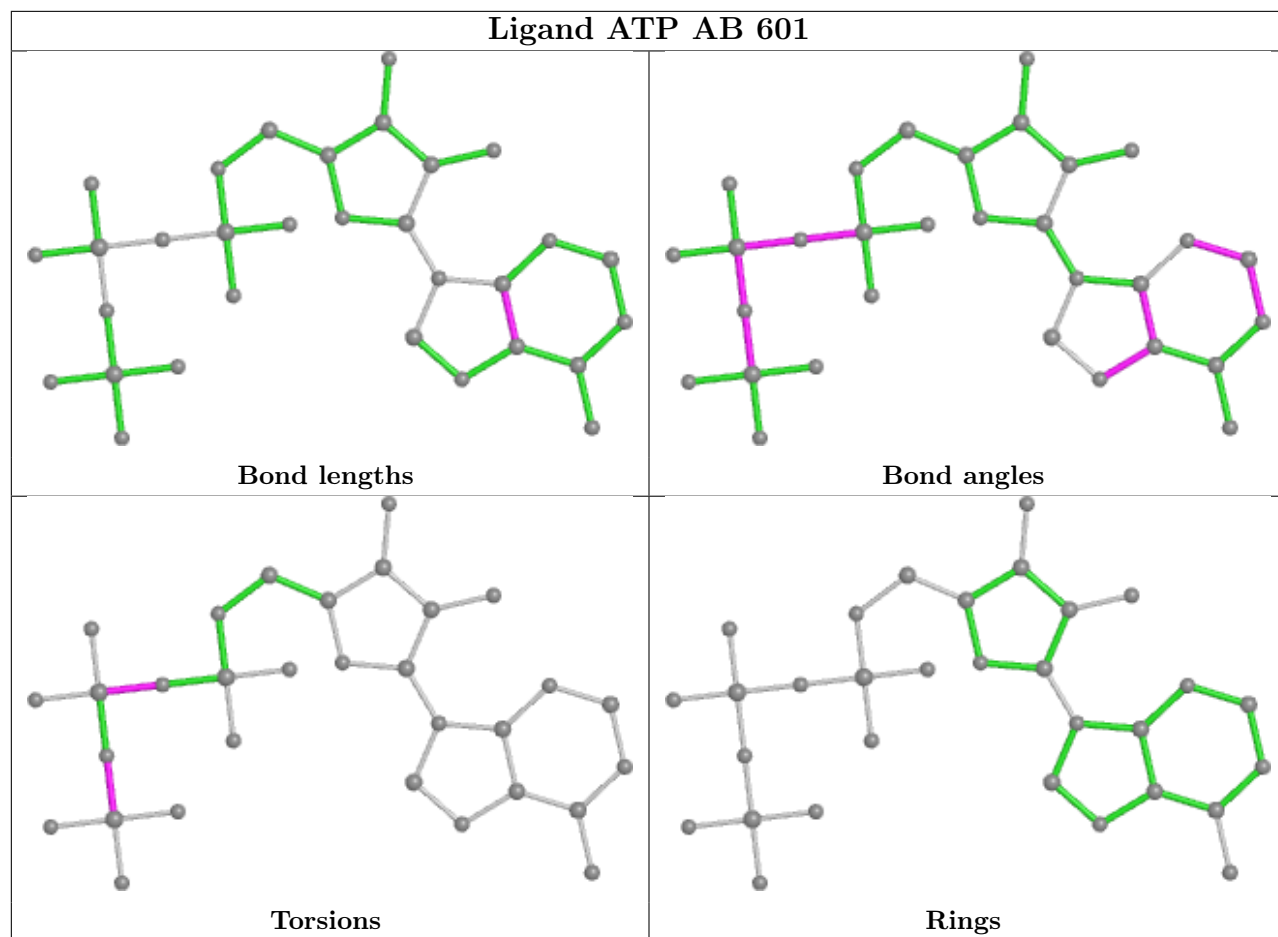
11 monomers are involved in 13 short contacts:

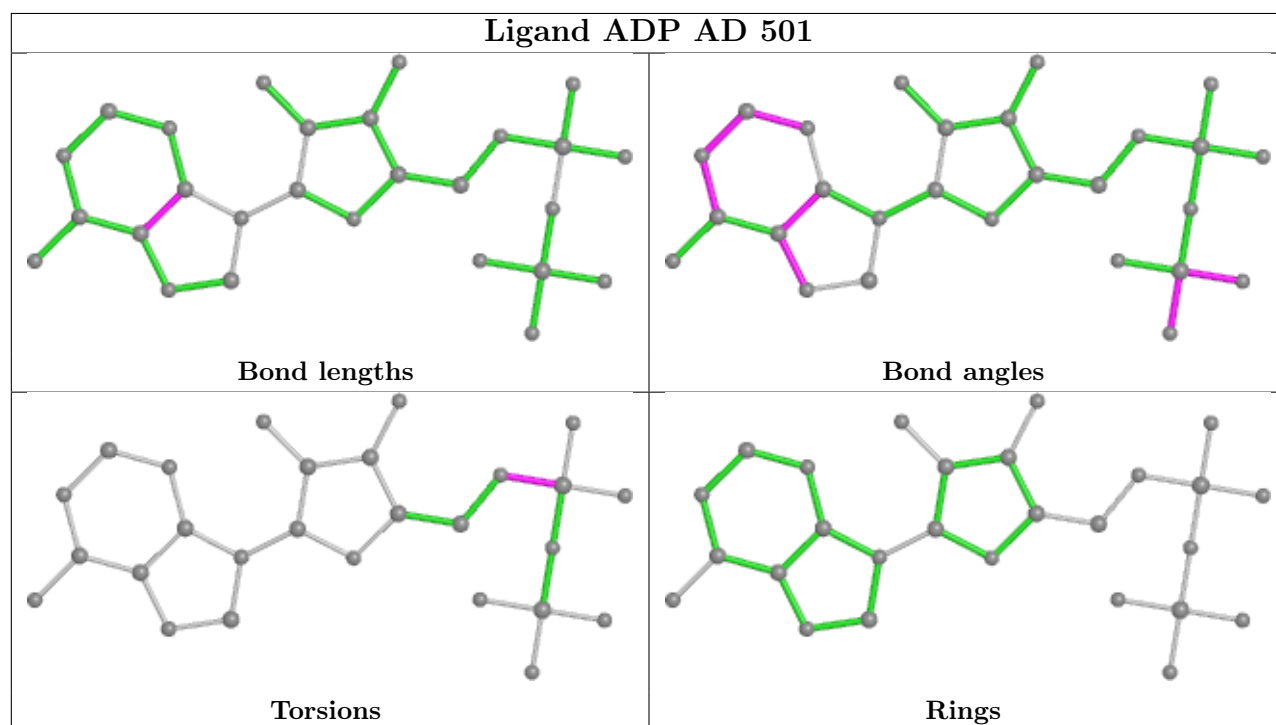
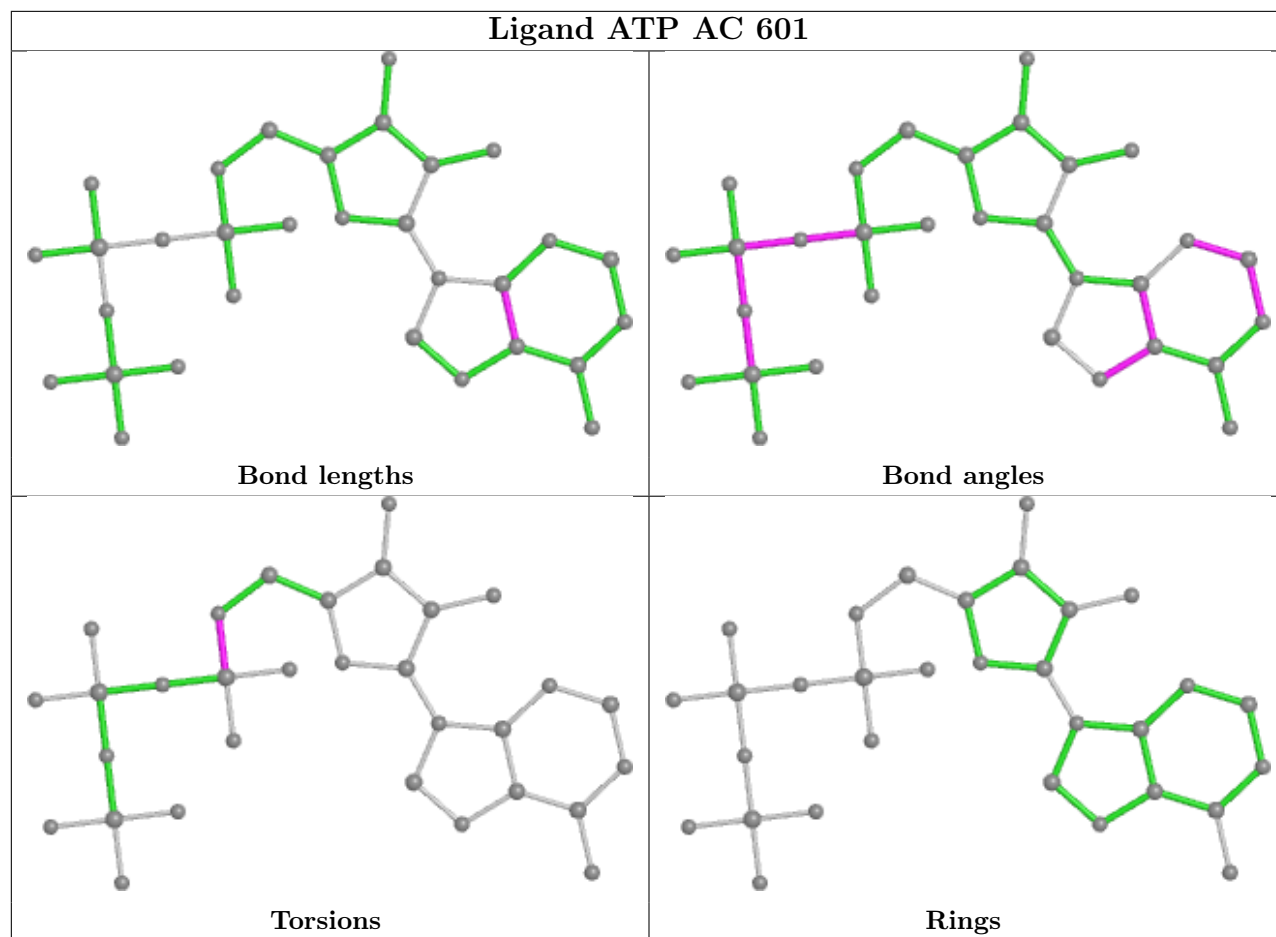
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AD	501	ADP	1	0
20	BA	601	ATP	1	0
20	BB	601	ATP	2	0
20	BC	601	ATP	1	0
22	BD	501	ADP	1	0
22	BF	501	ADP	1	0
20	CA	601	ATP	1	0
20	CB	601	ATP	2	0
20	CC	601	ATP	1	0
22	CD	501	ADP	1	0
22	D	501	ADP	1	0

