



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 9, 2019 – 02:53 AM EST

PDB ID : 6RDZ  
EMDB ID: : EMD-4836  
Title : Cryo-EM structure of Polytomella F-ATP synthase, Rotary substate 2A, composite map  
Authors : Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.  
Deposited on : 2019-04-12  
Resolution : 3.50 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](mailto: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.

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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

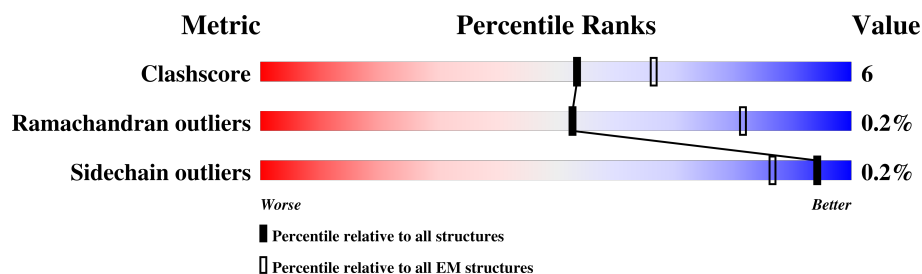
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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.





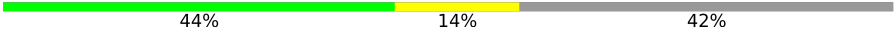
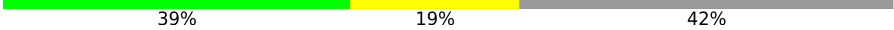
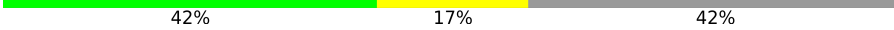
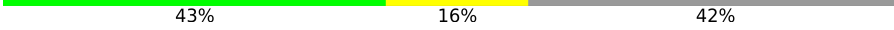
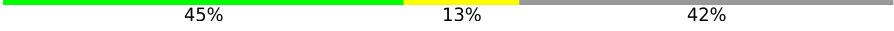
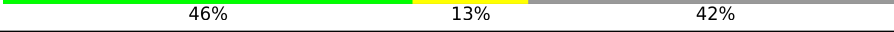
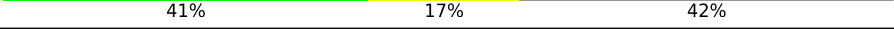
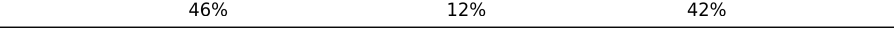

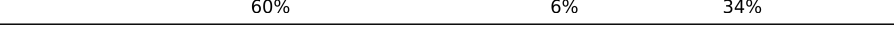







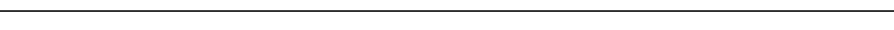

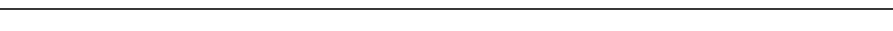
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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  $\geq 3$ , 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	0	82	88% 11% .
2	1	618	86% 11% .
3	2	441	88% 12%
4	3	325	68% 7% 25%
5	4	294	94% . .
6	5	123	86% 14%
7	6	151	75% 7% 18%
8	7	190	79% 14% 7%
9	8	89	87% 12% .

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Mol	Chain	Length	Quality of chain
10	9	97	 94% 6%
11	A	127	 49% 9% 42%
11	B	127	 44% 14% 42%
11	C	127	 39% 19% 42%
11	D	127	 42% 17% 42%
11	E	127	 43% 16% 42%
11	F	127	 45% 13% 42%
11	G	127	 46% 13% 42%
11	H	127	 41% 17% 42%
11	I	127	 46% 12% 42%
11	J	127	 50% 8% 42%
12	M	327	 60% 6% 34%
13	P	229	 69% 15% 16%
14	Q	74	 74% 23% .
15	R	199	 70% 19% 11%
16	S	317	 70% 17% 13%
17	T	562	 81% 11% . 7%
17	U	562	 77% 15% 7%
17	V	562	 77% 16% 7%
18	X	574	 82% 11% 6%
18	Y	574	 76% 14% 9%
18	Z	574	 79% 15% 6%

## 2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 53720 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 ASA-10: Polytomella F-ATP synthase associated subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	81	Total	C	N	O	S	0	0
			607	388	107	110	2		

- Molecule 2 is a protein called ATP synthase associated protein ASA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	595	Total	C	N	O	S	0	0
			4661	2958	798	900	5		

- Molecule 3 is a protein called ASA-2: Polytomella F-ATP synthase associated subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	2	441	Total	C	N	O	0	0
			3163	2020	532	611		

- Molecule 4 is a protein called Mitochondrial F1F0 ATP synthase associated 32 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	245	Total	C	N	O	S	0	0
			1874	1204	299	370	1		

- Molecule 5 is a protein called Mitochondrial ATP synthase associated protein ASA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	290	Total	C	N	O	S	0	0
			2177	1385	356	434	2		

- Molecule 6 is a protein called Mitochondrial F1F0 ATP synthase associated 14 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	123	Total	C	N	O	S	0	0
			986	640	172	170	4		

- Molecule 7 is a protein called Mitochondrial ATP synthase subunit ASA6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	124	Total	C	N	O	S	0	0
			926	599	154	172	1		

- Molecule 8 is a protein called Mitochondrial ATP synthase associated protein ASA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	176	Total	C	N	O	S	0	0
			1347	860	227	259	1		

- Molecule 9 is a protein called Mitochondrial ATP synthase subunit ASA8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	8	88	Total	C	N	O	0	0
			692	456	115	121		

- Molecule 10 is a protein called ASA-9: Polytomella F-ATP synthase associated subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	97	Total	C	N	O	S	0	0
			776	514	124	132	6		

- Molecule 11 is a protein called Mitochondrial ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	B	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	C	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	D	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	E	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	F	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	G	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	H	74	Total	C	N	O	S	0	0
			514	340	83	88	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	J	74	Total	C	N	O	S	0	0
			514	340	83	88	3		

- Molecule 12 is a protein called Mitochondrial ATP synthase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	217	Total	C	N	O	S	0	0
			1640	1077	267	288	8		

- Molecule 13 is a protein called Mitochondrial ATP synthase subunit OSCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	193	Total	C	N	O	S	0	0
			1532	988	250	290	4		

- Molecule 14 is a protein called epsilon: Polytomella F-ATP synthase epsilon subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	72	Total	C	N	O	S	0	0
			561	358	102	99	2		

- Molecule 15 is a protein called Mitochondrial ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	177	Total	C	N	O	S	0	0
			1303	833	213	256	1		

- Molecule 16 is a protein called ATP synthase gamma chain, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	277	Total	C	N	O	S	0	0
			2130	1327	377	416	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	523	Total	C	N	O	S	0	0
			3979	2537	703	728	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	523	Total	C	N	O	S	0	0
			3978	2537	702	728	11		
17	V	520	Total	C	N	O	S	0	0
			3961	2527	700	723	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	266	ARG	LYS	conflict	UNP A0ZW40
U	266	ARG	LYS	conflict	UNP A0ZW40
V	266	ARG	LYS	conflict	UNP A0ZW40

- Molecule 18 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	538	Total	C	N	O	S	0	0
			4087	2568	692	814	13		
18	Y	520	Total	C	N	O	S	0	0
			3952	2484	669	786	13		
18	Z	539	Total	C	N	O	S	0	0
			4095	2572	693	817	13		

