



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 17, 2017 – 04:08 PM EDT

PDB ID : 4B2Q
EMDB ID: : EMD-2161
Title : Model of the yeast F1Fo-ATP synthase dimer based on subtomogram average
Authors : Davies, K.M.; Kuehlbrandt, W.
Deposited on : unknown
Resolution : 37.00 Å(reported)
Based on PDB ID : 2WPD

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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

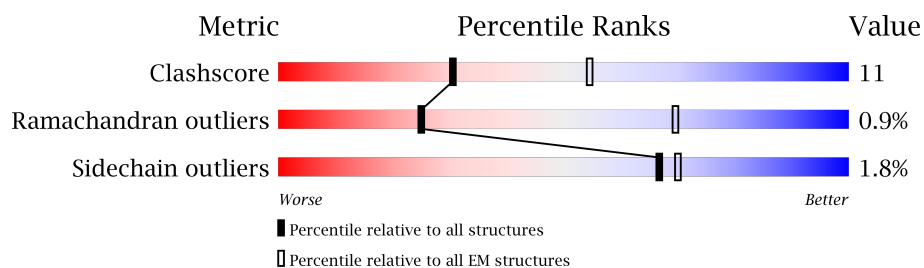
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 37.00 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.







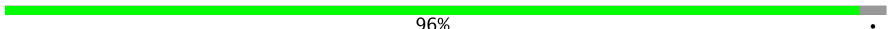

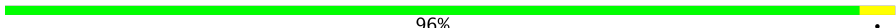












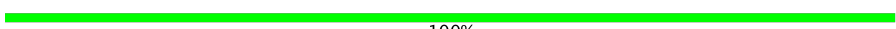
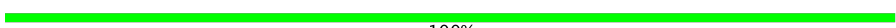

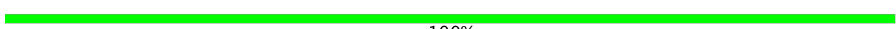


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	485	
1	C	485	
1	a	485	
1	c	485	
2	B	486	
2	b	486	
3	D	470	
3	d	470	
4	E	473	













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Mol	Chain	Length	Quality of chain
4	F	473	 59% 41%
4	e	473	 99%
4	f	473	 99%
5	G	278	 61% 35%
5	g	278	 96%
6	H	132	 51% 48%
6	h	132	 96%
7	I	59	 83% 17%
7	i	59	 100%
8	J	76	 71% 29%
8	K	76	 67% 33%
8	L	76	 70% 30%
8	M	76	 63% 37%
8	N	76	 63% 37%
8	O	76	 63% 37%
8	P	76	 64% 36%
8	Q	76	 68% 32%
8	R	76	 74% 26%
8	S	76	 74% 26%
8	j	76	 100%
8	k	76	 100%
8	l	76	 100%
8	m	76	 100%
8	n	76	 100%
8	o	76	 100%

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Mol	Chain	Length	Quality of chain
8	p	76	 100%
8	q	76	 100%
8	r	76	 100%
8	s	76	 100%
9	T	129	 39% 49% 11% .
9	t	129	 82% 16% .
10	U	120	 50% 38% 10% .
10	u	120	 84% 14% .
11	V	66	 48% 41% 9% .
11	v	66	 86% 12% .
12	W	120	 29% 43% 19% 8%
12	w	120	 64% 28% 8%

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 70306 atoms, of which 1786 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	485	Total	C	N	O	S	0	0
			3692	2334	651	704	3		
1	C	485	Total	C	N	O	S	0	0
			3692	2334	651	704	3		
1	a	485	Total	C	N	O	S	0	0
			3692	2334	651	704	3		
1	c	485	Total	C	N	O	S	0	0
			3692	2334	651	704	3		

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	485	Total	C	N	O	S	0	0
			3685	2328	651	703	3		
2	b	485	Total	C	N	O	S	0	0
			3685	2328	651	703	3		

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	470	Total	C	N	O	S	0	0
			3549	2250	604	689	6		
3	d	470	Total	C	N	O	S	0	0
			3549	2250	604	689	6		

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	473	Total	C	N	O	S	0	0
			3572	2262	608	696	6		
4	F	472	Total	C	N	O	S	0	0
			3566	2259	607	694	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	473	Total	C	N	O	S	0	0
			3572	2262	608	696	6		
4	f	472	Total	C	N	O	S	0	0
			3566	2259	607	694	6		

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	269	Total	C	N	O	S	0	0
			2086	1309	362	405	10		
5	g	269	Total	C	N	O	S	0	0
			2086	1309	362	405	10		

- Molecule 6 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	132	Total	C	N	O	S	0	0
			990	624	165	199	2		
6	h	132	Total	C	N	O	S	0	0
			990	624	165	199	2		

- Molecule 7 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	59	Total	C	N	O	0	0
			392	243	71	78		
7	i	59	Total	C	N	O	0	0
			392	243	71	78		

- Molecule 8 is a protein called ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	K	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	L	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	M	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	N	76	Total	C	N	O	S	0	0
			545	364	84	93	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	P	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	Q	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	R	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	S	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	j	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	k	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	l	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	m	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	n	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	o	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	p	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	q	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	r	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	s	76	Total	C	N	O	S	0	0
			545	364	84	93	4		

- Molecule 9 is a protein called ATP SYNTHASE SUBUNIT B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	129	Total	C	N	O	S	0	0
			1077	671	200	200	6		
9	t	129	Total	C	N	O	S	0	0
			1077	671	200	200	6		

- Molecule 10 is a protein called ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	120	Total	C	N	O	S	0	0
			969	620	161	186	2		
10	u	120	Total	C	N	O	S	0	0
			969	620	161	186	2		

