



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 20, 2018 – 08:15 pm GMT

PDB ID : 6B8H
EMDB ID: : EMD-7067
Title : Mosaic model of yeast mitochondrial ATP synthase monomer
Authors : Guo, H.; Bueler, S.A.; Rubinstein, J.L.
Deposited on : 2017-10-07
Resolution : 3.60 Å(reported)

This is a wwPDB/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 : 1.7.3 (157068), CSD as539be (2018)
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) : trunk30686

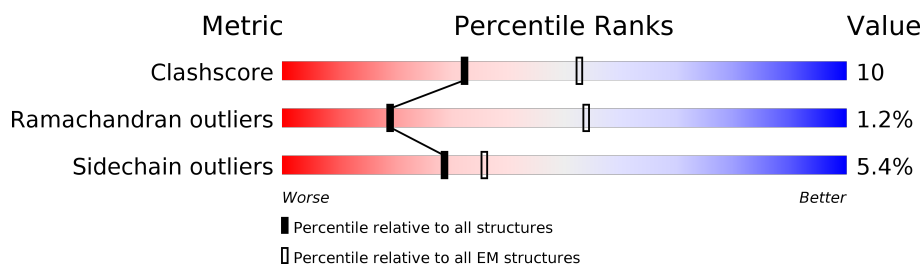
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
















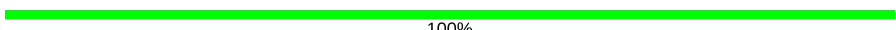
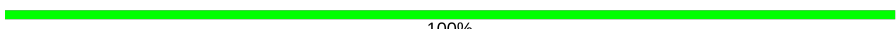




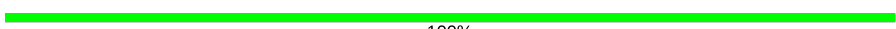
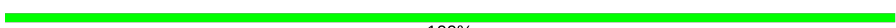




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

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	0	76	93% 5% .
1	1	76	96% ..
1	2	76	89% 8% ..
1	3	76	92% . . .
1	4	76	92% 7% .
1	5	76	88% 9% ..
1	6	76	88% 9% .
1	7	76	87% 9% .
1	8	76	93% 5% .


























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Mol	Chain	Length	Quality of chain
1	9	76	 92% 5% ..
1	J	76	 93% 5% ..
1	L	76	 96% ..
1	M	76	 88% 9% ..
1	N	76	 91% 5% ..
1	P	76	 91% 8% .
1	Q	76	 88% 9% ..
1	R	76	 89% 8% .
1	S	76	 91% 5% .
1	T	76	 95% ..
1	U	76	 92% 5% .
2	A	48	 88% 10% .
2	V	48	 88% 10% .
3	a	249	 100%
3	p	249	 100%
4	b	209	 93% ..
4	q	209	 93% ..
5	d	173	 88% . 9%
5	r	173	 88% . 9%
6	e	49	 100%
6	s	49	 100%
7	f	95	 85% . 12%
7	t	95	 85% . 12%
8	g	106	 99% .
8	u	106	 99% .


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Mol	Chain	Length	Quality of chain
9	i	59	 100%
9	w	59	 100%
10	k	68	 35% 65%
10	x	68	 35% 65%
11	B	510	 62% 31% . .
11	C	510	 69% 27% . .
11	K	510	 70% 27% . .
11	W	510	 63% 30% . .
11	X	510	 70% 26% . .
11	n	510	 94% 5% .
12	D	478	 73% 25% .
12	E	478	 67% 30% . .
12	F	478	 64% 31% . .
12	Y	478	 74% 24% . .
12	Z	478	 66% 31% . .
12	c	478	 92% 5% .
13	G	278	 62% 30% . 5%
13	j	278	 83% 12% 5%
14	H	138	 56% 22% 9% 14%
14	l	138	 72% 14% 14%
15	I	61	 43% 30% 5% . 21%
15	m	61	 62% 13% . 21%
16	O	195	 76% 5% . 17%
16	o	195	 78% . . 17%
17	h	21	 100%

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Mol	Chain	Length	Quality of chain
17	v	21	 100%

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 75614 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP synthase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	2	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	3	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	4	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	5	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	6	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	7	73	Total	C	N	O	S	0	0
			522	348	81	89	4		
1	8	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	9	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	0	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	L	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	M	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	N	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	P	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	Q	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	R	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	S	73	Total	C	N	O	S	0	0
			522	348	81	89	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	U	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	J	75	Total	C	N	O	S	0	0
			537	359	83	91	4		