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

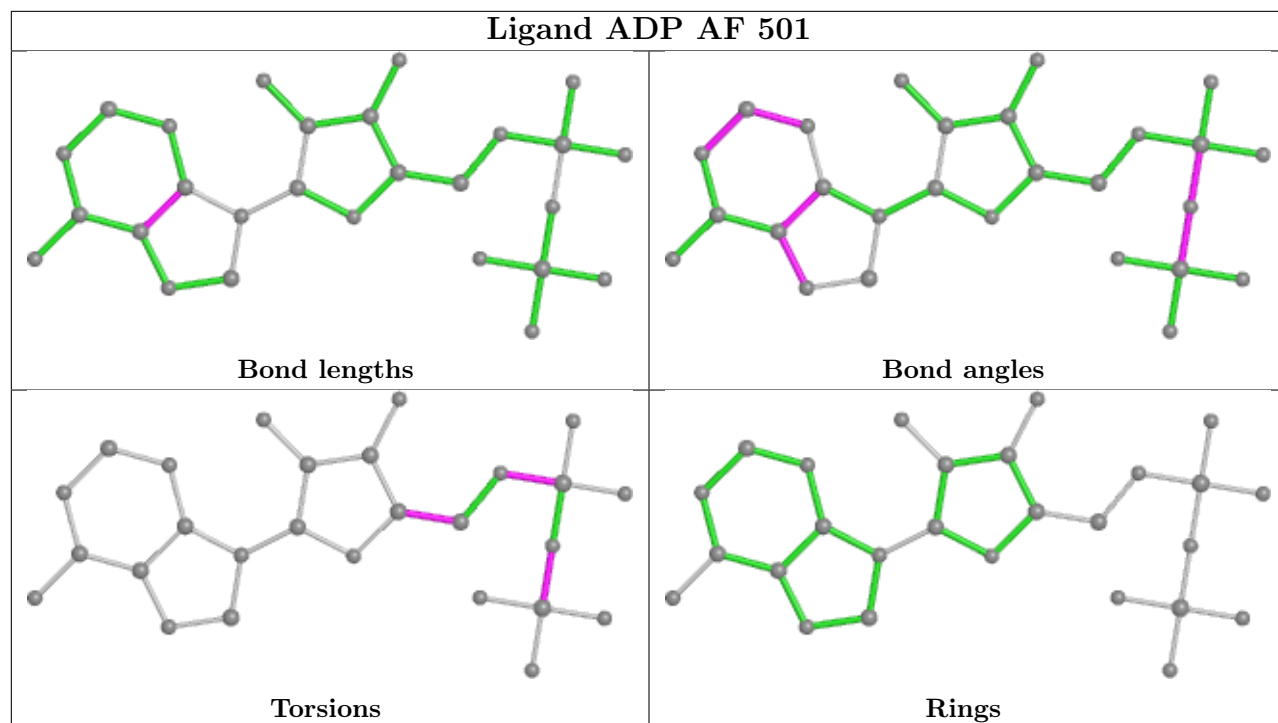