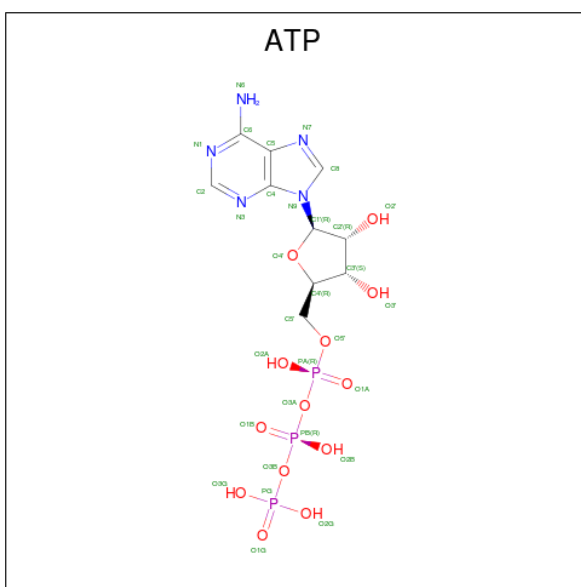
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	350	ALA	GLY	conflict	UNP A0ZW41
X	387	LEU	ARG	conflict	UNP A0ZW41
Y	350	ALA	GLY	conflict	UNP A0ZW41
Y	387	LEU	ARG	conflict	UNP A0ZW41
Z	350	ALA	GLY	conflict	UNP A0ZW41
Z	387	LEU	ARG	conflict	UNP A0ZW41

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	M	1	Total	Zn	0
			1	1	

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



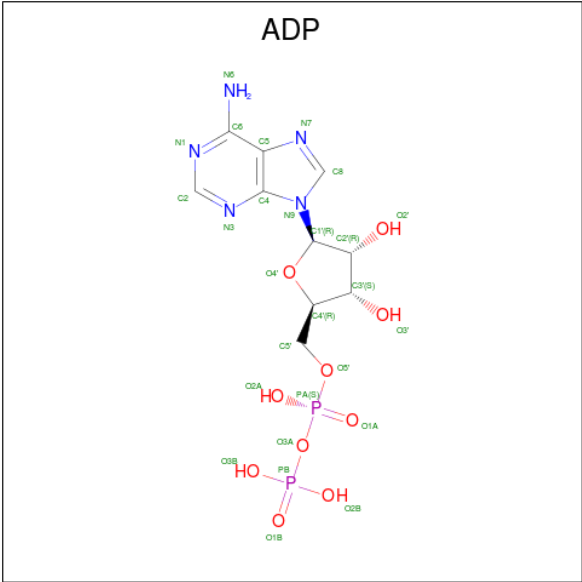
Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total 31	C 10	N 5	O 13	P 3	0
20	U	1	Total 31	C 10	N 5	O 13	P 3	0
20	V	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
21	Z	1	Total Mg 1 1	0
21	Y	1	Total Mg 1 1	0
21	T	1	Total Mg 1 1	0
21	V	1	Total Mg 1 1	0
21	U	1	Total Mg 1 1	0

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).






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

### 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.

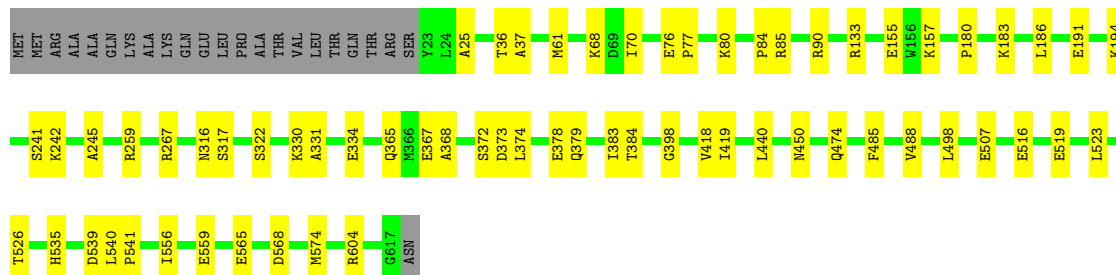
- Molecule 1: ASA-10: *Polytomella* F-ATP synthase associated subunit 10

Chain 0: 




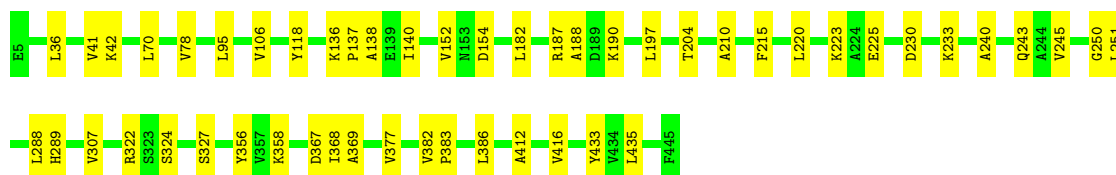
- Molecule 2: ATP synthase associated protein ASA1

Chain 1: 



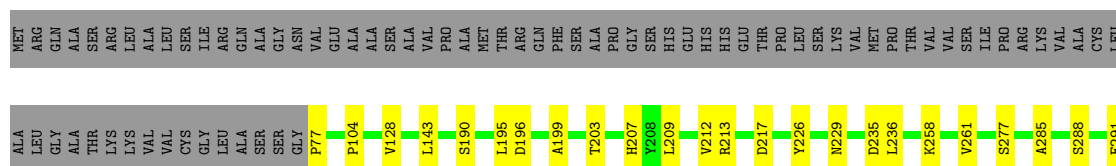
- Molecule 3: ASA-2: *Polytomella* F-ATP synthase associated subunit 2

Chain 2: 



- Molecule 4: Mitochondrial F1F0 ATP synthase associated 32 kDa protein

Chain 3: 





- Molecule 5: Mitochondrial ATP synthase associated protein ASA4

Chain 4: 94%



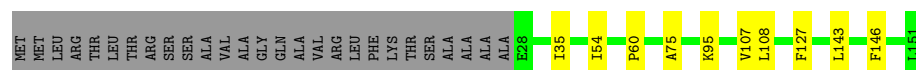
- Molecule 6: Mitochondrial F1F0 ATP synthase associated 14 kDa protein

Chain 5: 86%



- Molecule 7: Mitochondrial ATP synthase subunit ASA6

Chain 6: 75%



- Molecule 8: Mitochondrial ATP synthase associated protein ASA7

Chain 7: 79%



- Molecule 9: Mitochondrial ATP synthase subunit ASA8

Chain 8: 87%



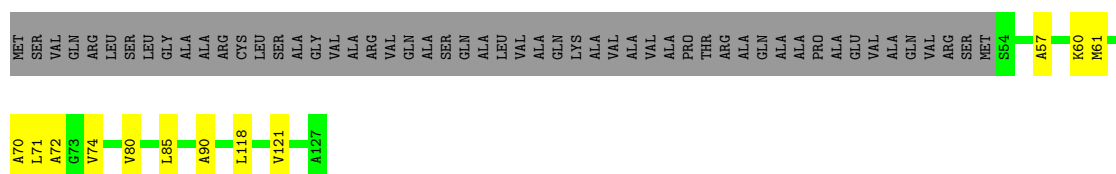
- Molecule 10: ASA-9: Polytomella F-ATP synthase associated subunit 9