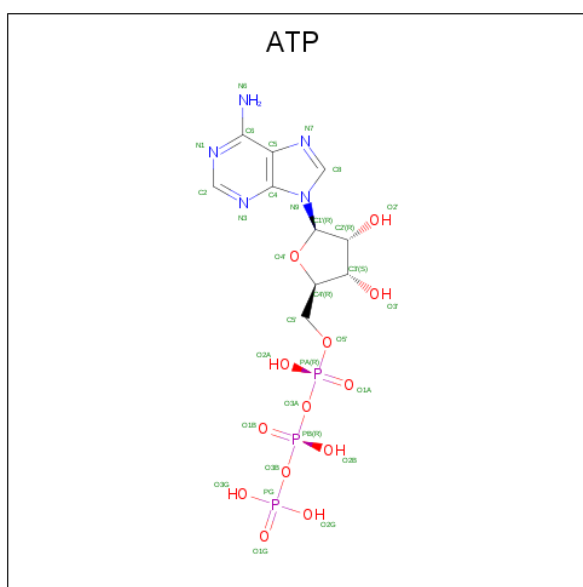
- Molecule 11 is a protein called ATP SYNTHASE-COUPPLING FACTOR 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	65	Total	C	N	O	S	0	0
			542	346	90	104	2		
11	v	65	Total	C	N	O	S	0	0
			542	346	90	104	2		

- Molecule 12 is a protein called ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	W	110	Total	C	H	N	O	S	0	0
			1739	535	893	146	160	5		
12	w	110	Total	C	H	N	O	S	0	0
			1739	535	893	146	160	5		

- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

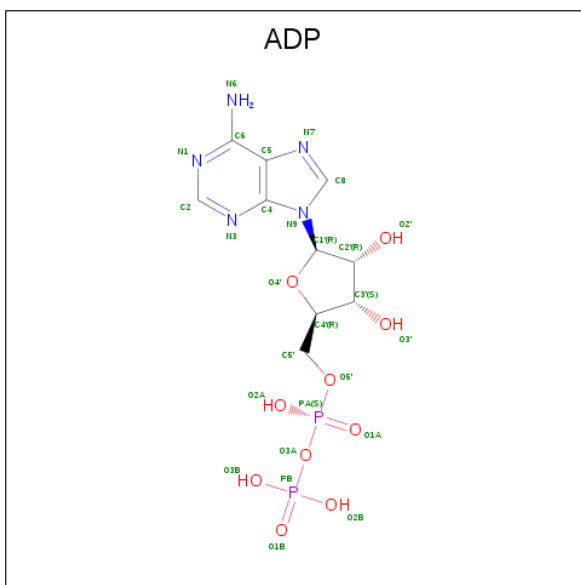


Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	a	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	b	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	c	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
14	D	1	Total	Mg	0
			1	1	
14	B	1	Total	Mg	0
			1	1	
14	C	1	Total	Mg	0
			1	1	
14	c	1	Total	Mg	0
			1	1	
14	A	1	Total	Mg	0
			1	1	
14	a	1	Total	Mg	0
			1	1	
14	f	1	Total	Mg	0
			1	1	
14	d	1	Total	Mg	0
			1	1	
14	b	1	Total	Mg	0
			1	1	
14	F	1	Total	Mg	0
			1	1	

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

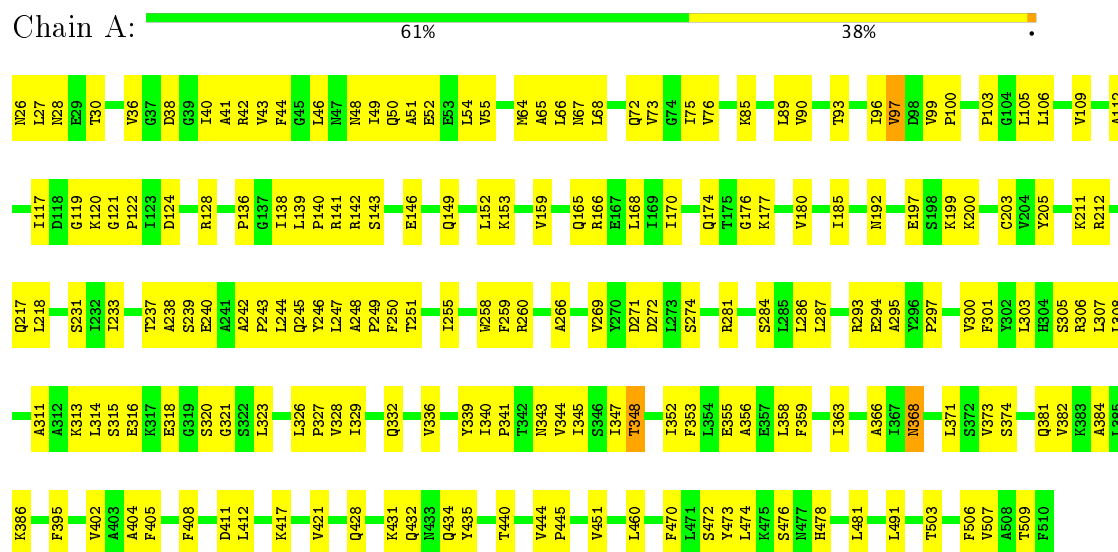


Mol	Chain	Residues	Atoms					AltConf
15	D	1	Total 27	C 10	N 5	O 10	P 2	0
15	F	1	Total 27	C 10	N 5	O 10	P 2	0
15	d	1	Total 27	C 10	N 5	O 10	P 2	0
15	f	1	Total 27	C 10	N 5	O 10	P 2	0