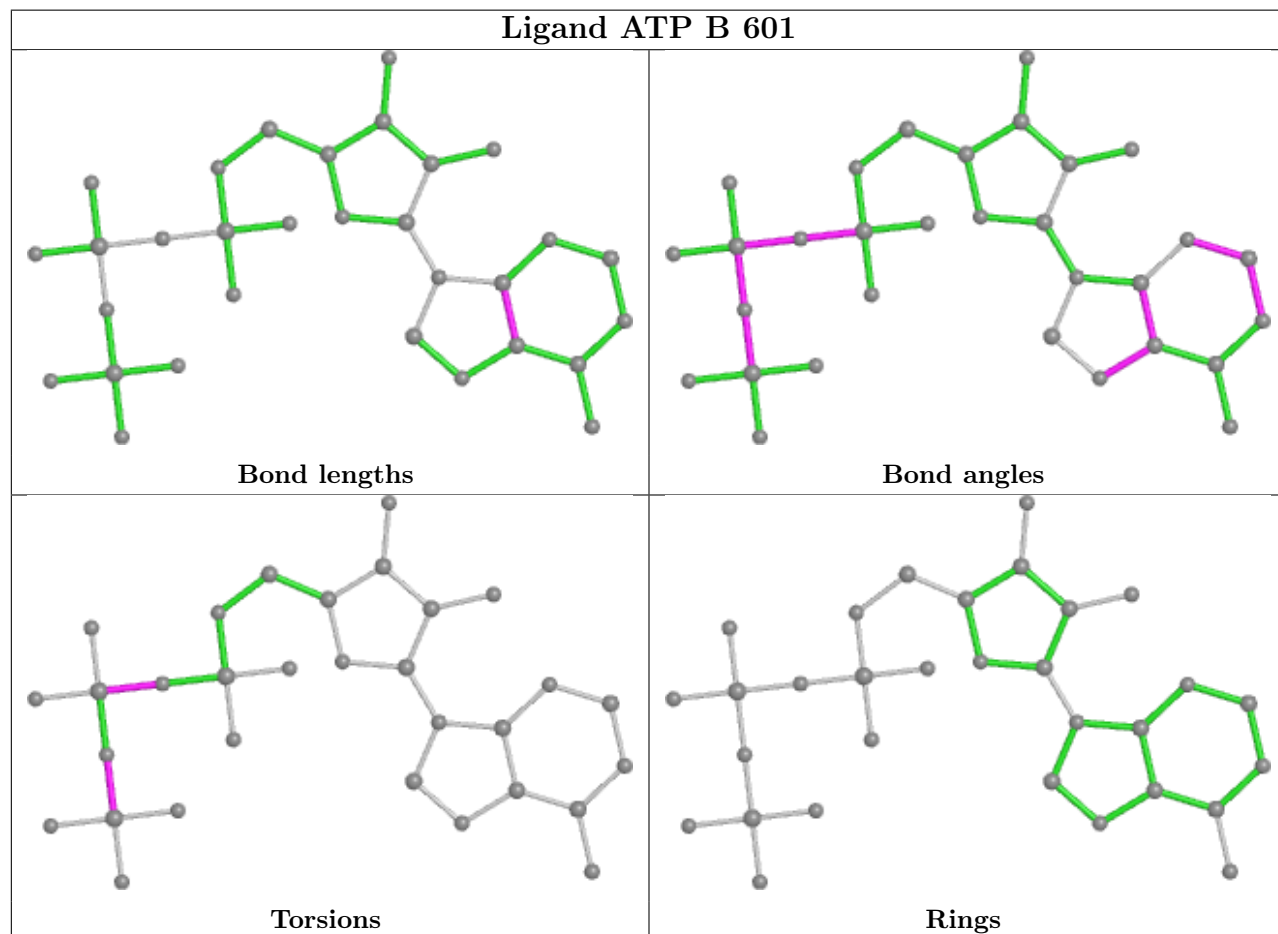


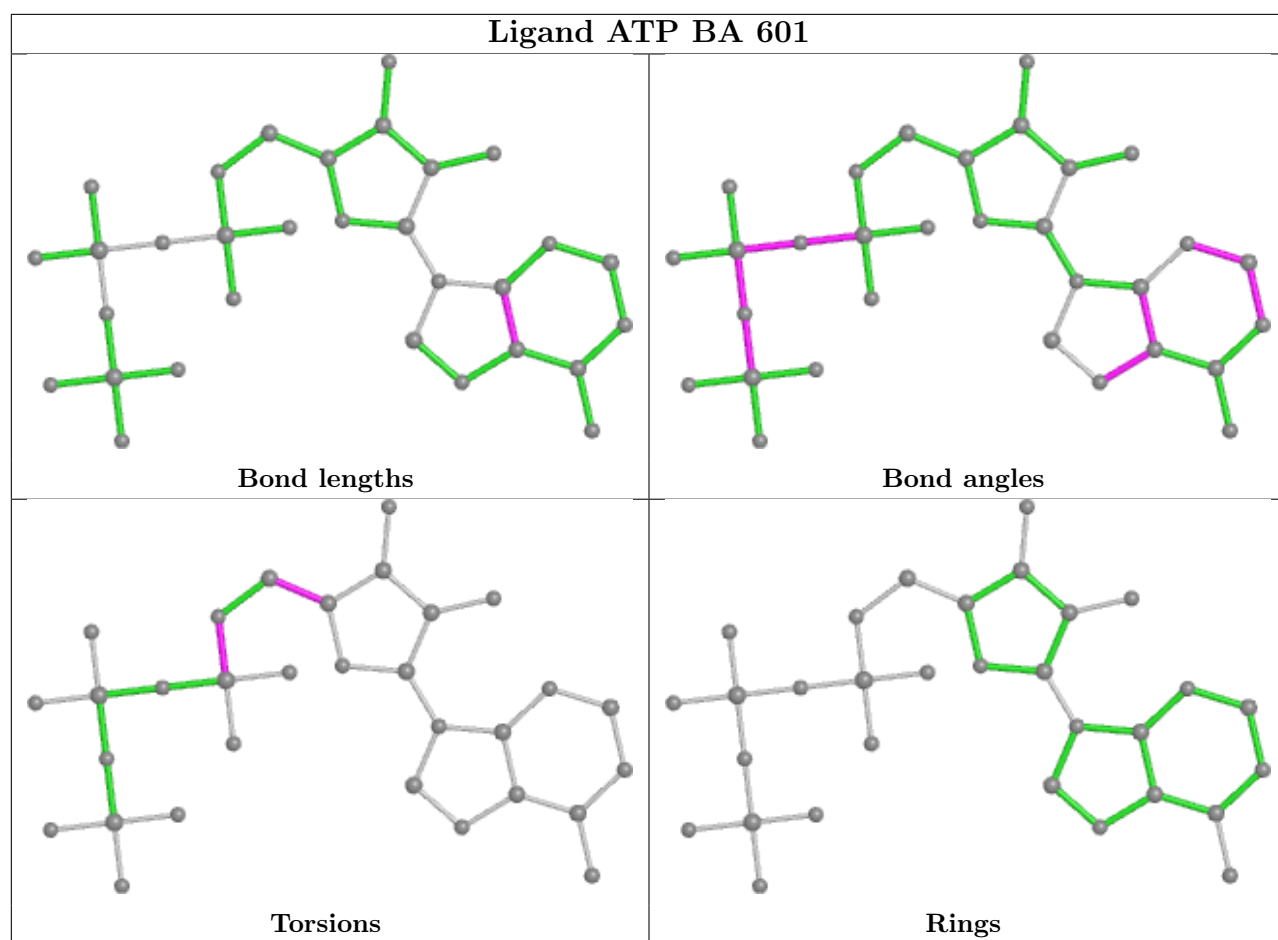


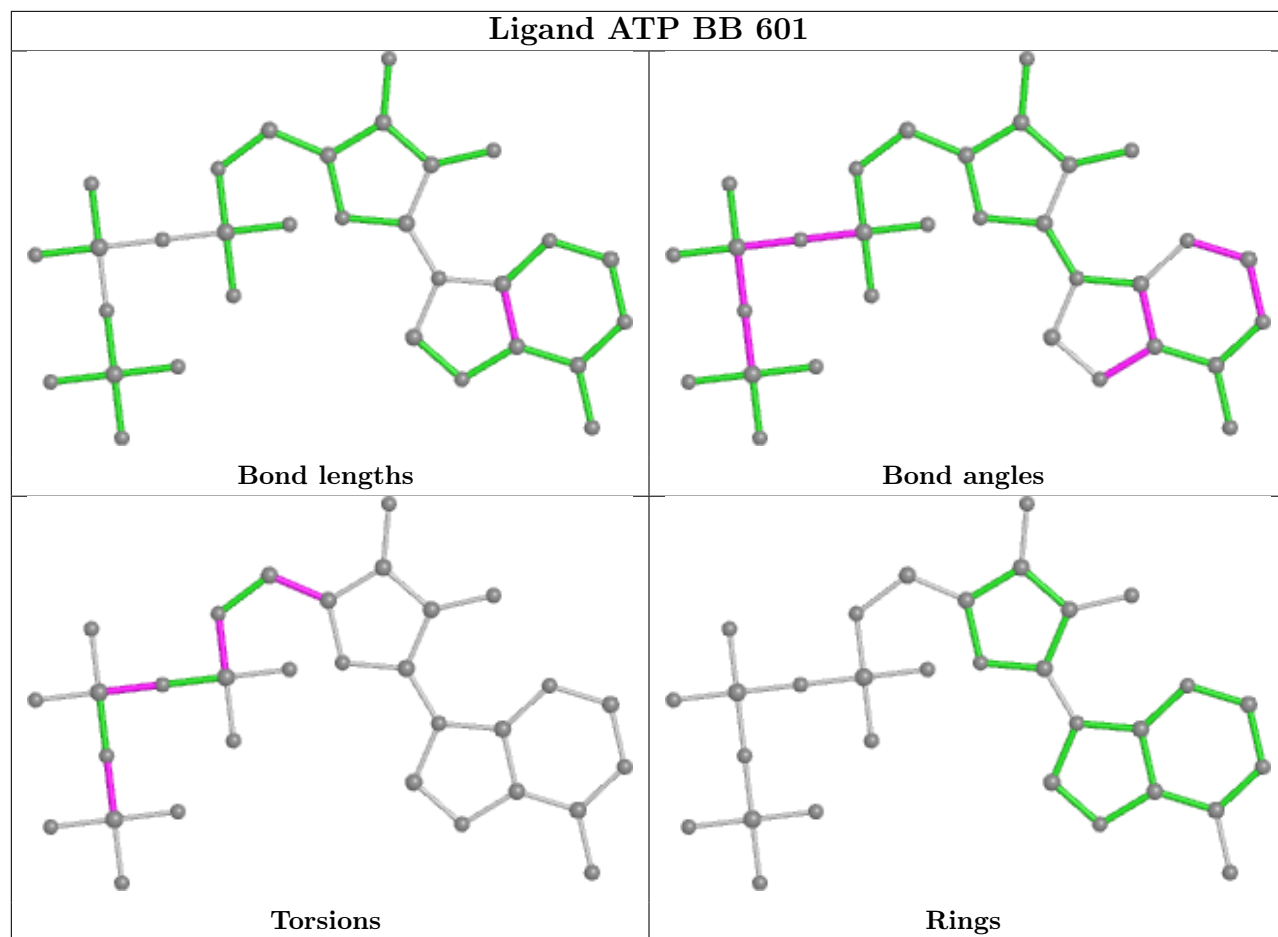