- Molecule 2 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	48	Total	C	N	O	S	0	0
			410	287	59	60	4		
2	V	48	Total	C	N	O	S	0	0
			410	287	59	60	4		

- Molecule 3 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	249	Total	C	N	O	S	0	0
			1971	1338	296	326	11		
3	p	249	Total	C	N	O	S	0	0
			1971	1338	296	326	11		

- Molecule 4 is a protein called ATP synthase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	200	Total	C	N	O	S	0	0
			1153	715	210	227	1		
4	q	200	Total	C	N	O	S	0	0
			1153	715	210	227	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	157	Total	C	N	O	S	0	0
			930	573	173	182	2		
5	r	157	Total	C	N	O	S	0	0
			930	573	173	182	2		

- Molecule 6 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	49	Total	C	N	O	0	0
			245	147	49	49		
6	s	49	Total	C	N	O	0	0
			245	147	49	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	84	Total	C	N	O	S	0	0
			607	396	108	102	1		
7	t	84	Total	C	N	O	S	0	0
			607	396	108	102	1		

- Molecule 8 is a protein called AATP synthase subunit g.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	g	106	Total	C	N	O	0	0
			530	318	106	106		
8	u	106	Total	C	N	O	0	0
			530	318	106	106		

- Molecule 9 is a protein called ATP synthase subunit J, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	59	Total	C	N	O	S	0	0
			473	313	78	80	2		
9	w	59	Total	C	N	O	S	0	0
			473	313	78	80	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	24	Total	C	N	O	S	0	0
			180	122	30	27	1		
10	x	24	Total	C	N	O	S	0	0
			180	122	30	27	1		

- Molecule 11 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	501	Total	C	N	O	S	0	0
			3745	2363	665	714	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	492	Total	C	N	O	S	0	0
			3700	2336	656	705	3		
11	C	500	Total	C	N	O	S	0	0
			3739	2359	664	713	3		
11	n	501	Total	C	N	O	S	0	0
			3745	2363	665	714	3		
11	W	492	Total	C	N	O	S	0	0
			3700	2336	656	705	3		
11	X	500	Total	C	N	O	S	0	0
			3739	2359	664	713	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	470	Total	C	N	O	S	0	0
			3549	2250	604	689	6		
12	E	468	Total	C	N	O	S	0	0
			3536	2243	602	685	6		
12	F	469	Total	C	N	O	S	0	0
			3543	2247	603	687	6		
12	Y	470	Total	C	N	O	S	0	0
			3549	2250	604	689	6		
12	Z	468	Total	C	N	O	S	0	0
			3536	2243	602	685	6		
12	c	469	Total	C	N	O	S	0	0
			3543	2247	603	687	6		

- Molecule 13 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	265	Total	C	N	O	S	0	0
			2030	1277	355	388	10		
13	j	265	Total	C	N	O	S	0	0
			2030	1277	355	388	10		

- Molecule 14 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	119	Total	C	N	O	S	0	0
			751	470	133	146	2		
14	l	119	Total	C	N	O	S	0	0
			751	470	133	146	2		

- Molecule 15 is a protein called ATP synthase catalytic sector F1 epsilon subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	I	48	Total	C	N	O	0	0
			324	201	56	67		
15	m	48	Total	C	N	O	0	0
			324	201	56	67		

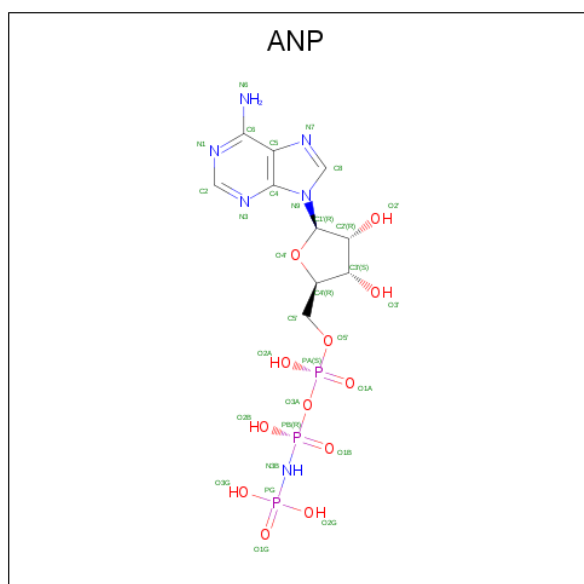
- Molecule 16 is a protein called ATP synthase subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	O	161	Total	C	N	O	0	0
			795	473	161	161		
16	o	161	Total	C	N	O	0	0
			795	473	161	161		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	h	21	Total	C	N	O	0	0
			105	63	21	21		
17	v	21	Total	C	N	O	0	0
			105	63	21	21		