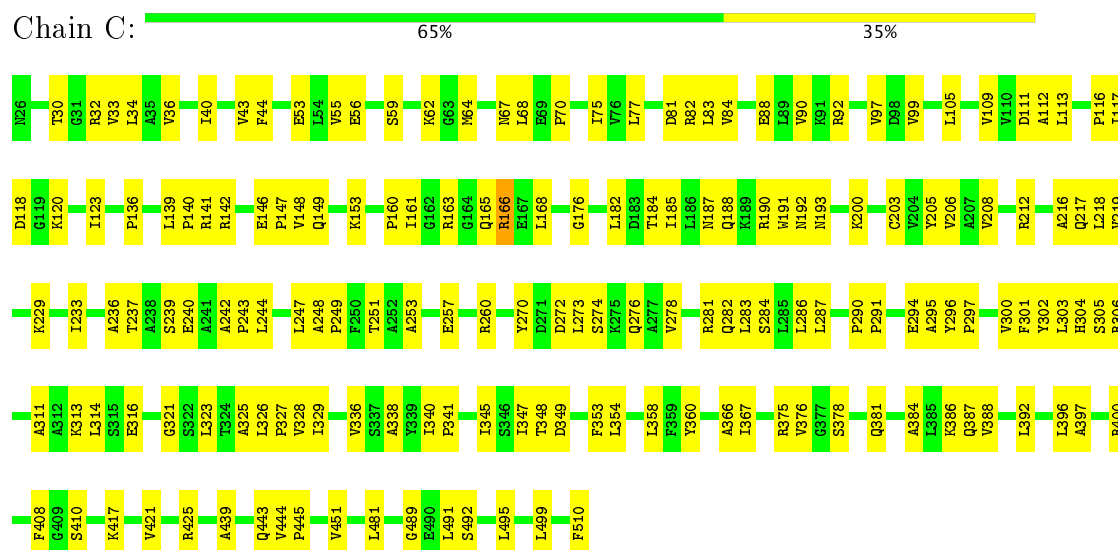
3 Residue-property plots

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 SUBUNIT ALPHA, MITOCHONDRIAL



• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain a:  99%



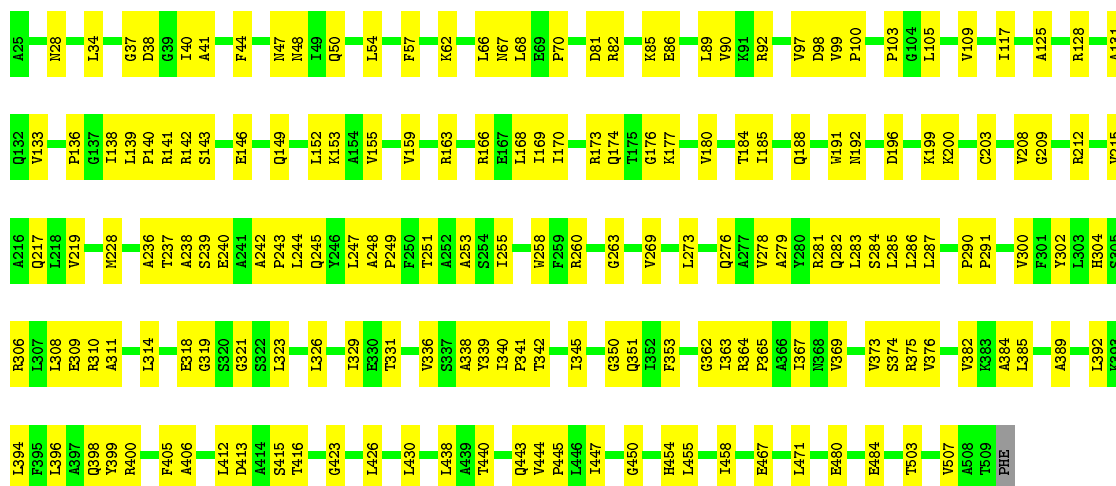
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain c: 100%



- Molecule 2: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain B:  63% 37%



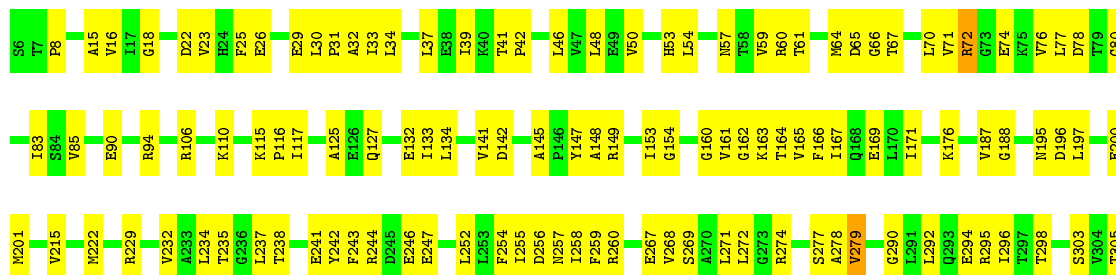
- Molecule 2: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

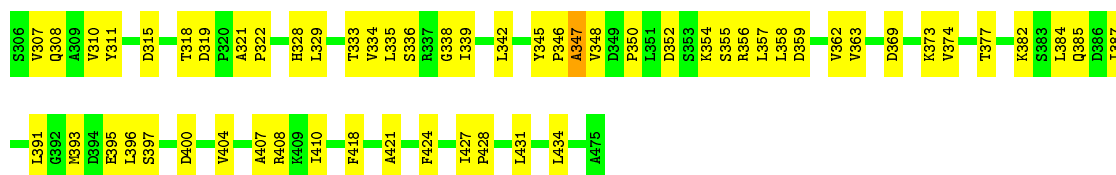
Chain b: 100%



- Molecule 3: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain D:  63% 37%





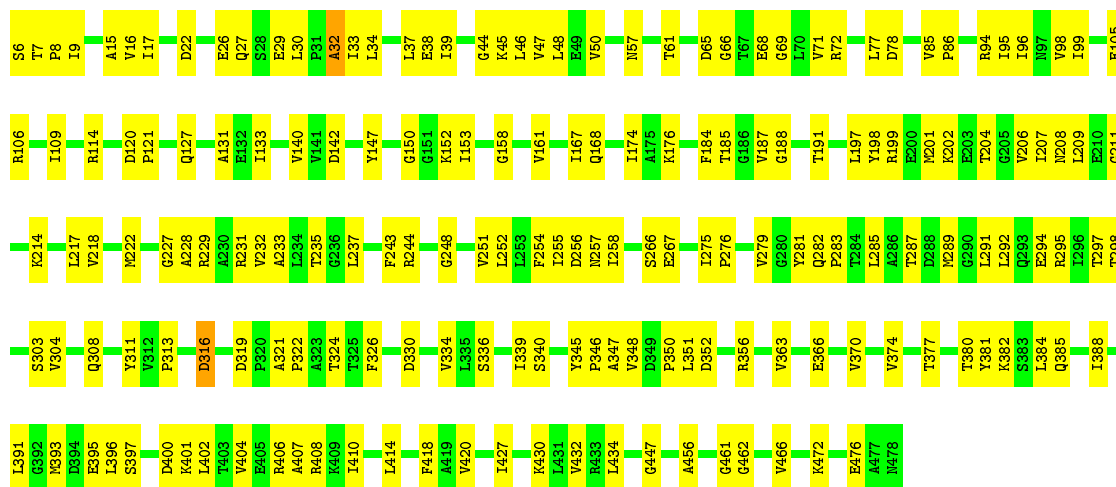
• Molecule 3: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain d: 99%