Ligand ADP AF 501

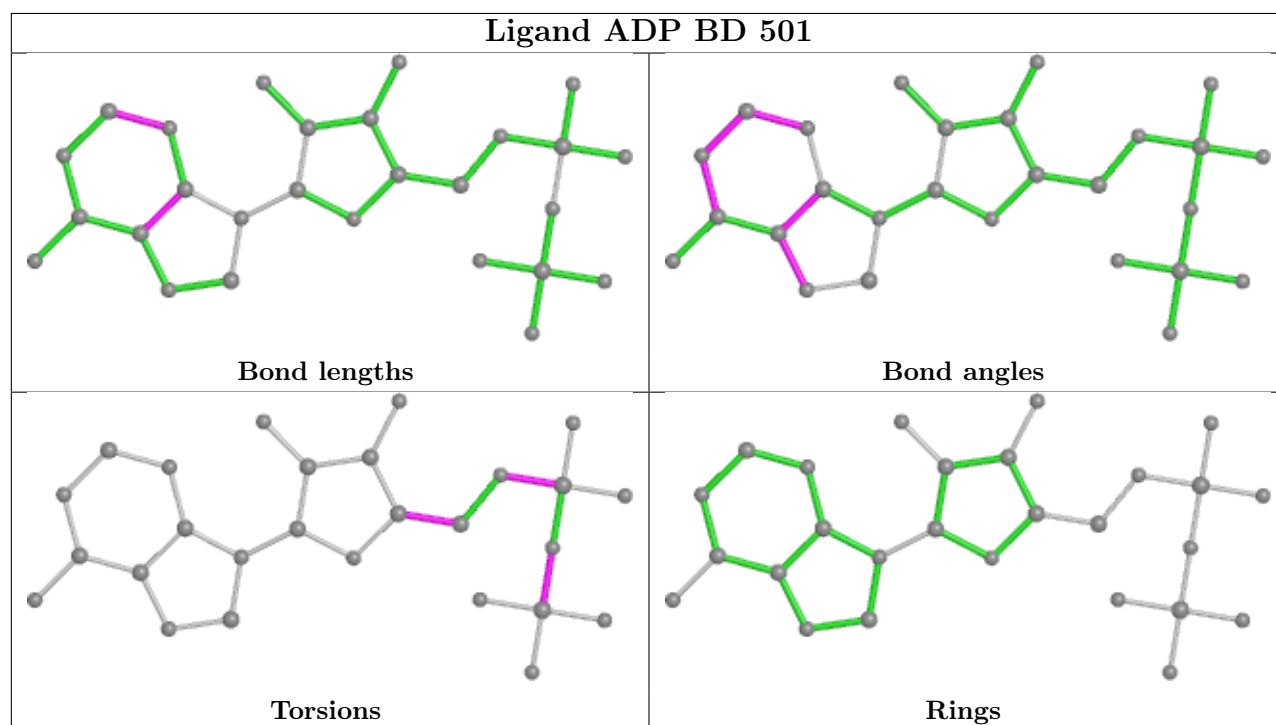
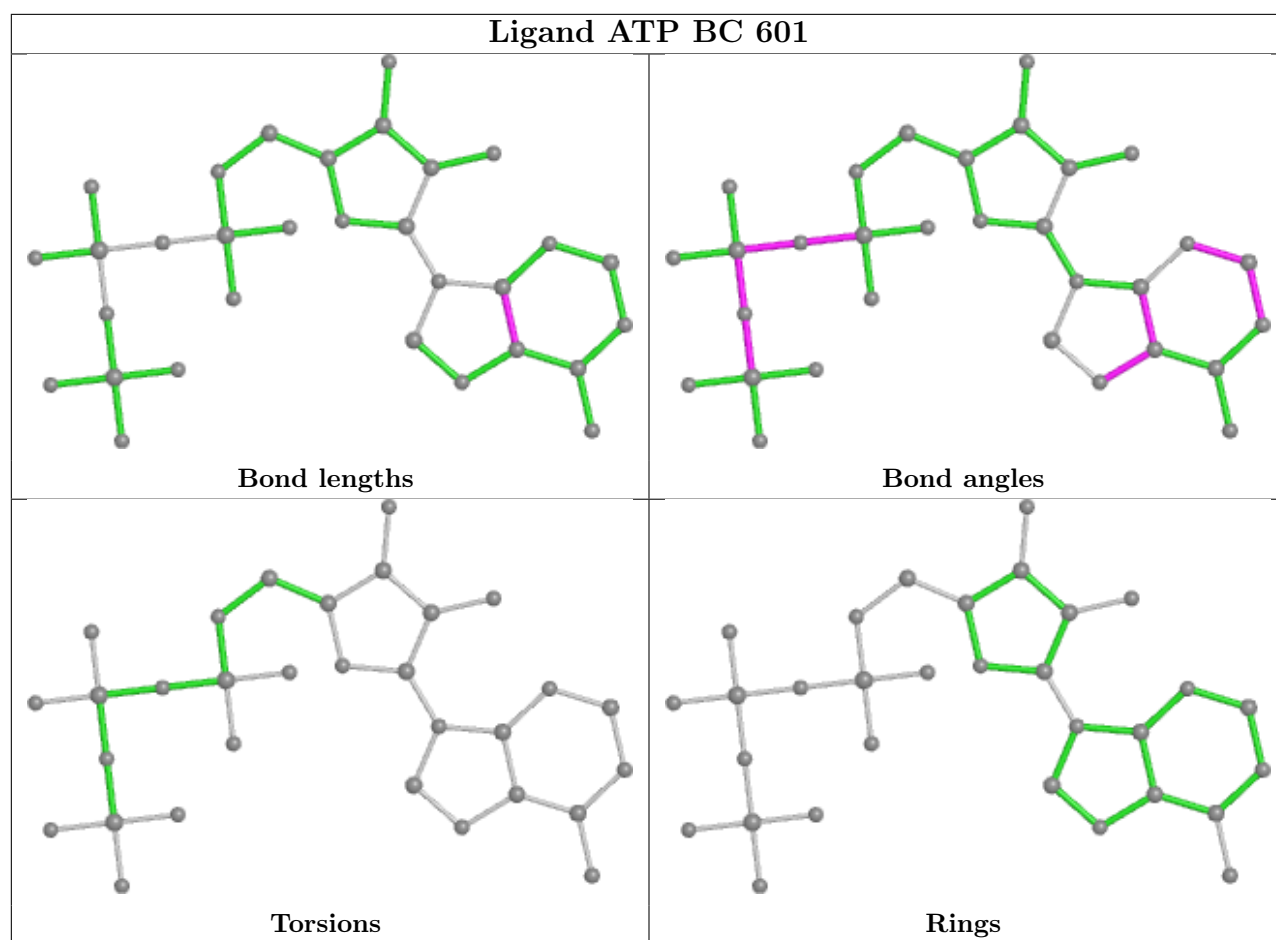