- Molecule 18 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
18	K	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	B	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	C	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	D	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	F	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	n	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	W	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	X	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	Y	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	c	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
19	D	1	Total	Mg	0
			1	1	
19	K	1	Total	Mg	0
			1	1	
19	B	1	Total	Mg	0
			1	1	
19	C	1	Total	Mg	0
			1	1	
19	c	1	Total	Mg	0
			1	1	
19	W	1	Total	Mg	0
			1	1	
19	n	1	Total	Mg	0
			1	1	
19	X	1	Total	Mg	0
			1	1	
19	Y	1	Total	Mg	0
			1	1	
19	F	1	Total	Mg	0
			1	1	

3 Residue-property plots [i](#)


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.

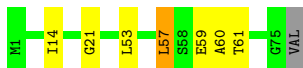
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 1:  96% ..



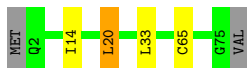
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 2:  89% 8% ..



- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 3:  92% ...




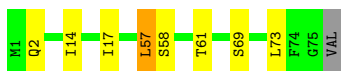
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 4:  92% 7% .




- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 5:  88% 9% ..




- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 6:  88% 9% .



- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 7:  87% 9% .



- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 8:  93% 5% .



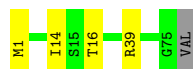
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 9:  92% 5% .



- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 0:  93% 5% .




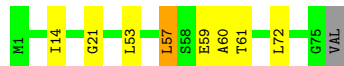
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain L:  96% . .



- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain M:  88% 9% . .



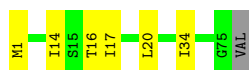
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain N:  91% 5% . .




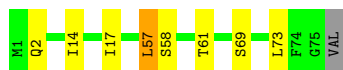
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain P:  91% 8% .




- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain Q:  88% 9% ..



- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain R:  89% 8% .



- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain S:  91% 5% .



- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain T:  95% ..



- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain U:  92% 5% .




- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain J:  93% 5% .




- Molecule 2: ATP synthase protein 8

Chain A:  88% 10% .



- Molecule 2: ATP synthase protein 8

Chain V:  88% 10% .



- Molecule 3: ATP synthase subunit a

Chain a:  100%



- Molecule 3: ATP synthase subunit a

Chain p:  100%



- Molecule 4: ATP synthase subunit 4, mitochondrial

Chain b:  93% ..




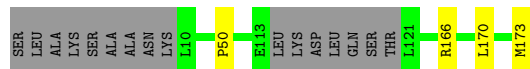
- Molecule 4: ATP synthase subunit 4, mitochondrial

Chain q:  93% ..




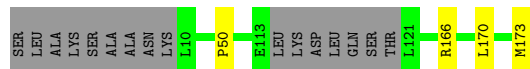
- Molecule 5: ATP synthase subunit d, mitochondrial

Chain d:  88% . 9%



- Molecule 5: ATP synthase subunit d, mitochondrial

Chain r:  88% . 9%



- Molecule 6: ATP synthase subunit e, mitochondrial

Chain e:  100%


There are no outlier residues recorded for this chain.

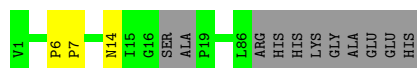
- Molecule 6: ATP synthase subunit e, mitochondrial

Chain s:  100%


There are no outlier residues recorded for this chain.

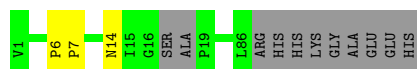
- Molecule 7: ATP synthase subunit f, mitochondrial

Chain f:  85% 12%



- Molecule 7: ATP synthase subunit f, mitochondrial

Chain t:  85% 12%



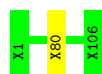
- Molecule 8: AATP synthase subunit g

Chain g:  99%



- Molecule 8: AATP synthase subunit g

Chain u:  99%



- Molecule 9: ATP synthase subunit J, mitochondrial

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: ATP synthase subunit J, mitochondrial

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: ATP synthase subunit K, mitochondrial

Chain k: 

MET	GLY	ALA	ALA	Y5	L28	VAL	VAL	PRO	ASN	PRO	PHE	LYS	SER	ALA	LYS	PRO	PRO	LYS	THR	VAL	ASP	ILE	LYS	THR	ASP	ASN	LYS	ASP	GLU	GLU	LYS	PHE	ILE	GLU	ASN	TYR	LEU	LYS	LYS	HIS	SER	GLU	LYS	GLN	ASP	ALA
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- Molecule 10: ATP synthase subunit K, mitochondrial