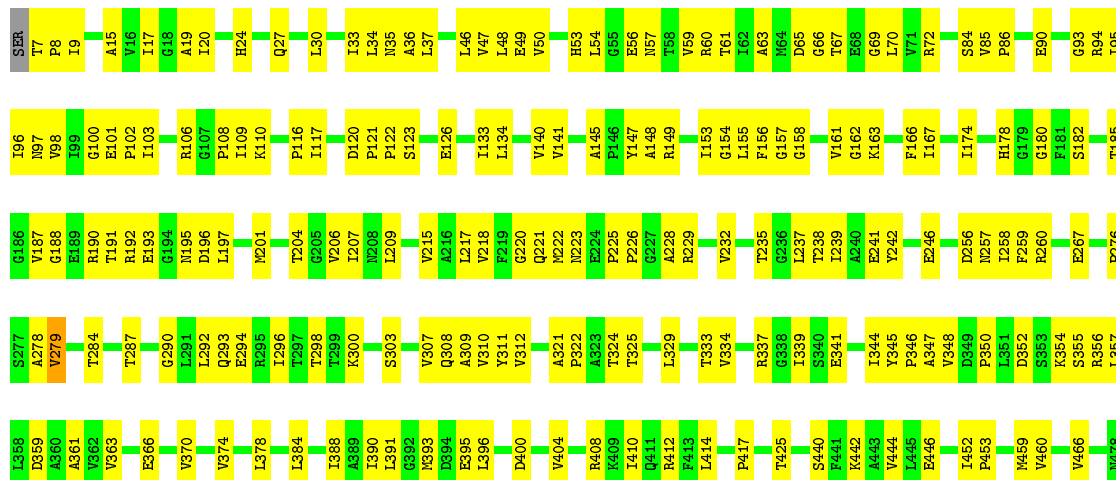
• Molecule 4: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain E: 62% 37%

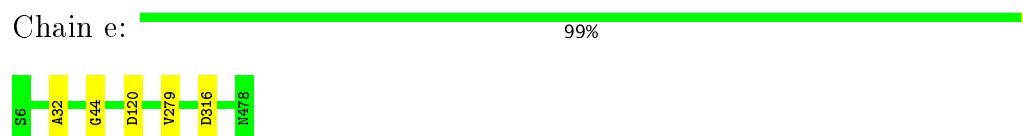


• Molecule 4: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

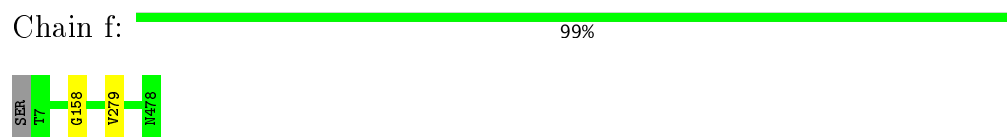
Chain F: 59% 41%



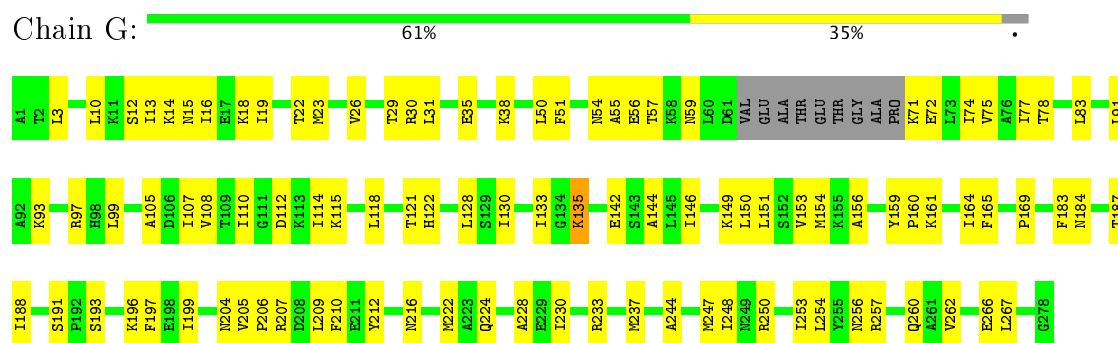
• Molecule 4: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



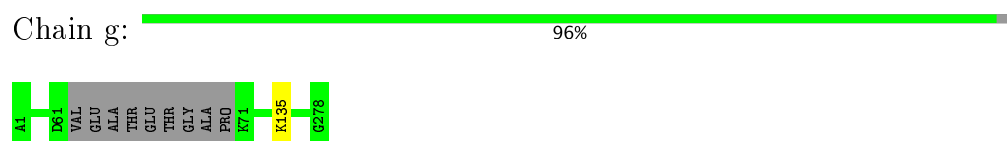
- Molecule 4: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



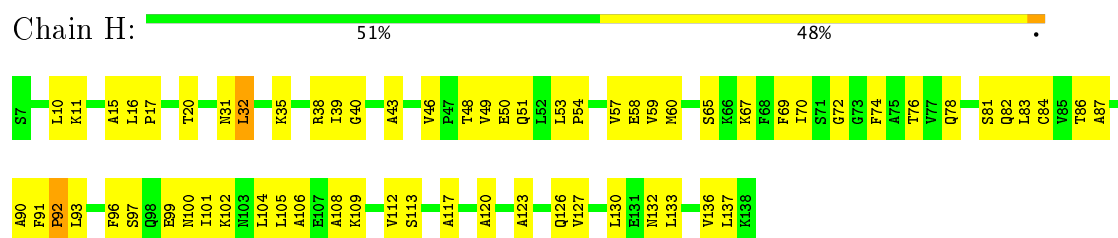
- Molecule 5: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