Ligand ATP B 601

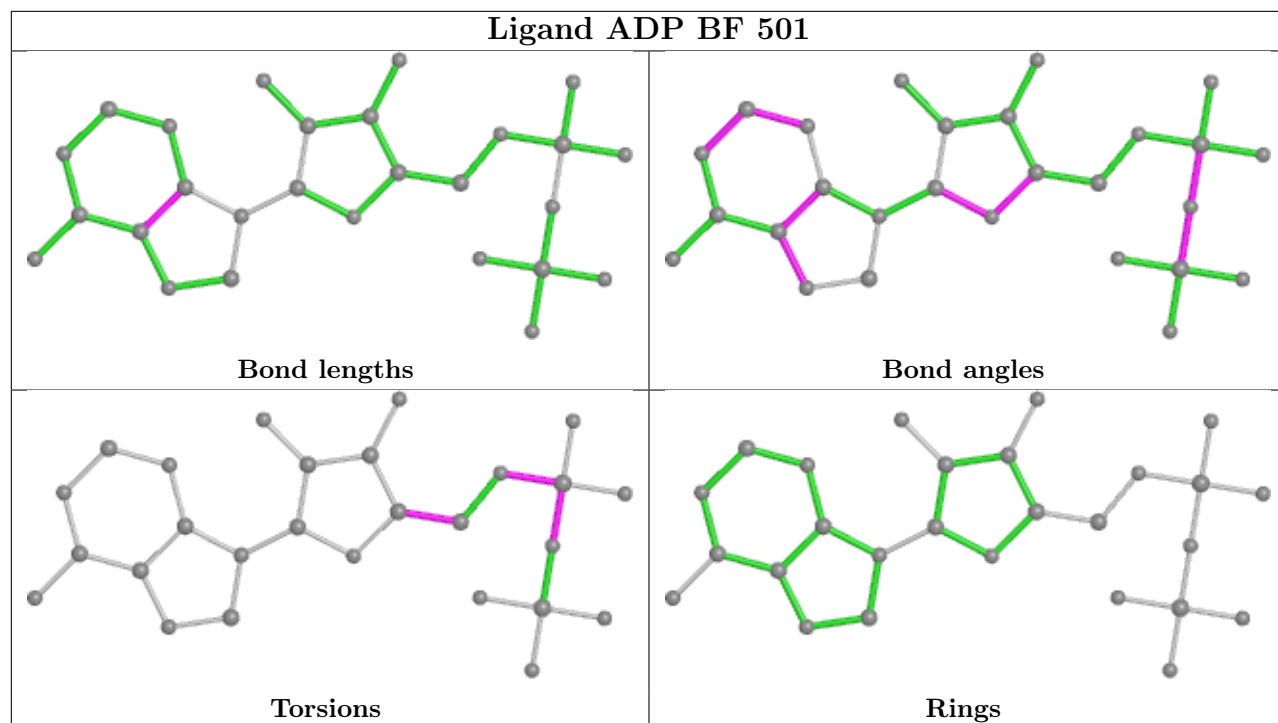




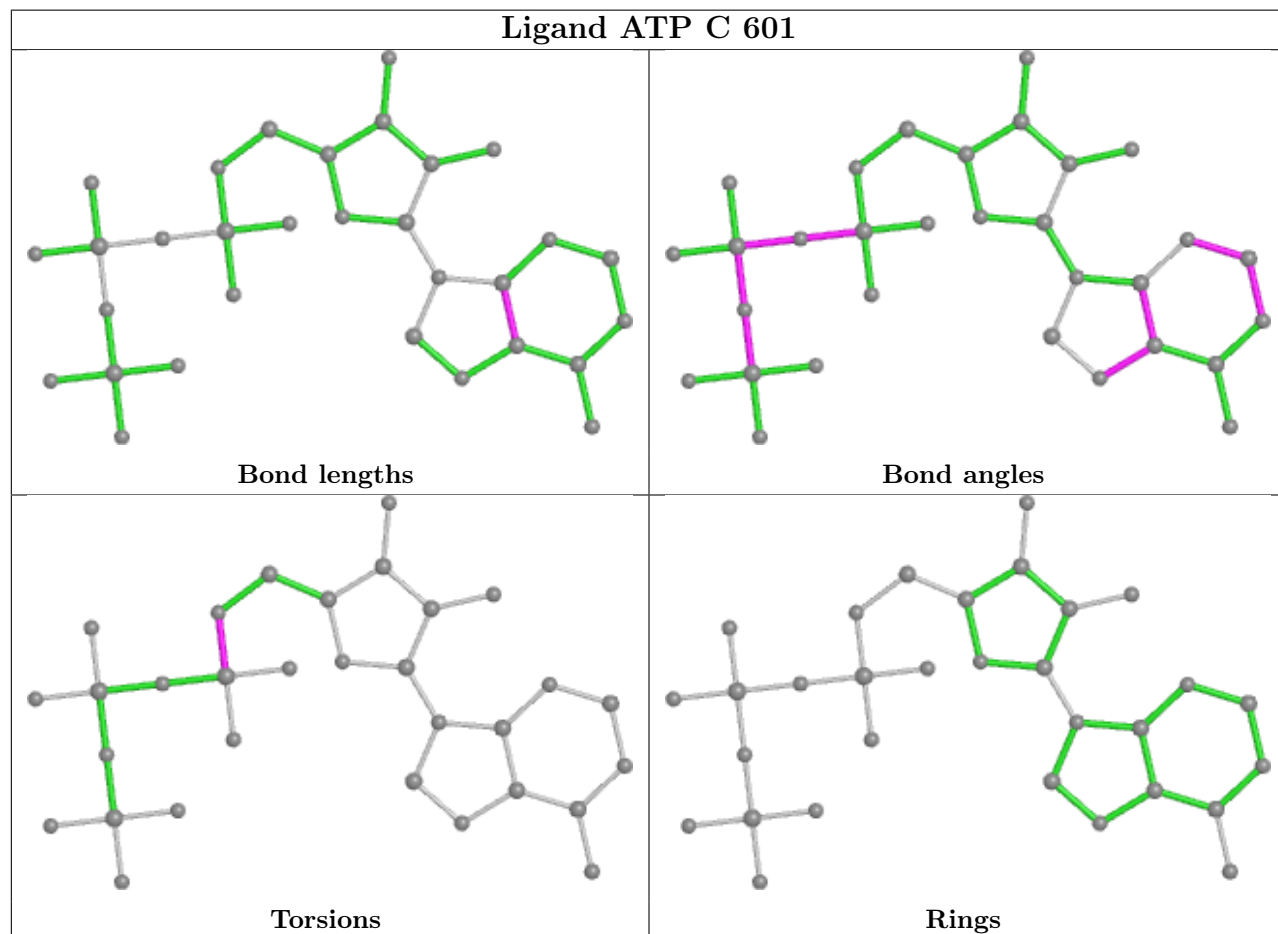