Chain x: 

MET	GLY	ALA	ALA	Y5	L28	VAL	VAL	PRO	ASN	PRO	PHE	LYS	SER	ALA	LYS	PRO	PRO	LYS	THR	VAL	ASP	ILE	LYS	THR	ASP	ASN	LYS	ASP	GLU	GLU	LYS	PHE	ILE	GLU	ASN	TYR	LEU	LYS	LYS	HIS	SER	GLU	LYS	GLN	ASP	ALA
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- Molecule 11: ATP synthase subunit alpha, mitochondrial

Chain K: 

ALA	SER	THR	K4	P7	S11	D23	N26	LEU	ASN	T30	G31	R32	V43	L34	A35	D38	R42	T49	Q50	A51	E52	E53	L54	V55	L66	N67	L68	E69	P70	V76	L77	D81	R82	K85	E86	L89	R92	T93	G94	V101	G102	P103	G104	L105
R108	V109	V110	D111	A112	N115	P116	I117	I138	R141	R142	S143	E146	G151	L152	L158	R163	G164	Q165	R166	E167	L168	I169	R173	Q174	L182	I185	C203	V204	K211	R212	S213	Q217	L218	V219	Q220	T221	K229	G239	I233	T237	A238	S239	E240	
A241	A242	P243	L244	Q245	T251	W258	L267	I268	V269	Y270	D271	L273	S274	L286	R293	E294	A295	L308	A311	A312	E316	R317	G319	G321	S322	L323	L326	P327	V328	I329	T340	P341	T348	D349	E355	L358	E459	L460	I363	R364	P365	A366	R375	
S378	V382	K383	Q387	S391	L394	F395	L396	A397	Q398	Y399	R400	E401	V402	F405	A406	Q407	PHE	S410	D411	L412	K417	V421	R422	G423	E424	R425	Q432	P437	T440	V444	P445	L446	V451	L455	T458	E459	L460	S461	E467	L471				
K475	M479	E480	L481	S492	L495	S501	F506	T509	PHE																																			

- Molecule 11: ATP synthase subunit alpha, mitochondrial

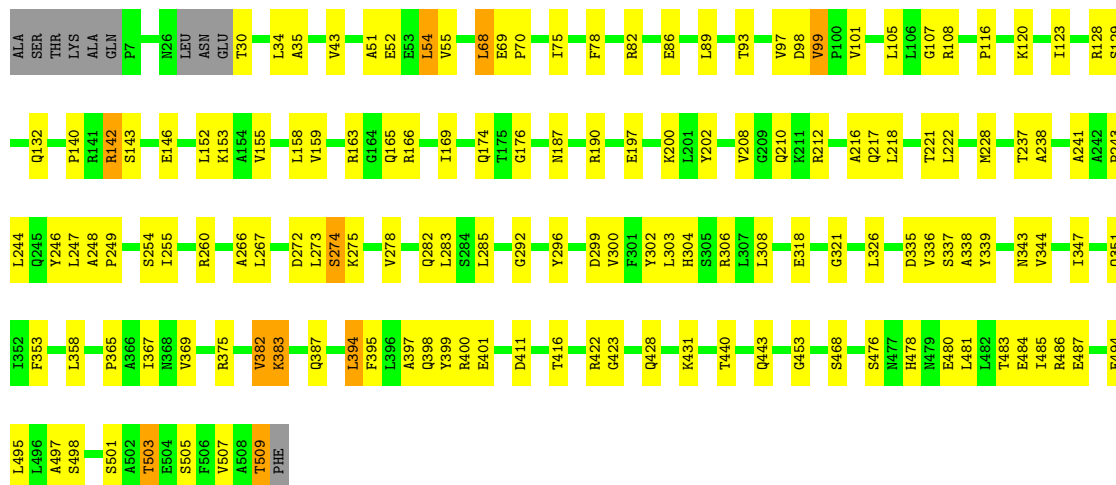
Chain B: 