Chain 9: 94%

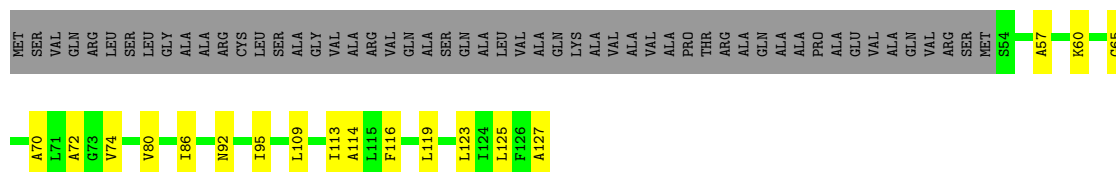


- Molecule 11: Mitochondrial ATP synthase subunit c

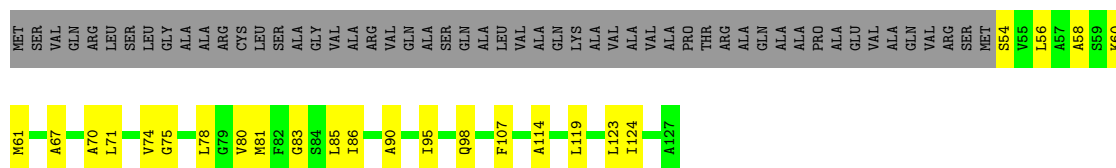
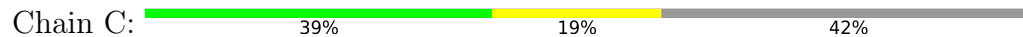
Chain A: 49%



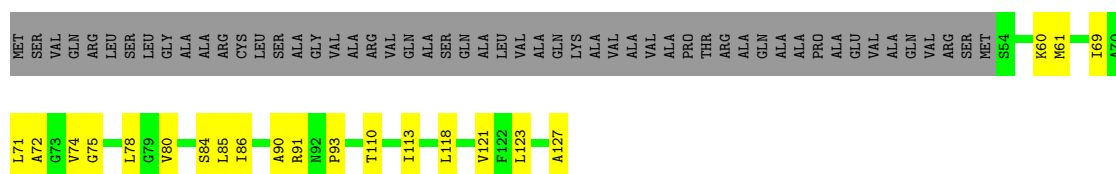
- Molecule 11: Mitochondrial ATP synthase subunit c



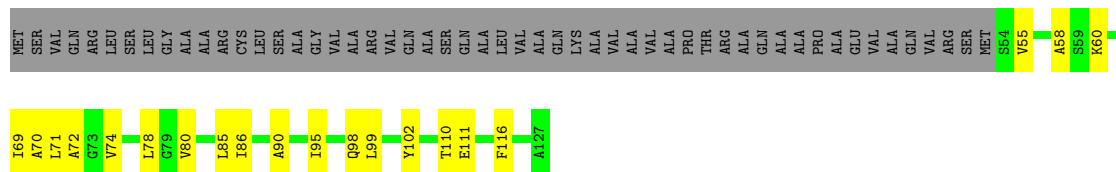
- Molecule 11: Mitochondrial ATP synthase subunit c



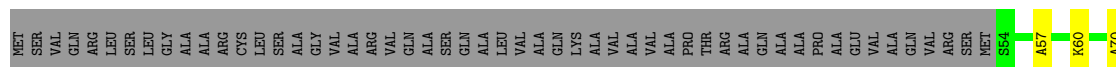
- Molecule 11: Mitochondrial ATP synthase subunit c

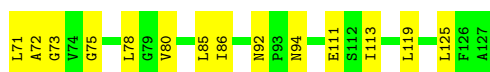


- Molecule 11: Mitochondrial ATP synthase subunit c



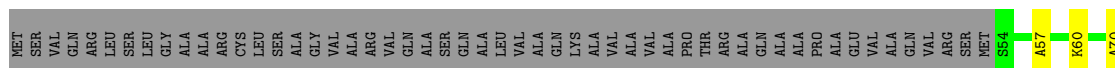
- Molecule 11: Mitochondrial ATP synthase subunit c





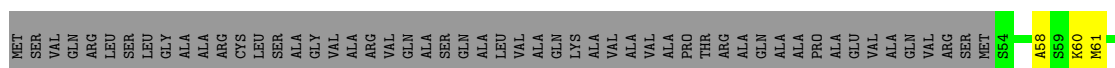
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain G: 46% 13% 42%



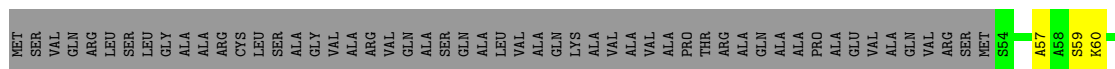
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain H: 41% 17% 42%



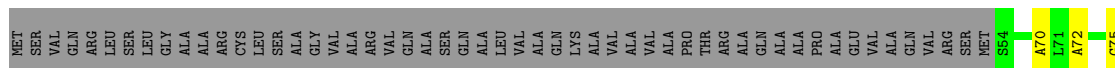
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain I: 46% 12% 42%



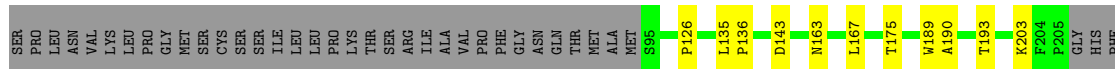
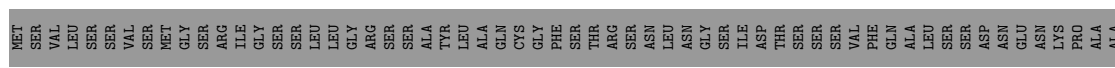
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain J: 50% 8% 42%



- Molecule 12: Mitochondrial ATP synthase subunit 6

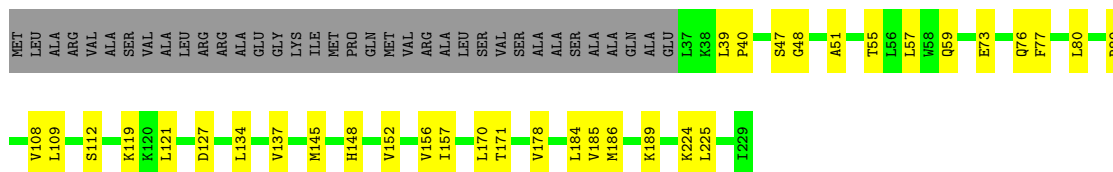
Chain M: 60% 6% 34%





• Molecule 13: Mitochondrial ATP synthase subunit OSCP

Chain P: 69% 15% 16%



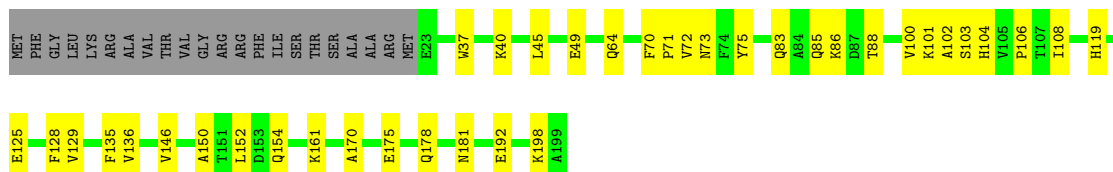
• Molecule 14: epsilon: Polytomella F-ATP synthase epsilon subunit

Chain Q: 74% 23% .