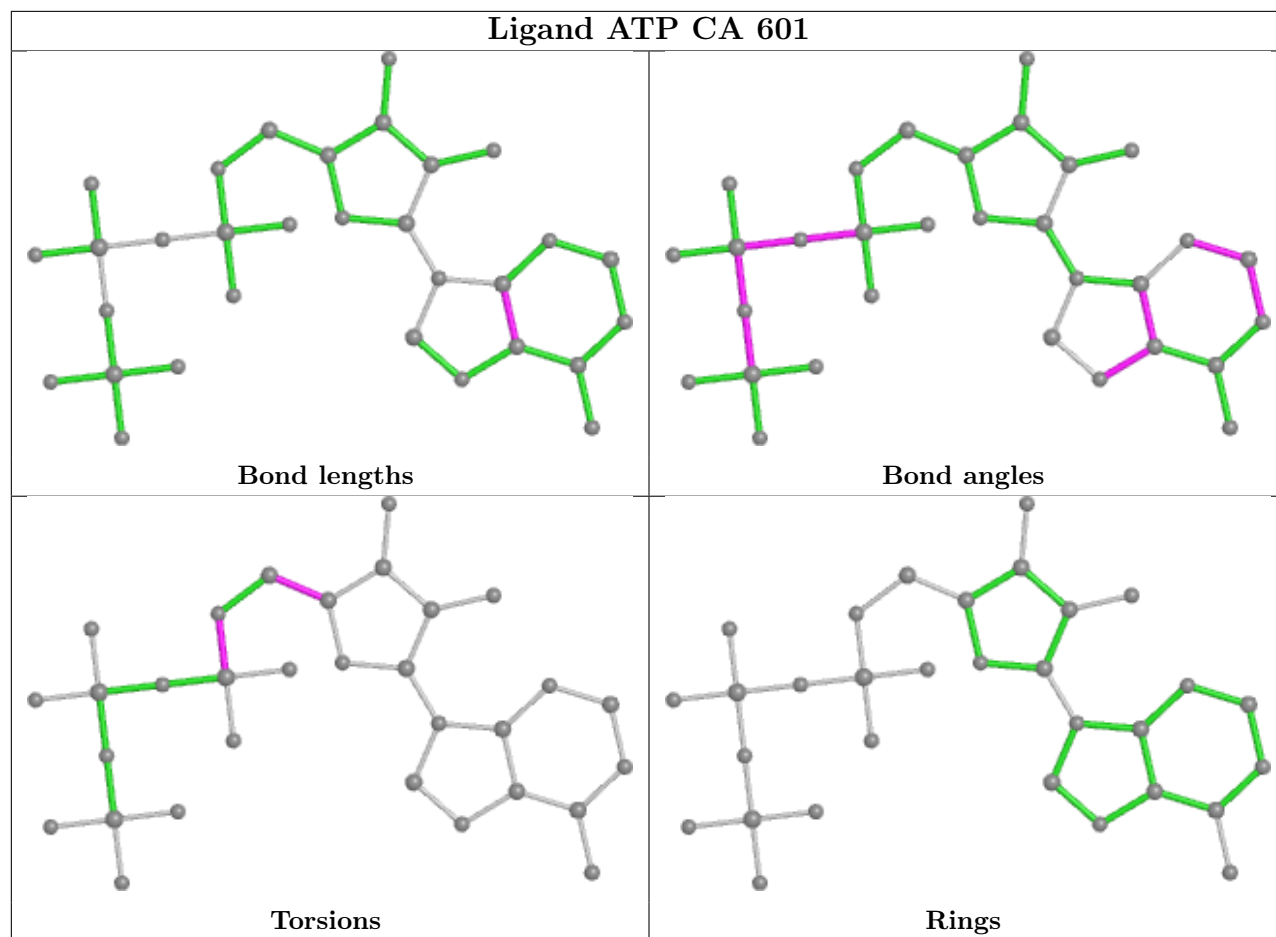


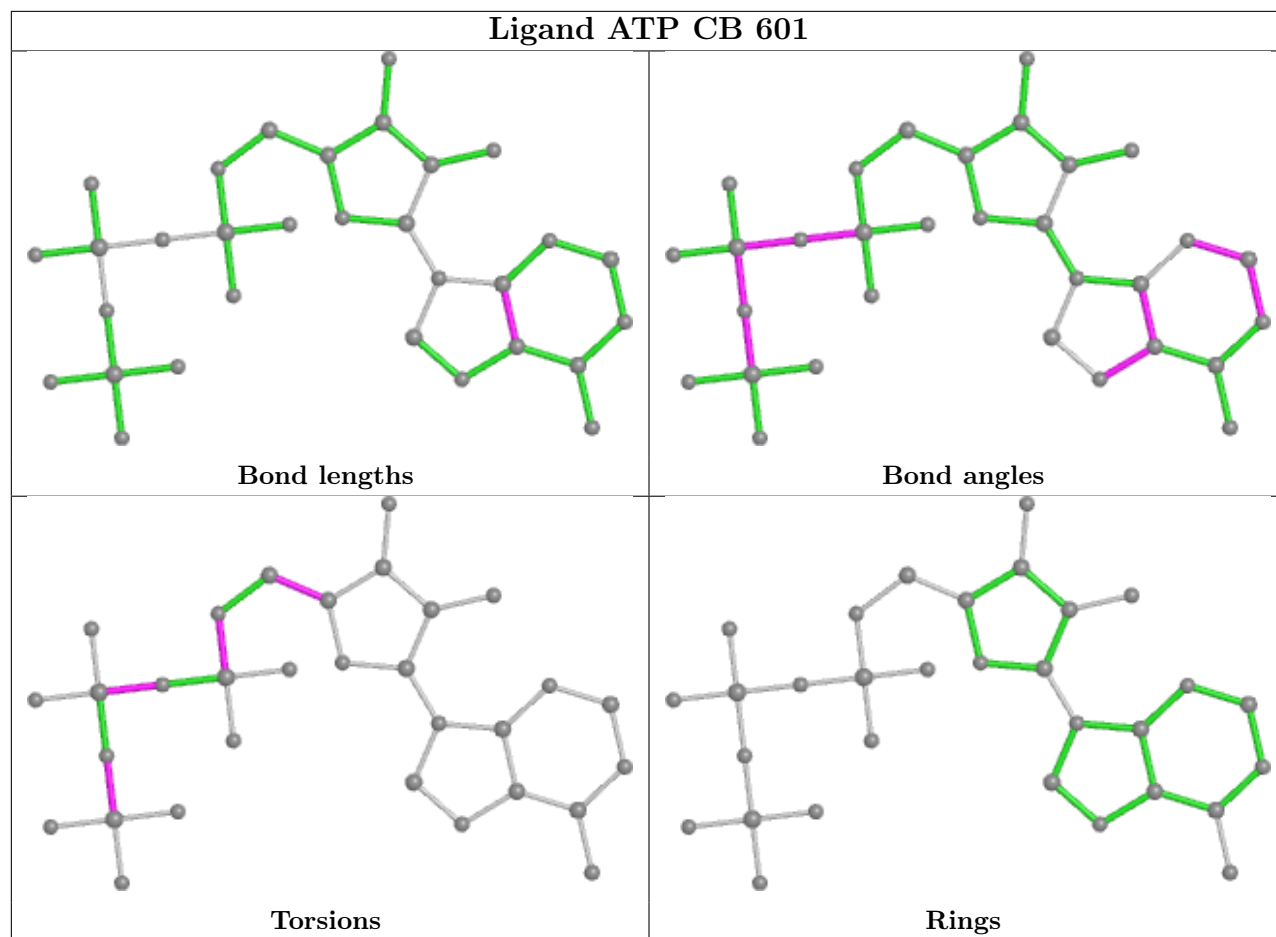