ALA	SER	THR	LYS	ALA	GLN	PRO	THR	VAL	SER	I13	N26	LEU	V110	D111	GLU	T30	L34	G37	I40	V43	L46	I49	Q50	E53	L54	V55	E56	F57	V61	M64	A65	L66	N67	V73	G74	I75	V76	L77	S80	D81	R82	K85	L89	V90		
T93	I96	I99	V99	P100	V101	G102	P103	L106	G107	R108	V109	V110	D111	N115	P116	I123	A126	S129	M128	A135	L139	S231	P140	R141	R142	P147	V148	Q149	T150	G151	D156	R163	G164	Q165	I170	G171	D172	R173	Q174	G176	K177	V180	A181	L182	D183	T184
I185	Q188	K189	R190	V191	N192	C203	V206	A207	V208	K211	V215	L218	T221	E223	D226	A227	M228	K229	V230	S231	I232	I233	V234	A235	A242	P243	Y246	L247	A248	P249	F250	A253	S254	I255	V258	F259	R260	H265	A266	L267	I268	V269	Y270	D271	D272	
L273	S274	V278	A279	Q282	P290	P291	G292	R293	S305	L308	E309	L314	S315	E318	G321	T324	A325	L326	P327	V328	I329	E330	V336	S337	A338	P341	V344	I347	T348	Q351	I352	F353	L358	A366	R375	V376	G377	L378	S378	A379	A380	Q381	Y382			
K383	A384	L385	S391	L392	K393	L394	F395	A397	Q398	Y399	Q407	PHE	GLY	S410	A414	S415	T416	K417	V421	R422	G423	E424	R425	L426	T427	Q428	L429	Q432	P437	V444	P445	L446	I447	Y448	L460	I463	F466	F470	L471	S472	Y473	L474	K475	H478	M479	E480



- Molecule 11: ATP synthase subunit alpha, mitochondrial

Chain C: 69% 27%



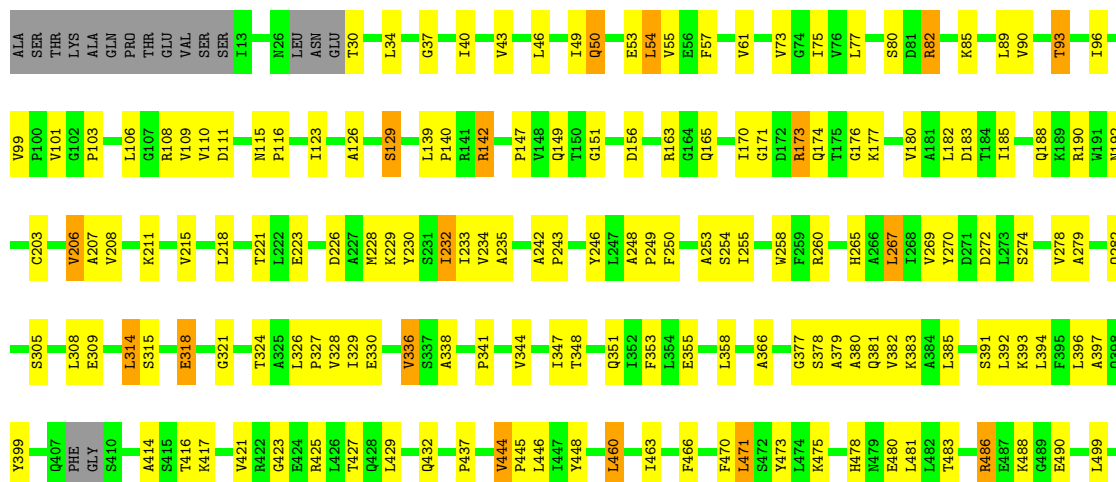
- Molecule 11: ATP synthase subunit alpha, mitochondrial

Chain n: 94% 5%



- Molecule 11: ATP synthase subunit alpha, mitochondrial

Chain W: 63% 30%



A502
T503
E504
S505
F506
V507
A508
T509
PHE

● Molecule 11: ATP synthase subunit alpha, mitochondrial

Chain X: 70% 26% . .

ALA SER THR LYS ALA GLN P7 R26 L26 LEU ASN GLU T30 L34 V43 A51 E52 E53 L54 V55 L68 E69 F70 I75 I78 F78 E86 L89 L93 T93 V97 D98 V99 P100 V101 L105 L106 G107 R108 V109 V110 G114 N115 P116 K120 I123 R128

S129 Q132 P140 R141 R142 R143 E146 L152 K153 A154 V155 L158 V159 R163 G164 L165 R166 I169 Q174 T175 G176 N187 R190 E197 L200 K200 L201 Y202 V208 G209 Q210 K211 R212 A216 Q217 S337 L218 L221 L222 M228 T237 A238 A241 A242

P243 L244 Q245 Y246 L247 A248 P249 S254 L255 R260 A266 L267 D272 L273 L274 S274 K275 V278 L283 G292 Y296 D299 V300 F301 Y302 L303 H304 S305 R306 L307 L308 E318 G321 L326 V336 S337 L338 Y339 N343 V344 I347 Q351 F353

P365 A366 N367 N368 V369 G375 V382 K383 Q387 L394 F395 L396 Q397 Q398 Y399 R400 E401 D411 T416 R422 G423 Q428 K431 T440 Q443 G453 S468 S476 N477 H478 R479 E480 L481 L482 T483 E484 E485 R486 E487 E494 L495 L496 S497 S498

S501 A502 T503 E504 S505 F506 V507 A508 T509 PHE

● Molecule 12: ATP synthase subunit beta, mitochondrial

Chain D: 73% 25% .