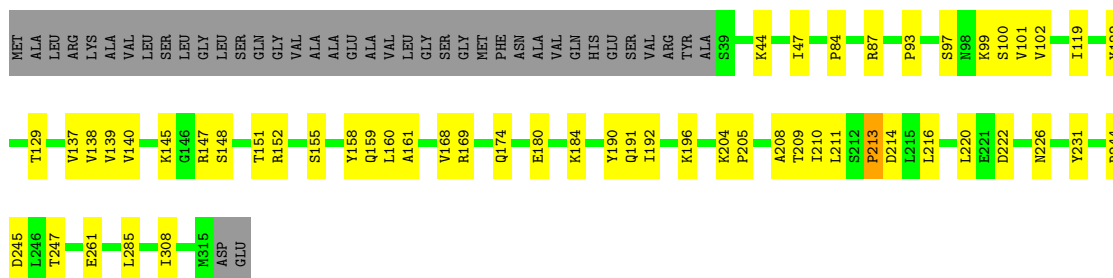
• Molecule 15: Mitochondrial ATP synthase subunit delta

Chain R: 70% 19% 11%



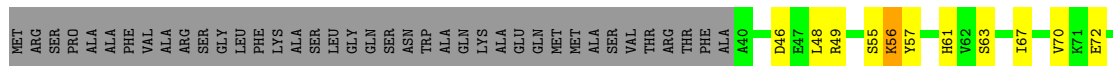
• Molecule 16: ATP synthase gamma chain, mitochondrial

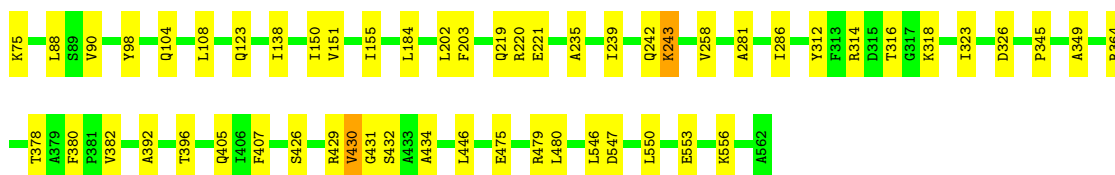
Chain S: 70% 17% 13%



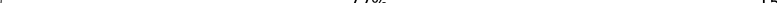
• Molecule 17: ATP synthase subunit alpha

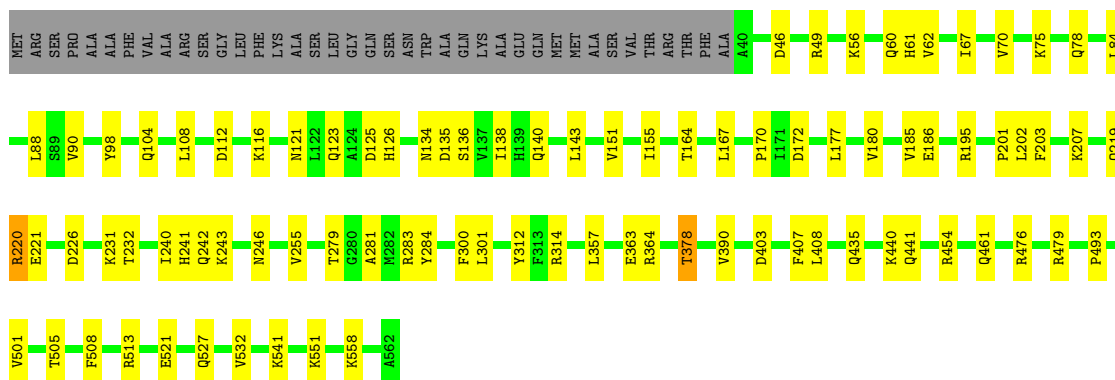
Chain T: 81% 11% . 7%





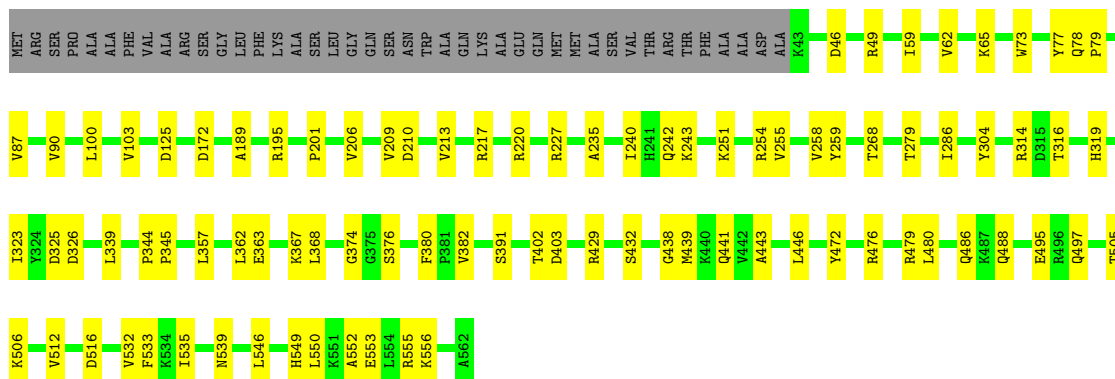
- Molecule 17: ATP synthase subunit alpha

Chain U:  77% 15% 7%

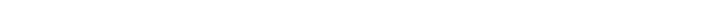


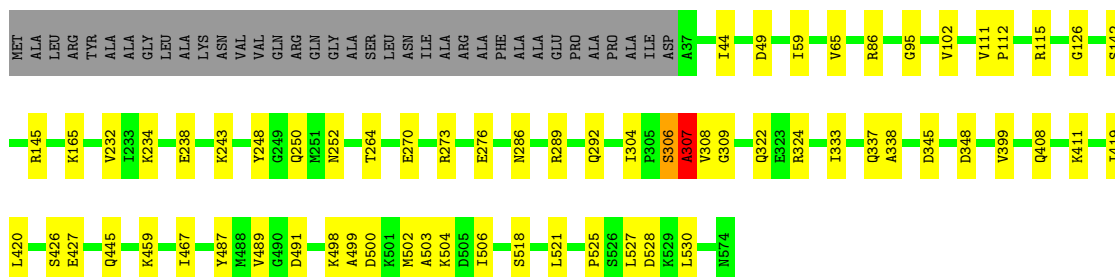
- Molecule 17: ATP synthase subunit alpha

Chain V:  77% 16% 7%




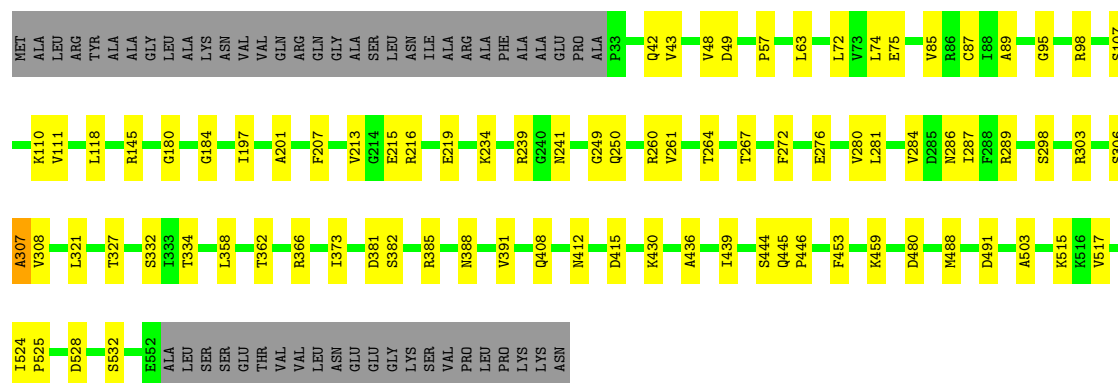
- Molecule 18: ATP synthase subunit beta