Ligand ADP BF 501

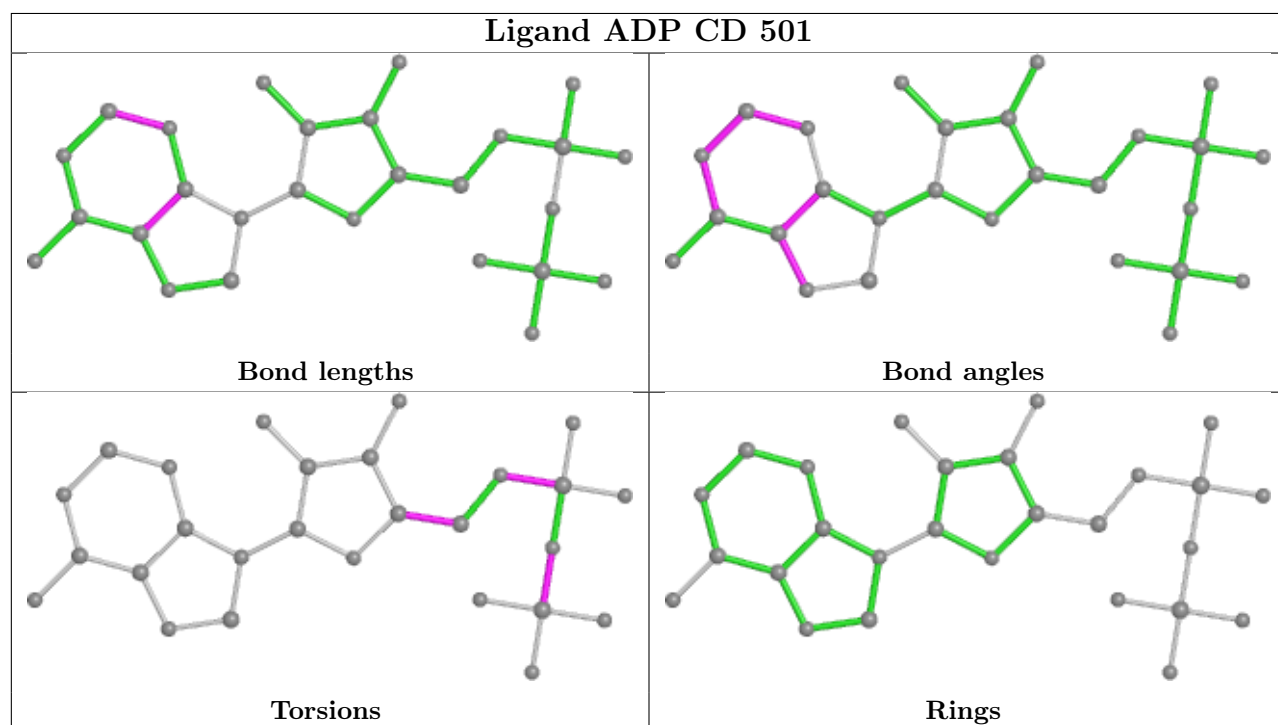
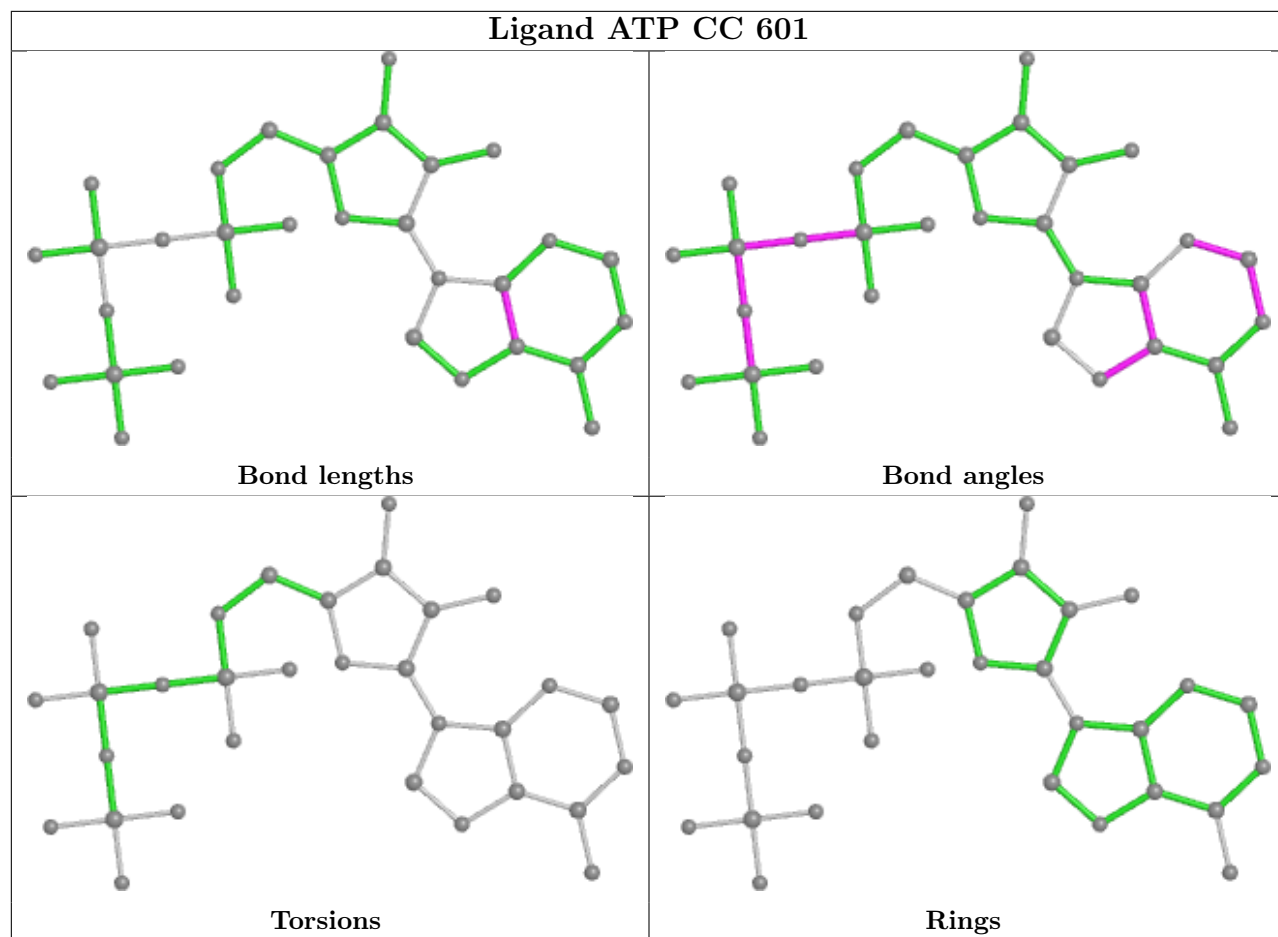