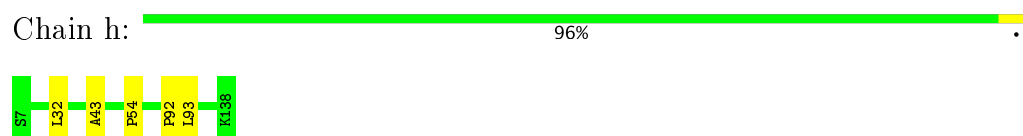
- Molecule 5: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL




- Molecule 6: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL

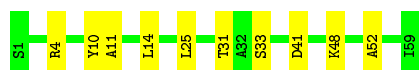


- Molecule 6: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



- Molecule 7: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

Chain I:  83% 17%



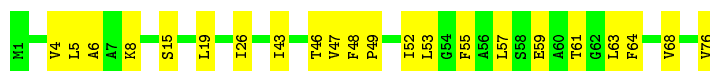
- Molecule 7: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain J:  71% 29%



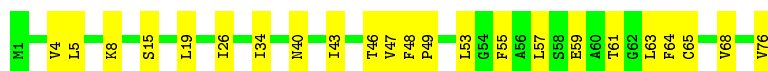
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain K:  67% 33%



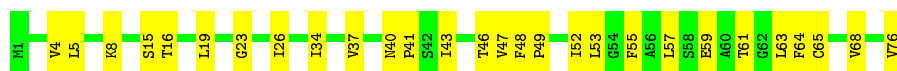
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain L:  70% 30%



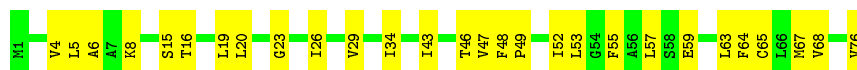
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain M:  63% 37%



- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain N:  63% 37%



- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain O:  63% 37%



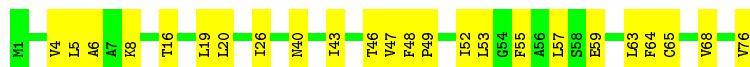
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain P:  64% 36%



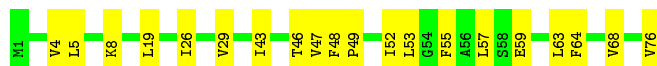
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain Q:  68% 32%



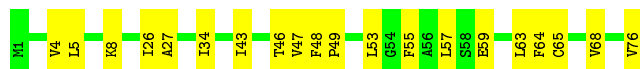
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain R:  74% 26%



- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain S:  74% 26%



- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain m:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain r:  100%

There are no outlier residues recorded for this chain.

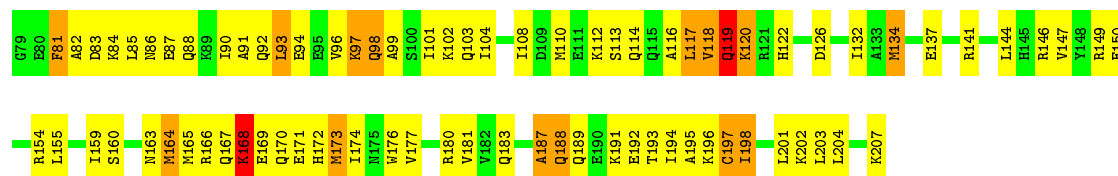
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain s:  100%


There are no outlier residues recorded for this chain.

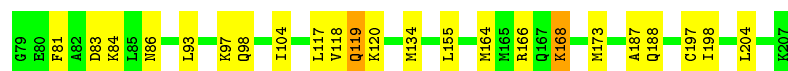
- Molecule 9: ATP SYNTHASE SUBUNIT B, MITOCHONDRIAL

Chain T:  39% 49% 11%

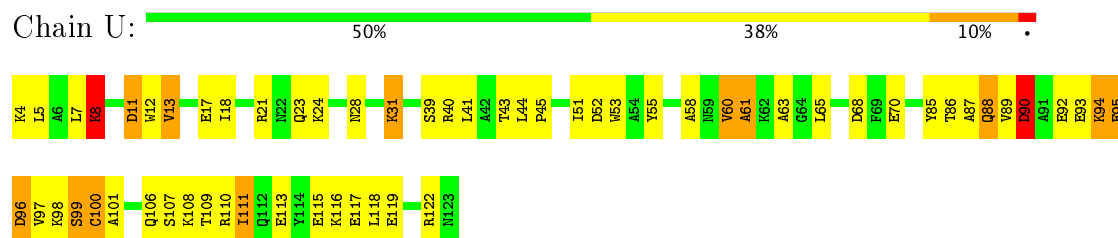


- Molecule 9: ATP SYNTHASE SUBUNIT B, MITOCHONDRIAL

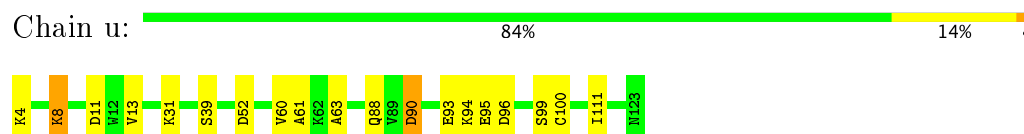
Chain t:  82% 16%



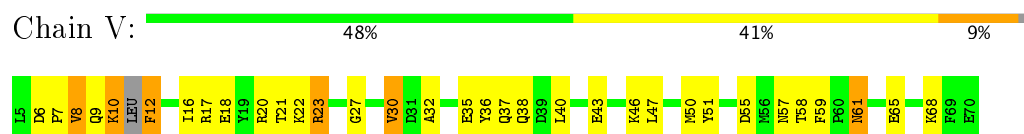
- Molecule 10: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL



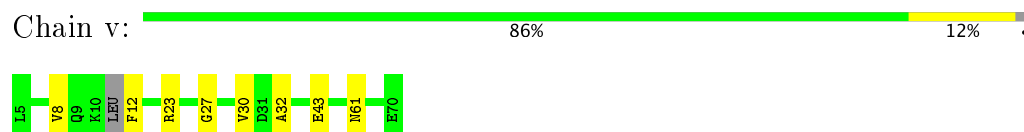
• Molecule 10: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL



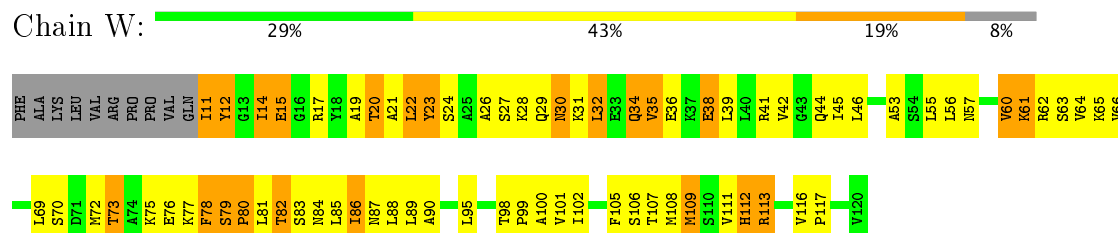
• Molecule 11: ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL



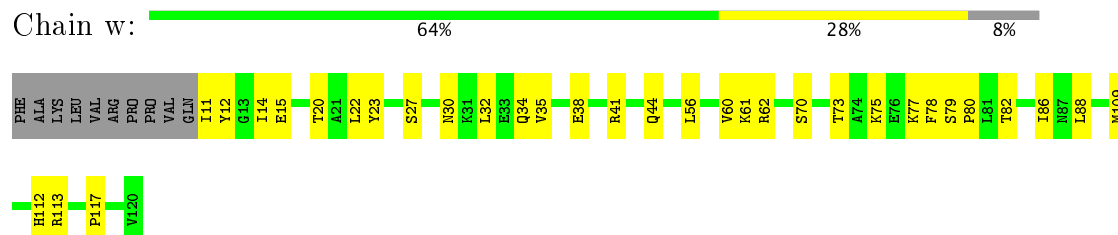
• Molecule 11: ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL



• Molecule 12: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL



• Molecule 12: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL



4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of tilted images used	121	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	160	Depositor
Minimum defocus (nm)	6500	Depositor
Maximum defocus (nm)	7500	Depositor
Magnification	24500	Depositor
Image detector	GATAN ULTRASCAN 1000 (2k x 2k)	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	0.28	0/3749	0.43	0/5073
1	C	0.27	0/3749	0.43	0/5073
1	a	0.28	0/3749	0.43	0/5073
1	c	0.27	0/3749	0.43	0/5073
10	U	0.61	0/988	0.76	1/1335 (0.1%)
10	u	0.61	0/988	0.76	1/1335 (0.1%)
11	V	19.73	1/553 (0.2%)	0.82	1/738 (0.1%)
11	v	0.58	0/554	0.71	0/741
12	W	0.26	0/857	0.36	0/1154
12	w	0.26	0/857	0.36	0/1154
2	B	0.24	0/3741	0.39	0/5064
2	b	0.25	0/3741	0.39	0/5064
3	D	0.28	0/3605	0.44	0/4889
3	d	0.28	0/3605	0.44	0/4889
4	E	0.24	0/3628	0.41	0/4919
4	F	0.26	0/3622	0.43	0/4911
4	e	0.24	0/3628	0.41	0/4919
4	f	0.27	0/3622	0.43	0/4911
5	G	0.25	0/2111	0.39	0/2838
5	g	0.24	0/2111	0.39	0/2838
6	H	0.24	0/1004	0.39	0/1359
6	h	0.24	0/1004	0.39	0/1359
7	I	0.23	0/398	0.34	0/547
7	i	0.23	0/398	0.34	0/547
8	J	0.23	0/553	0.35	0/747
8	K	0.24	0/553	0.37	0/747
8	L	0.22	0/553	0.35	0/747
8	M	0.23	0/553	0.36	0/747
8	N	0.23	0/553	0.35	0/747
8	O	0.23	0/553	0.35	0/747
8	P	0.23	0/553	0.35	0/747
8	Q	0.23	0/553	0.34	0/747