Chain X:  82% 11% 6%




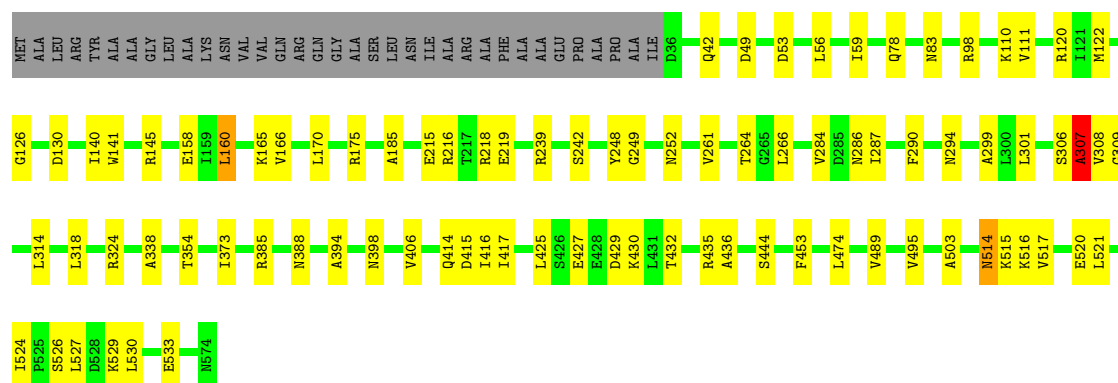
- Molecule 18: ATP synthase subunit beta

Chain Y:  76% 14% 9%



● Molecule 18: ATP synthase subunit beta

Chain Z:  79% 15% 6%





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46820	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	-400	Depositor
Maximum defocus (nm)	-5000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (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: ATP, ZN, MG, 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	0	0.39	0/628	0.53	0/856
10	9	0.36	0/802	0.51	0/1084
11	A	0.29	0/520	0.57	0/704
11	B	0.31	0/520	0.61	2/704 (0.3%)
11	C	0.32	0/519	0.56	0/701
11	D	0.32	0/520	0.56	0/704
11	E	0.30	0/520	0.58	0/704
11	F	0.31	0/520	0.57	1/704 (0.1%)
11	G	0.30	0/520	0.62	0/704
11	H	0.34	0/520	0.56	0/704
11	I	0.34	0/520	0.53	0/704
11	J	0.31	0/520	0.52	0/704
12	M	0.44	0/1683	0.58	0/2295
13	P	0.37	0/1553	0.54	0/2093
14	Q	0.32	0/574	0.49	0/774
15	R	0.34	0/1336	0.57	0/1827
16	S	0.35	0/2153	0.56	0/2901
17	T	0.49	0/4048	0.58	0/5481
17	U	0.46	0/4047	0.58	0/5479
17	V	0.47	0/4030	0.58	0/5456
18	X	0.46	0/4147	0.56	0/5619
18	Y	0.48	0/4011	0.57	0/5435
18	Z	0.42	0/4155	0.58	1/5630 (0.0%)
2	1	0.41	0/4750	0.52	0/6434
3	2	0.37	0/3212	0.53	0/4371
4	3	0.38	0/1911	0.52	1/2601 (0.0%)
5	4	0.40	0/2216	0.51	0/3000
6	5	0.49	0/1011	0.61	0/1376
7	6	0.45	0/946	0.54	0/1287
8	7	0.46	0/1374	0.54	0/1865
9	8	0.46	0/715	0.58	0/974
All	All	0.42	0/54501	0.56	5/73875 (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
11	H	0	1
18	X	0	1
18	Y	0	2
18	Z	0	2
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	77	PRO	N-CA-CB	5.92	110.41	103.30
11	B	95	ILE	CG1-CB-CG2	-5.55	99.19	111.40
18	Z	521	LEU	CA-CB-CG	5.50	127.94	115.30
11	B	119	LEU	CA-CB-CG	5.39	127.69	115.30
11	F	119	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	H	61	MET	Peptide
18	X	307	ALA	Peptide
18	Y	307	ALA	Peptide
18	Y	503	ALA	Mainchain
18	Z	307	ALA	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	607	0	584	6	0
2	1	4661	0	4695	45	0
3	2	3163	0	3262	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3	1874	0	1826	17	0
5	4	2177	0	2169	11	0
6	5	986	0	1021	15	0
7	6	926	0	941	9	0
8	7	1347	0	1345	21	0
9	8	692	0	694	7	0
10	9	776	0	757	6	0
11	A	514	0	554	11	0
11	B	514	0	554	14	0
11	C	514	0	553	21	0
11	D	514	0	554	28	0
11	E	514	0	554	29	0
11	F	514	0	554	16	0
11	G	514	0	554	20	0
11	H	514	0	554	16	0
11	I	514	0	554	12	0
11	J	514	0	554	9	0
12	M	1640	0	1665	17	0
13	P	1532	0	1602	34	0
14	Q	561	0	565	13	0
15	R	1303	0	1266	26	0
16	S	2130	0	2180	38	0
17	T	3979	0	4119	56	0
17	U	3978	0	4115	56	0
17	V	3961	0	4105	58	0
18	X	4087	0	4110	46	0
18	Y	3952	0	3965	59	0
18	Z	4095	0	4113	57	0
19	M	1	0	0	0	0
20	T	31	0	12	0	0
20	U	31	0	12	3	0
20	V	31	0	12	1	0
21	T	1	0	0	0	0
21	U	1	0	0	0	0
21	V	1	0	0	0	0
21	Y	1	0	0	0	0
21	Z	1	0	0	0	0
22	Y	27	0	12	2	0
22	Z	27	0	12	0	0
All	All	53720	0	54698	652	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 652 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)
13:P:171:THR:HG22	13:P:186:MET:CE	1.22	1.58
13:P:171:THR:CG2	13:P:186:MET:CE	1.95	1.44
17:T:429:ARG:HD2	18:Y:453:PHE:CG	1.66	1.29
11:D:61:MET:HG3	11:E:60:LYS:CG	1.61	1.29
13:P:171:THR:CG2	13:P:186:MET:HE1	1.58	1.28

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	0	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
2	1	593/618 (96%)	565 (95%)	28 (5%)	0	100	100
3	2	439/441 (100%)	416 (95%)	22 (5%)	1 (0%)	49	83
4	3	243/325 (75%)	236 (97%)	7 (3%)	0	100	100
5	4	288/294 (98%)	277 (96%)	11 (4%)	0	100	100
6	5	121/123 (98%)	110 (91%)	11 (9%)	0	100	100
7	6	122/151 (81%)	109 (89%)	13 (11%)	0	100	100
8	7	174/190 (92%)	166 (95%)	8 (5%)	0	100	100
9	8	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
10	9	95/97 (98%)	82 (86%)	13 (14%)	0	100	100
11	A	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	B	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	C	71/127 (56%)	69 (97%)	2 (3%)	0	100	100
11	D	72/127 (57%)	71 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	E	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	F	72/127 (57%)	68 (94%)	4 (6%)	0	100	100
11	G	72/127 (57%)	69 (96%)	3 (4%)	0	100	100
11	H	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	I	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	J	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
12	M	213/327 (65%)	207 (97%)	6 (3%)	0	100	100
13	P	191/229 (83%)	179 (94%)	12 (6%)	0	100	100
14	Q	70/74 (95%)	63 (90%)	7 (10%)	0	100	100
15	R	175/199 (88%)	159 (91%)	16 (9%)	0	100	100
16	S	275/317 (87%)	263 (96%)	11 (4%)	1 (0%)	36	75
17	T	521/562 (93%)	489 (94%)	30 (6%)	2 (0%)	36	75
17	U	521/562 (93%)	497 (95%)	23 (4%)	1 (0%)	49	83
17	V	518/562 (92%)	492 (95%)	26 (5%)	0	100	100
18	X	536/574 (93%)	505 (94%)	28 (5%)	3 (1%)	27	68
18	Y	518/574 (90%)	480 (93%)	37 (7%)	1 (0%)	49	83
18	Z	537/574 (94%)	493 (92%)	40 (7%)	4 (1%)	24	65
All	All	7034/8234 (85%)	6639 (94%)	382 (5%)	13 (0%)	53	83