ALA SER ALA ALA ALA S6 A15 T20 V23 H24 F25 E26 Q27 S28 E29 F30 F31 A32 I33 L34 L46 Q52 H53 E56 N57 R60 T61 I62 D65 E74 R75 V76 L77 V85 G88 R89 E90 T91 L92 V98 I99 K110 S111 P121 P122 R244

L133 L134 E135 T136 P146 Y147 G154 L155 F156 G157 V158 V161 G162 T167 Q168 Q169 I174 S182 G188 E189 R190 T191 L197 M201 T204 G205 V206 T207 N208 G211 K214 M222 N223 E224 R229 V232 T235 L237 E241 Y242 F243 R244

D245 Q249 D250 V251 L252 T255 D256 N257 I258 F259 R260 Q263 S266 E267 F268 L271 L272 V279 L292 R295 I296 V304 T305 A309 Y310 G311 Y312 P313 A321 P322 L329 T332 S340 A347 Y348 D349 P350 R356 L357 F358 D359 V362

L378 I388 G392 L396 S397 R408 K409 I410 Q411 R412 F418 V423 F424 T425 G426 P428 L434 V438 G447 Y449 A456 E464 K469 A475 GLU ALA ASN

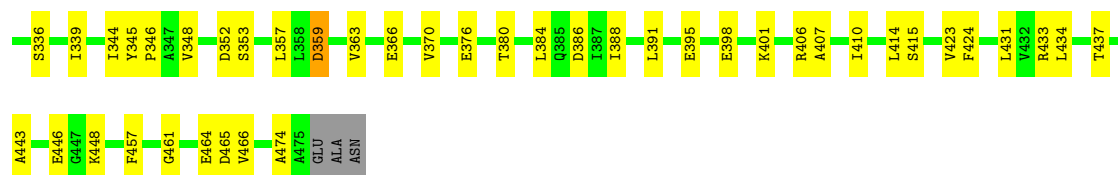
● Molecule 12: ATP synthase subunit beta, mitochondrial

Chain E: 67% 30% . .

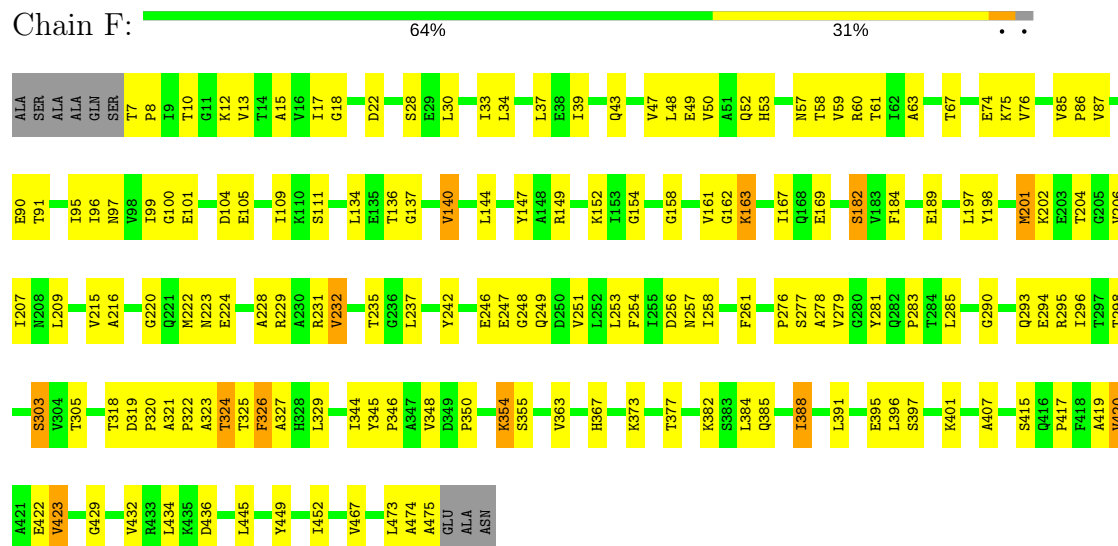
ALA SER ALA ALA GLN SER THR P8 A15 I20 V21 D22 E26 Q27 S28 E29 L30 P31 A32 I33 L34 L37 E38 I39 L48 F49 V50 A51 Q52 H53 L54 G55 E56 N57 R60 T61 G69 V76 V85 R89 T95 V98 I99 G100 E101 P102 I103 D104