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
8	R	0.23	0/553	0.34	0/747
8	S	0.23	0/553	0.35	0/747
8	j	0.23	0/553	0.35	0/747
8	k	0.23	0/553	0.37	0/747
8	l	0.23	0/553	0.35	0/747
8	m	0.23	0/553	0.36	0/747
8	n	0.22	0/553	0.35	0/747
8	o	0.23	0/553	0.35	0/747
8	p	0.23	0/553	0.35	0/747
8	q	0.23	0/553	0.34	0/747
8	r	0.23	0/553	0.34	0/747
8	s	0.23	0/553	0.35	0/747
9	T	0.72	2/1088 (0.2%)	0.69	1/1453 (0.1%)
9	t	0.72	2/1088 (0.2%)	0.69	1/1453 (0.1%)
All	All	1.79	5/69247 (0.0%)	0.44	5/93649 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	V	10	LYS	N-CA	463.87	10.74	1.46
9	T	168	LYS	C-N	-14.85	0.99	1.34
9	t	168	LYS	C-N	-14.84	0.99	1.34
9	T	173	MET	CG-SD	5.98	1.96	1.81
9	t	173	MET	CG-SD	5.97	1.96	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	V	10	LYS	N-CA-CB	-11.15	90.52	110.60
9	t	173	MET	CG-SD-CE	6.80	111.08	100.20
9	T	173	MET	CG-SD-CE	6.79	111.06	100.20
10	U	90	ASP	CB-CG-OD1	6.38	124.05	118.30
10	u	90	ASP	CB-CG-OD1	6.37	124.03	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3692	0	3769	241	0
1	C	3692	0	3772	134	0
1	a	3692	0	3769	0	0
1	c	3692	0	3772	0	0
2	B	3685	0	3768	139	0
2	b	3685	0	3768	0	0
3	D	3549	0	3621	138	0
3	d	3549	0	3621	0	0
4	E	3572	0	3638	160	0
4	F	3566	0	3633	175	0
4	e	3572	0	3638	0	0
4	f	3566	0	3633	0	0
5	G	2086	0	2156	87	0
5	g	2086	0	2156	0	0
6	H	990	0	999	64	0
6	h	990	0	999	0	0
7	I	392	0	306	10	0
7	i	392	0	306	0	0
8	J	545	0	591	17	0
8	K	545	0	591	25	0
8	L	545	0	591	28	0
8	M	545	0	591	33	0
8	N	545	0	591	30	0
8	O	545	0	591	29	0
8	P	545	0	591	28	0
8	Q	545	0	591	25	0
8	R	545	0	591	20	0
8	S	545	0	591	18	0
8	j	545	0	591	0	0
8	k	545	0	591	0	0
8	l	545	0	591	0	0
8	m	545	0	591	0	0
8	n	545	0	591	0	0
8	o	545	0	591	0	0
8	p	545	0	591	0	0
8	q	545	0	591	0	0
8	r	545	0	591	0	0
8	s	545	0	591	0	0
9	T	1077	0	1104	166	0
9	t	1077	0	1104	0	0
10	U	969	0	980	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	u	969	0	980	0	0
11	V	542	0	520	94	0
11	v	542	0	521	0	0
12	W	846	893	889	146	0
12	w	846	893	889	0	0
13	A	31	0	12	5	0
13	B	31	0	12	1	0
13	C	31	0	12	1	0
13	a	31	0	12	0	0
13	b	31	0	12	0	0
13	c	31	0	12	0	0
14	A	1	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	D	1	0	0	0	0
14	F	1	0	0	0	0
14	a	1	0	0	0	0
14	b	1	0	0	0	0
14	c	1	0	0	0	0
14	d	1	0	0	0	0
14	f	1	0	0	0	0
15	D	27	0	12	2	0
15	F	27	0	12	2	0
15	d	27	0	12	0	0
15	f	27	0	12	0	0
All	All	68520	1786	70251	1554	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 1554 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)
1:A:122:PRO:CD	9:T:159:ILE:CG2	1.78	1.59
1:A:27:LEU:CD2	9:T:202:LYS:HE2	1.35	1.56
4:F:56:GLU:CD	12:W:53:ALA:HB2	1.25	1.55
9:T:203:LEU:HD21	12:W:84:ASN:CB	1.45	1.47
9:T:201:LEU:HD13	11:V:7:PRO:CG	1.01	1.47

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	483/485 (100%)	444 (92%)	35 (7%)	4 (1%)	22	67
1	C	483/485 (100%)	450 (93%)	33 (7%)	0	100	100
1	a	483/485 (100%)	444 (92%)	35 (7%)	4 (1%)	22	67
1	c	483/485 (100%)	450 (93%)	33 (7%)	0	100	100
2	B	483/486 (99%)	447 (92%)	35 (7%)	1 (0%)	51	84
2	b	483/486 (99%)	447 (92%)	35 (7%)	1 (0%)	51	84
3	D	468/470 (100%)	443 (95%)	22 (5%)	3 (1%)	28	71
3	d	468/470 (100%)	443 (95%)	22 (5%)	3 (1%)	28	71
4	E	471/473 (100%)	436 (93%)	32 (7%)	3 (1%)	28	71
4	F	470/473 (99%)	438 (93%)	30 (6%)	2 (0%)	38	77
4	e	471/473 (100%)	436 (93%)	32 (7%)	3 (1%)	28	71
4	f	470/473 (99%)	438 (93%)	30 (6%)	2 (0%)	38	77
5	G	265/278 (95%)	247 (93%)	17 (6%)	1 (0%)	38	77
5	g	265/278 (95%)	247 (93%)	17 (6%)	1 (0%)	38	77
6	H	130/132 (98%)	115 (88%)	11 (8%)	4 (3%)	5	37
6	h	130/132 (98%)	115 (88%)	11 (8%)	4 (3%)	5	37
7	I	57/59 (97%)	48 (84%)	9 (16%)	0	100	100
7	i	57/59 (97%)	48 (84%)	9 (16%)	0	100	100
8	J	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
8	K	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
8	L	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	M	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
8	N	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
8	O	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	P	74/76 (97%)	68 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Q	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	R	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	S	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
8	j	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
8	k	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
8	l	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	m	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
8	n	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
8	o	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	p	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
8	q	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	r	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	s	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
9	T	127/129 (98%)	100 (79%)	19 (15%)	8 (6%)	1	22
9	t	127/129 (98%)	100 (79%)	19 (15%)	8 (6%)	1	22
10	U	118/120 (98%)	88 (75%)	24 (20%)	6 (5%)	2	26
10	u	118/120 (98%)	88 (75%)	24 (20%)	6 (5%)	2	26
11	V	60/66 (91%)	52 (87%)	6 (10%)	2 (3%)	4	35
11	v	61/66 (92%)	52 (85%)	7 (12%)	2 (3%)	4	35
12	W	108/120 (90%)	92 (85%)	8 (7%)	8 (7%)	1	18
12	w	108/120 (90%)	92 (85%)	8 (7%)	8 (7%)	1	18
All	All	8927/9072 (98%)	8182 (92%)	661 (7%)	84 (1%)	25	63

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	72	ARG
3	D	279	VAL
4	E	32	ALA
4	E	279	VAL
4	F	279	VAL