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	T	430	VAL
18	X	308	VAL
18	Y	308	VAL
18	Z	308	VAL
3	2	383	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	0	63/64 (98%)	63 (100%)	0	100	100
2	1	493/512 (96%)	493 (100%)	0	100	100
3	2	312/312 (100%)	312 (100%)	0	100	100
4	3	195/258 (76%)	195 (100%)	0	100	100
5	4	220/223 (99%)	220 (100%)	0	100	100
6	5	107/107 (100%)	107 (100%)	0	100	100
7	6	96/115 (84%)	96 (100%)	0	100	100
8	7	140/150 (93%)	140 (100%)	0	100	100
9	8	71/72 (99%)	71 (100%)	0	100	100
10	9	79/79 (100%)	78 (99%)	1 (1%)	71	88
11	A	50/86 (58%)	50 (100%)	0	100	100
11	B	50/86 (58%)	50 (100%)	0	100	100
11	C	50/86 (58%)	50 (100%)	0	100	100
11	D	50/86 (58%)	49 (98%)	1 (2%)	58	82
11	E	50/86 (58%)	50 (100%)	0	100	100
11	F	50/86 (58%)	50 (100%)	0	100	100
11	G	50/86 (58%)	50 (100%)	0	100	100
11	H	50/86 (58%)	48 (96%)	2 (4%)	34	67
11	I	50/86 (58%)	50 (100%)	0	100	100
11	J	50/86 (58%)	50 (100%)	0	100	100
12	M	178/272 (65%)	178 (100%)	0	100	100
13	P	171/196 (87%)	171 (100%)	0	100	100
14	Q	56/58 (97%)	56 (100%)	0	100	100
15	R	134/151 (89%)	134 (100%)	0	100	100
16	S	235/265 (89%)	234 (100%)	1 (0%)	92	96
17	T	419/448 (94%)	417 (100%)	2 (0%)	90	95
17	U	419/448 (94%)	416 (99%)	3 (1%)	85	94
17	V	418/448 (93%)	416 (100%)	2 (0%)	90	95
18	X	446/469 (95%)	446 (100%)	0	100	100
18	Y	429/469 (92%)	429 (100%)	0	100	100
18	Z	447/469 (95%)	445 (100%)	2 (0%)	92	96
All	All	5628/6445 (87%)	5614 (100%)	14 (0%)	94	98

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	T	243	LYS
17	U	220	ARG
17	V	316	THR
17	T	220	ARG
17	V	243	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
14	Q	46	HIS
16	S	267	HIS
18	Y	388	ASN
15	R	104	HIS
16	S	186	ASN

### 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 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	T	1001	21	26,33,33	0.91	1 (3%)	27,52,52	1.51	4 (14%)
20	ATP	U	1001	21	26,33,33	0.92	1 (3%)	27,52,52	1.57	4 (14%)
20	ATP	V	1001	21	26,33,33	0.96	1 (3%)	27,52,52	1.66	4 (14%)
22	ADP	Y	601	21	24,29,29	0.97	1 (4%)	25,45,45	1.43	3 (12%)
22	ADP	Z	601	21	24,29,29	0.94	1 (4%)	25,45,45	1.40	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	T	1001	21	-	2/18/38/38	0/3/3/3
20	ATP	U	1001	21	-	2/18/38/38	0/3/3/3
20	ATP	V	1001	21	-	5/18/38/38	0/3/3/3
22	ADP	Y	601	21	-	3/12/32/32	0/3/3/3
22	ADP	Z	601	21	-	3/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	601	ADP	C5-C4	2.93	1.47	1.40
22	Y	601	ADP	C5-C4	2.87	1.47	1.40
20	V	1001	ATP	C5-C4	2.71	1.46	1.40
20	U	1001	ATP	C5-C4	2.71	1.46	1.40
20	T	1001	ATP	C5-C4	2.66	1.46	1.40

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	U	1001	ATP	PB-O3B-PG	-4.13	119.46	132.57
20	V	1001	ATP	PA-O3A-PB	-3.93	120.06	132.57
20	V	1001	ATP	PB-O3B-PG	-3.75	120.66	132.57
20	T	1001	ATP	PB-O3B-PG	-3.49	121.48	132.57
22	Z	601	ADP	N3-C2-N1	-3.27	123.41	128.68

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

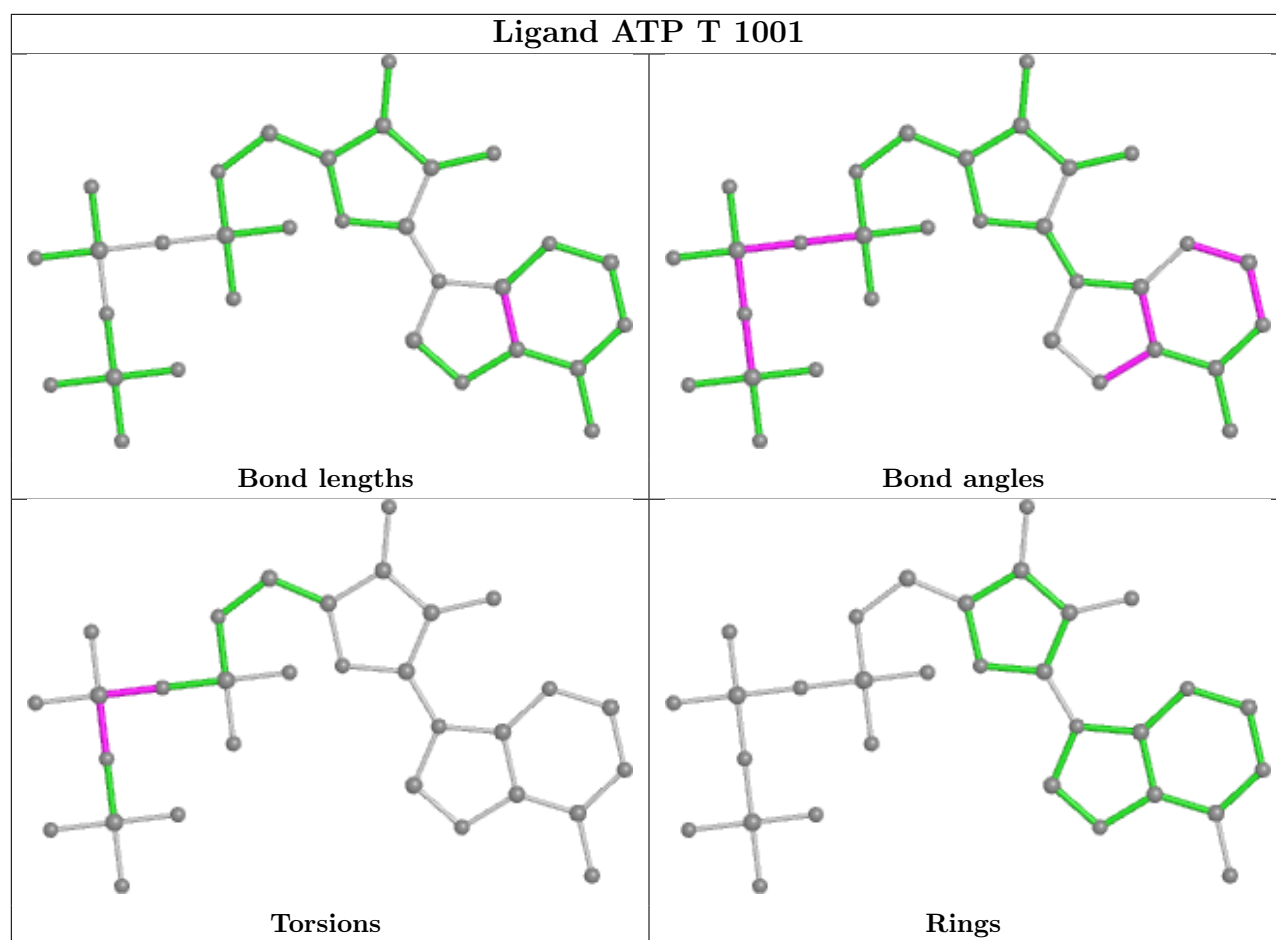
Mol	Chain	Res	Type	Atoms
22	Z	601	ADP	C5'-O5'-PA-O2A
22	Z	601	ADP	C5'-O5'-PA-O3A
20	V	1001	ATP	C5'-O5'-PA-O1A
20	V	1001	ATP	C5'-O5'-PA-O2A
20	V	1001	ATP	O4'-C4'-C5'-O5'