Ligand ATP C 601

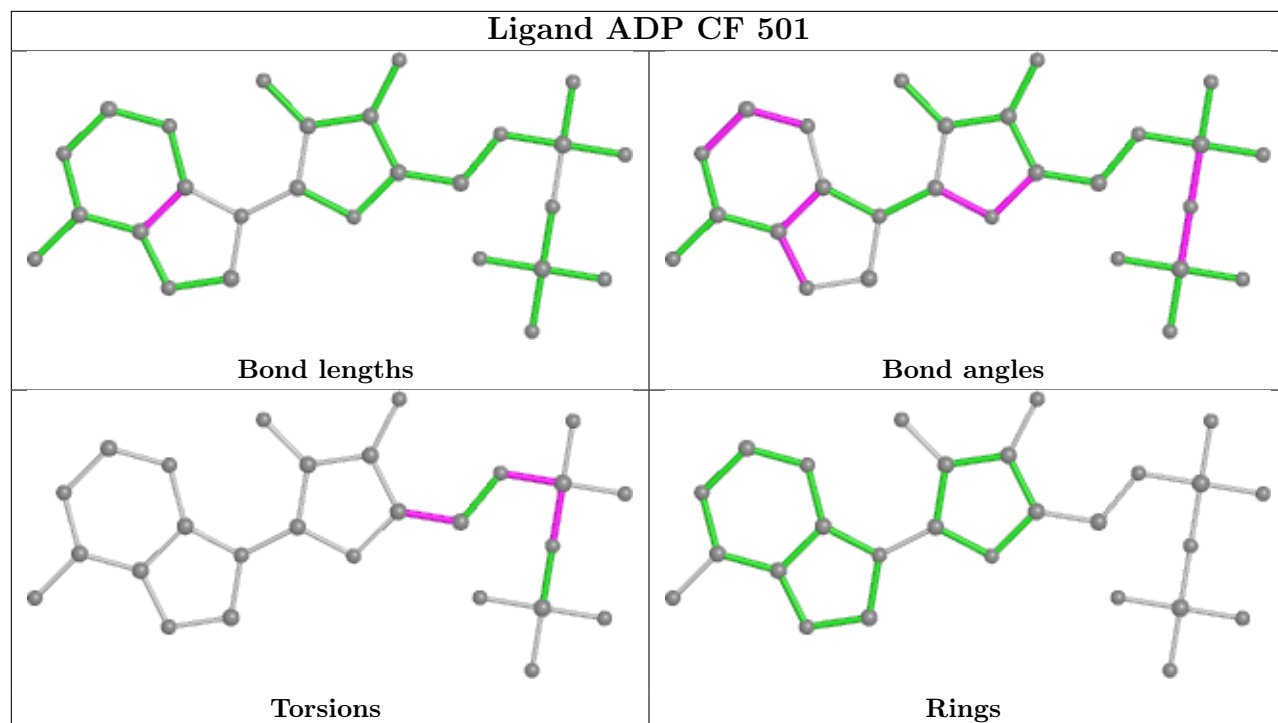




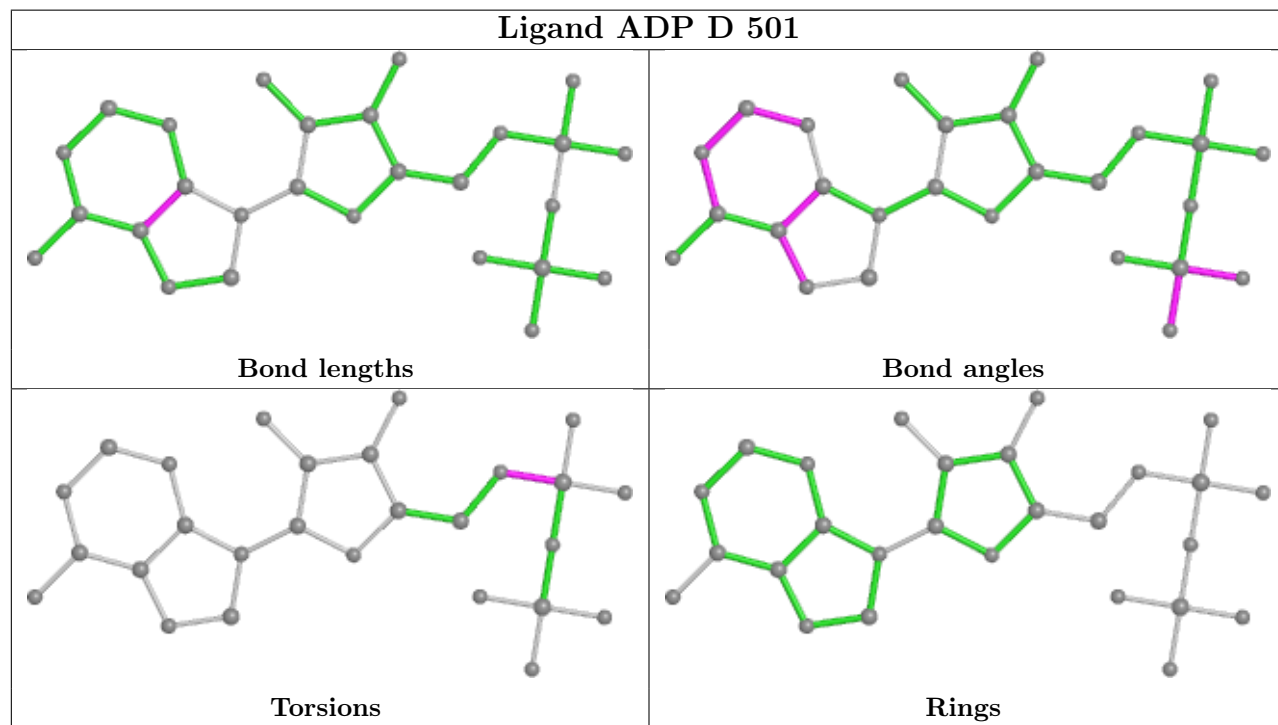


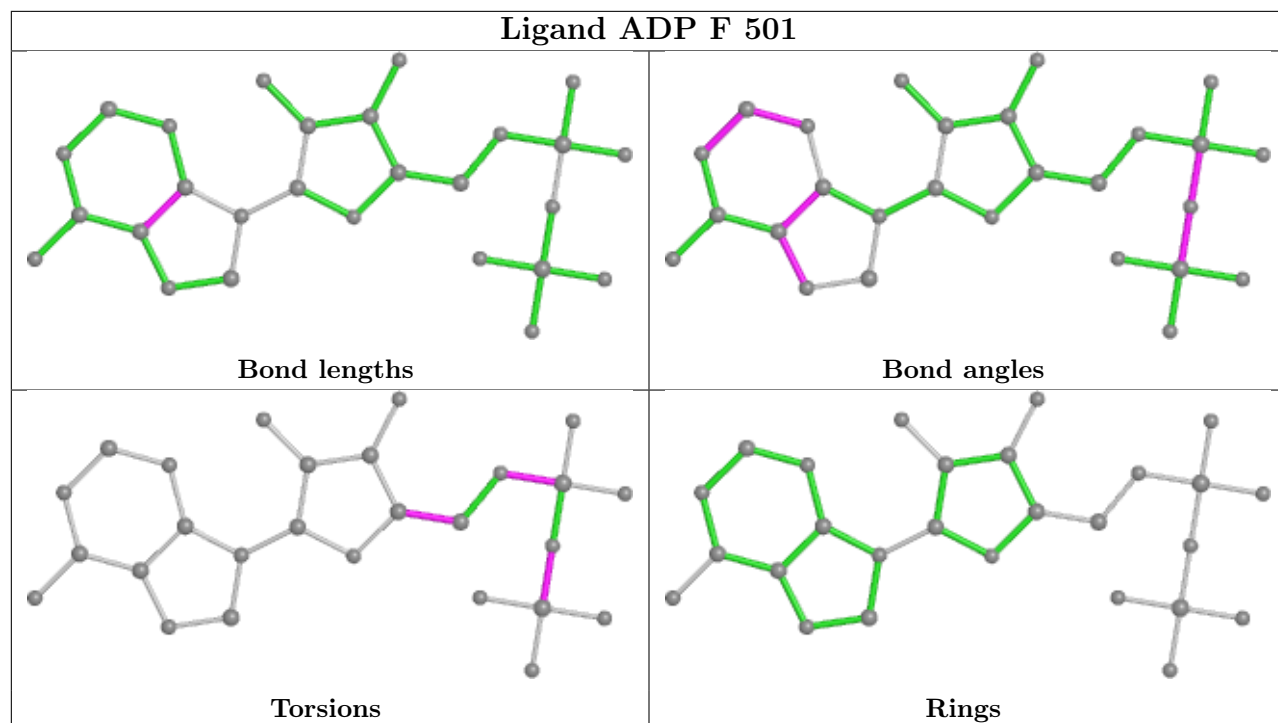


Ligand ADP CF 501



Ligand ADP D 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.