P108 A119 S123 E126 Q127 S128 T129 E132 I133 I138 K139 V140 F141 D142 L143 P146 Y147 A148 R149 G150 G151 K152 I153 V165 F166 T167 Q168 E169 L170 G171 A177 G180 F181 S182 V187 T191 R191 L197 Y198 M201 T204 V215 F219

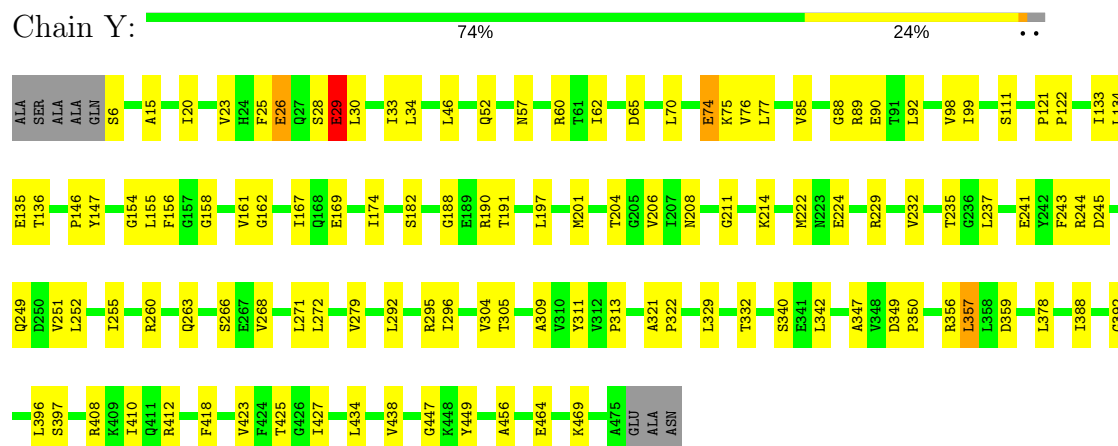
G220 R229 V232 T235 G236 L237 E241 Y242 F243 R244 Q249 D250 V251 T255 D256 N257 L258 F259 Y147 A148 R149 G150 G151 K152 I153 L271 S277 A278 P283 T284 L285 R295 I296 T297 T298 T299 K300 S303 V304 Q308 D319 P320 A321 P322 A323 T324 A331



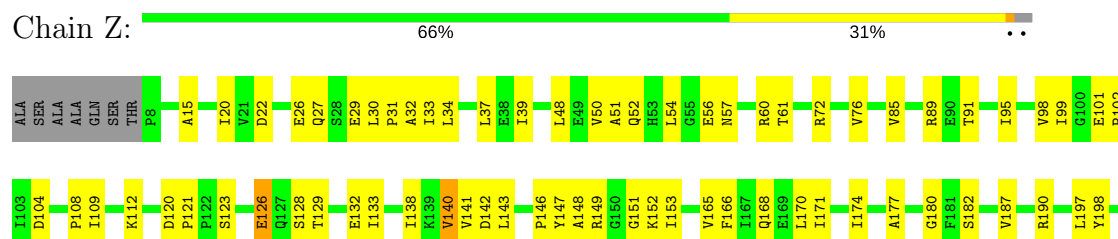
- Molecule 12: ATP synthase subunit beta, mitochondrial