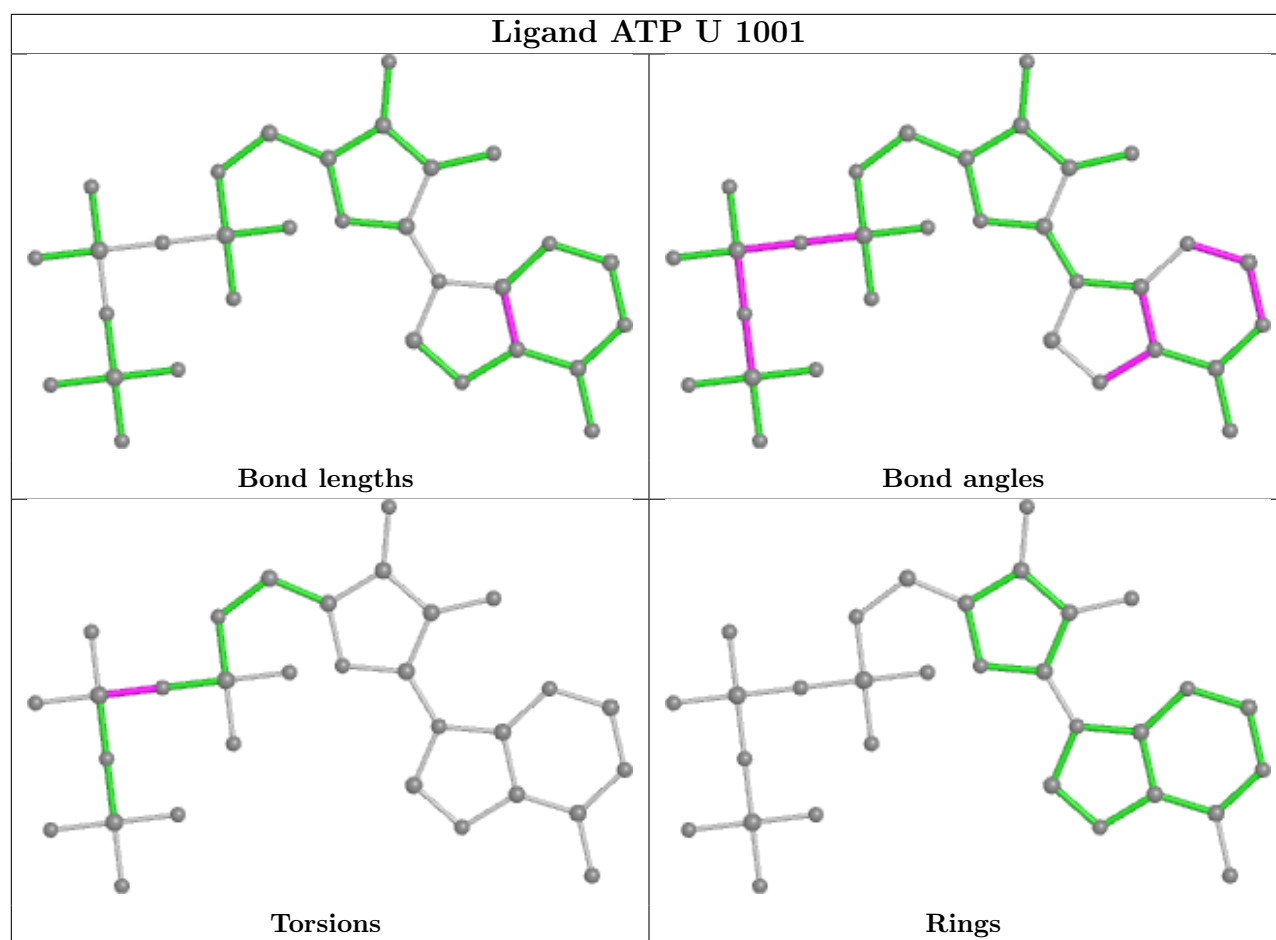
There are no ring outliers.