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	391/391 (100%)	390 (100%)	1 (0%)	94	96
1	C	391/391 (100%)	390 (100%)	1 (0%)	94	96
1	a	391/391 (100%)	390 (100%)	1 (0%)	94	96
1	c	391/391 (100%)	390 (100%)	1 (0%)	94	96
2	B	390/391 (100%)	390 (100%)	0	100	100
2	b	390/391 (100%)	390 (100%)	0	100	100
3	D	380/380 (100%)	379 (100%)	1 (0%)	94	96
3	d	380/380 (100%)	379 (100%)	1 (0%)	94	96
4	E	382/382 (100%)	380 (100%)	2 (0%)	91	95
4	F	381/382 (100%)	381 (100%)	0	100	100
4	e	382/382 (100%)	380 (100%)	2 (0%)	91	95
4	f	381/382 (100%)	381 (100%)	0	100	100
5	G	230/236 (98%)	230 (100%)	0	100	100
5	g	230/236 (98%)	230 (100%)	0	100	100
6	H	111/111 (100%)	110 (99%)	1 (1%)	82	91
6	h	111/111 (100%)	110 (99%)	1 (1%)	82	91
7	I	25/46 (54%)	25 (100%)	0	100	100
7	i	25/46 (54%)	25 (100%)	0	100	100
8	J	56/56 (100%)	56 (100%)	0	100	100
8	K	56/56 (100%)	56 (100%)	0	100	100
8	L	56/56 (100%)	56 (100%)	0	100	100
8	M	56/56 (100%)	56 (100%)	0	100	100
8	N	56/56 (100%)	56 (100%)	0	100	100
8	O	56/56 (100%)	56 (100%)	0	100	100
8	P	56/56 (100%)	56 (100%)	0	100	100
8	Q	56/56 (100%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	R	56/56 (100%)	56 (100%)	0	100	100
8	S	56/56 (100%)	56 (100%)	0	100	100
8	j	56/56 (100%)	56 (100%)	0	100	100
8	k	56/56 (100%)	56 (100%)	0	100	100
8	l	56/56 (100%)	56 (100%)	0	100	100
8	m	56/56 (100%)	56 (100%)	0	100	100
8	n	56/56 (100%)	56 (100%)	0	100	100
8	o	56/56 (100%)	56 (100%)	0	100	100
8	p	56/56 (100%)	56 (100%)	0	100	100
8	q	56/56 (100%)	56 (100%)	0	100	100
8	r	56/56 (100%)	56 (100%)	0	100	100
8	s	56/56 (100%)	56 (100%)	0	100	100
9	T	118/118 (100%)	103 (87%)	15 (13%)	5	25
9	t	118/118 (100%)	103 (87%)	15 (13%)	5	25
10	U	104/104 (100%)	90 (86%)	14 (14%)	4	24
10	u	104/104 (100%)	90 (86%)	14 (14%)	4	24
11	V	58/60 (97%)	52 (90%)	6 (10%)	8	32
11	v	58/60 (97%)	52 (90%)	6 (10%)	8	32
12	W	95/104 (91%)	70 (74%)	25 (26%)	0	4
12	w	95/104 (91%)	70 (74%)	25 (26%)	0	4
All	All	7232/7312 (99%)	7100 (98%)	132 (2%)	67	84

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	W	75	LYS
9	t	84	LYS
12	w	56	LEU
12	W	86	ILE
1	c	166	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
8	S	40	ASN
1	a	381	GLN
8	n	40	ASN
9	T	98	GLN
1	a	48	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	ATP	A	1511	14	27,33,33	0.94	1 (3%)	25,52,52	1.57	2 (8%)
13	ATP	B	1510	14	27,33,33	0.98	1 (3%)	25,52,52	1.60	2 (8%)
13	ATP	C	1511	14	27,33,33	0.98	1 (3%)	25,52,52	1.64	2 (8%)
15	ADP	D	1476	14	25,29,29	1.03	1 (4%)	24,45,45	1.66	2 (8%)
15	ADP	F	1479	14	25,29,29	0.94	1 (4%)	24,45,45	1.71	3 (12%)
13	ATP	a	1511	14	27,33,33	0.93	1 (3%)	25,52,52	1.56	2 (8%)
13	ATP	b	1510	14	27,33,33	0.98	1 (3%)	25,52,52	1.60	2 (8%)
13	ATP	c	1511	14	27,33,33	0.97	1 (3%)	25,52,52	1.64	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	ADP	d	1476	14	25,29,29	1.04	1 (4%)	24,45,45	1.68	2 (8%)
15	ADP	f	1479	14	25,29,29	0.95	1 (4%)	24,45,45	1.72	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
13	ATP	A	1511	14	-	0/18/38/38	0/3/3/3
13	ATP	B	1510	14	-	0/18/38/38	0/3/3/3
13	ATP	C	1511	14	-	0/18/38/38	0/3/3/3
15	ADP	D	1476	14	-	0/12/32/32	0/3/3/3
15	ADP	F	1479	14	-	0/12/32/32	0/3/3/3
13	ATP	a	1511	14	-	0/18/38/38	0/3/3/3
13	ATP	b	1510	14	-	0/18/38/38	0/3/3/3
13	ATP	c	1511	14	-	0/18/38/38	0/3/3/3
15	ADP	d	1476	14	-	0/12/32/32	0/3/3/3
15	ADP	f	1479	14	-	0/12/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	1479	ADP	C5-C4	2.95	1.47	1.40
15	f	1479	ADP	C5-C4	2.97	1.47	1.40
13	A	1511	ATP	C5-C4	3.06	1.47	1.40
13	b	1510	ATP	C5-C4	3.06	1.47	1.40
13	a	1511	ATP	C5-C4	3.07	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	f	1479	ADP	N3-C2-N1	-6.17	123.49	128.86
15	F	1479	ADP	N3-C2-N1	-6.11	123.53	128.86
13	c	1511	ATP	N3-C2-N1	-5.96	123.67	128.86
15	d	1476	ADP	N3-C2-N1	-5.96	123.67	128.86
13	B	1510	ATP	N3-C2-N1	-5.93	123.69	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	1511	ATP	5	0
13	B	1510	ATP	1	0
13	C	1511	ATP	1	0
15	D	1476	ADP	2	0
15	F	1479	ADP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	t	1
9	T	1
11	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	9:GLN	C	10:LYS	N	9.37
1	T	168:LYS	C	169:GLU	N	0.99
1	t	168:LYS	C	169:GLU	N	0.99