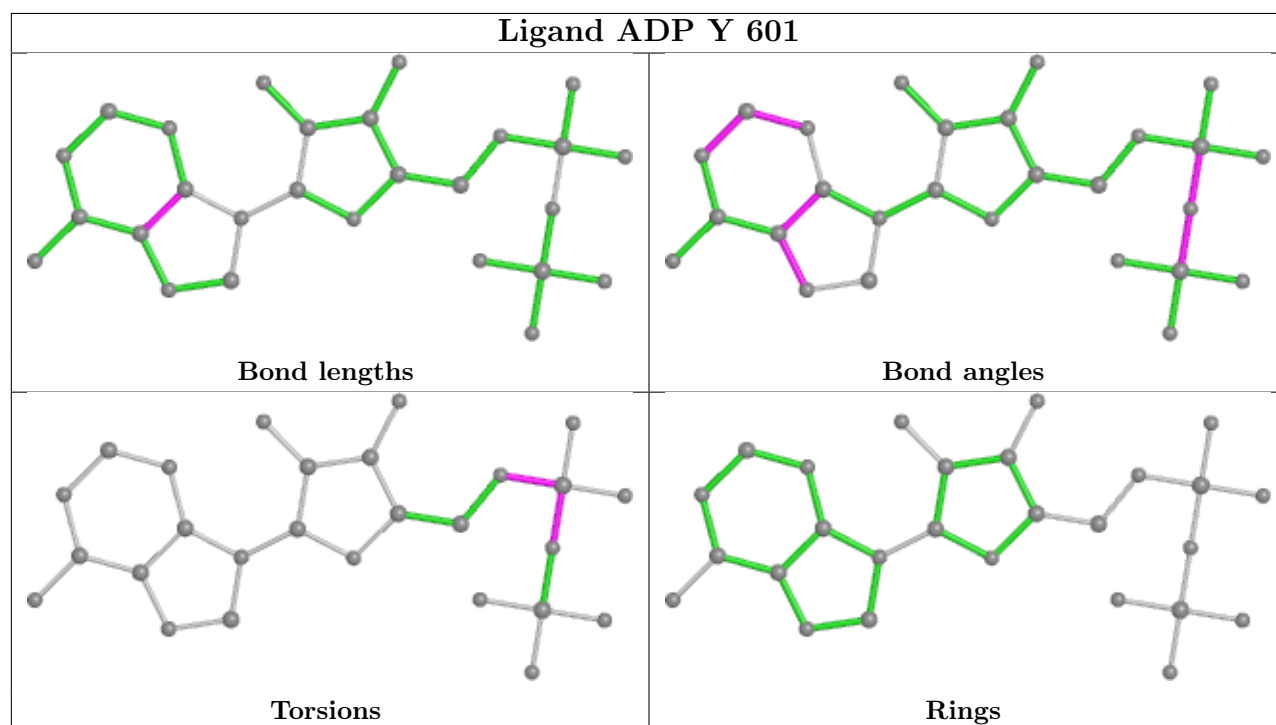
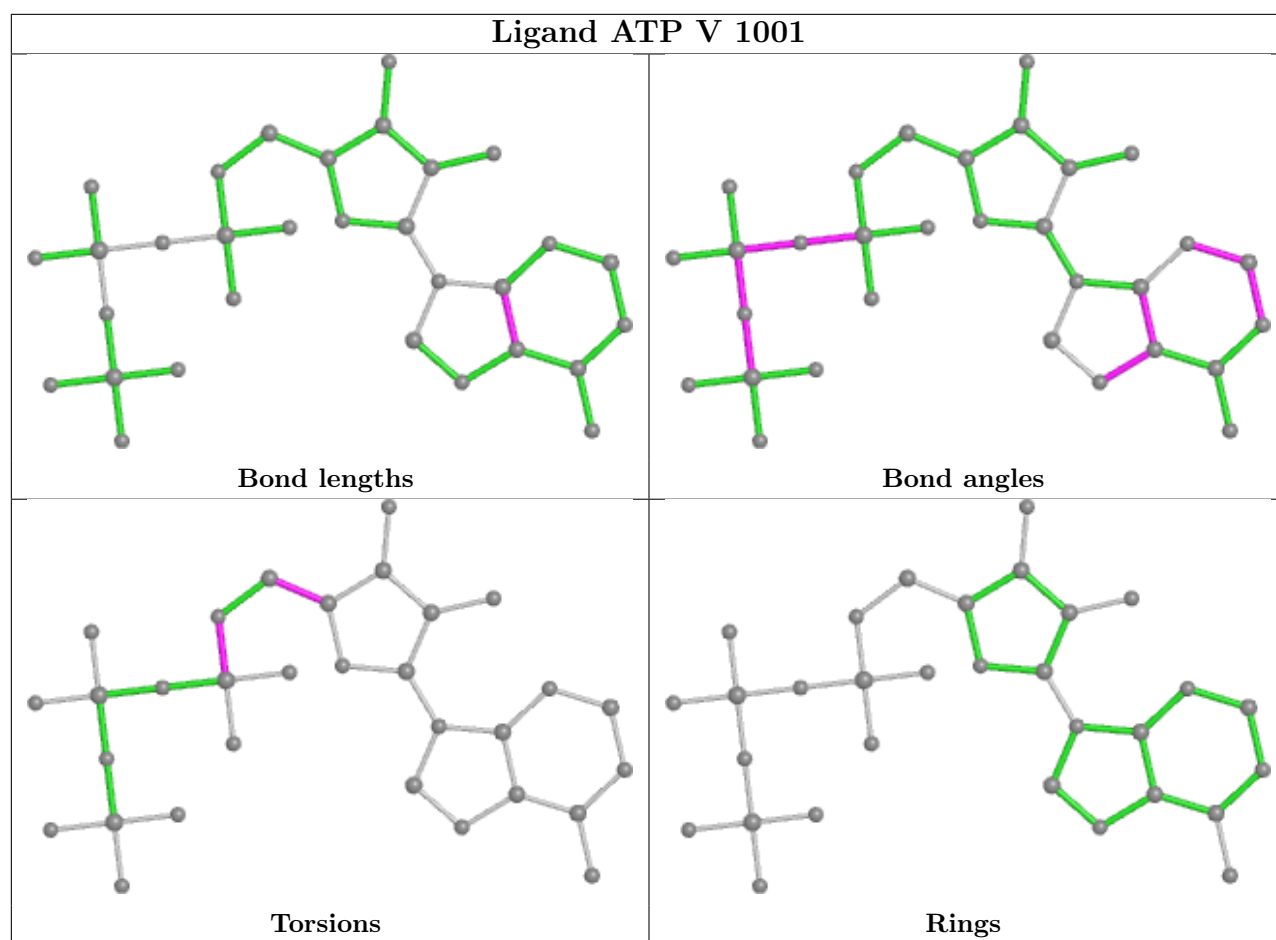
3 monomers are involved in 6 short contacts:

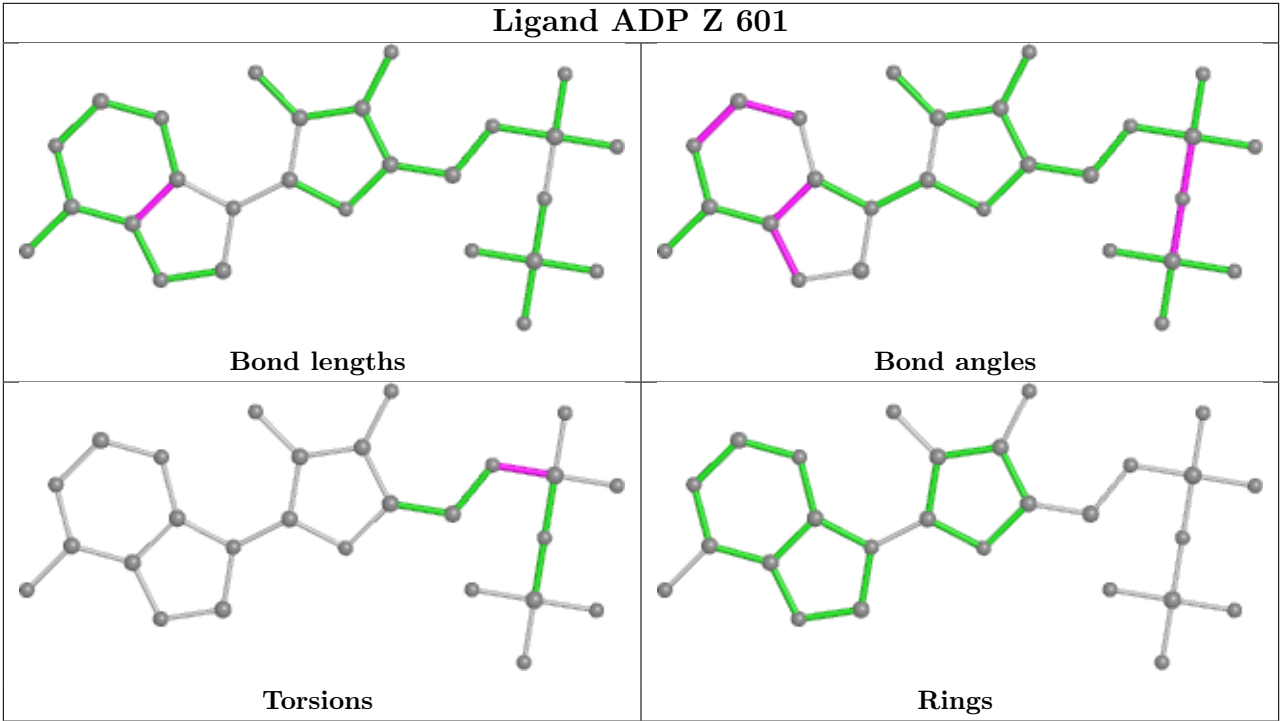
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	U	1001	ATP	3	0
20	V	1001	ATP	1	0
22	Y	601	ADP	2	0

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.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	126:PHE	C	127:ALA	N	4.05