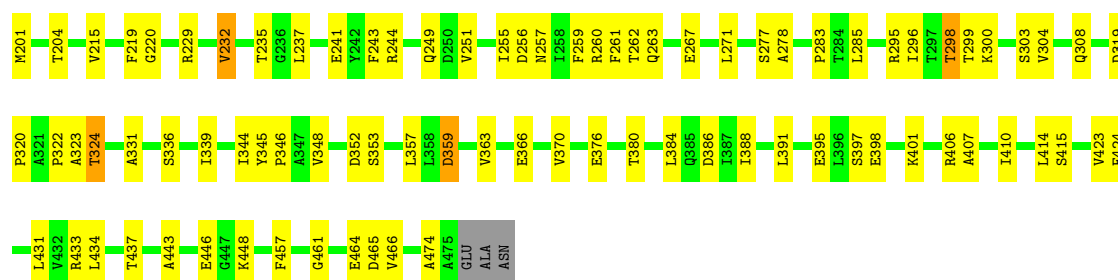


- Molecule 12: ATP synthase subunit beta, mitochondrial



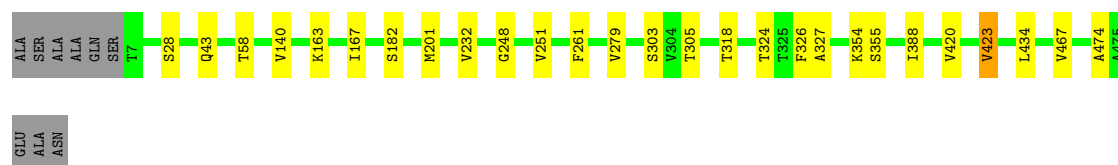
- Molecule 12: ATP synthase subunit beta, mitochondrial





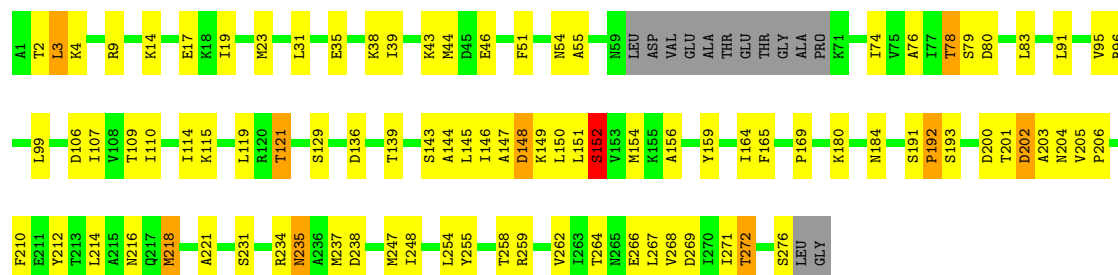
- Molecule 12: ATP synthase subunit beta, mitochondrial

Chain c: 92% 5% •



- Molecule 13: ATP synthase subunit gamma, mitochondrial

Chain G: 62% 30% 5% •



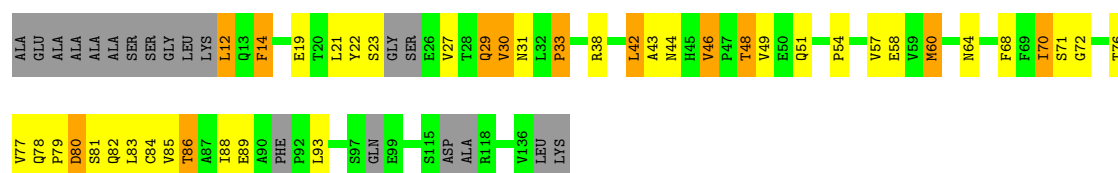
- Molecule 13: ATP synthase subunit gamma, mitochondrial

Chain j: 83% 12% 5% •

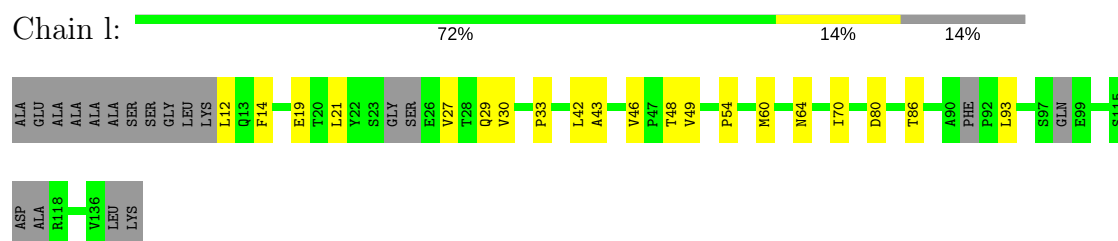


- Molecule 14: ATP synthase subunit delta, mitochondrial

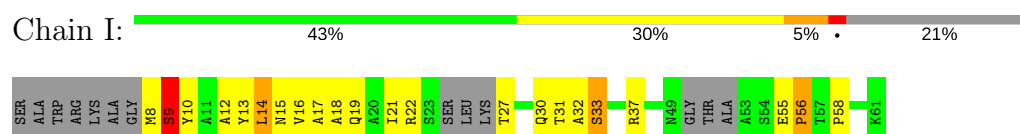
Chain H: 56% 22% 9% 14% •



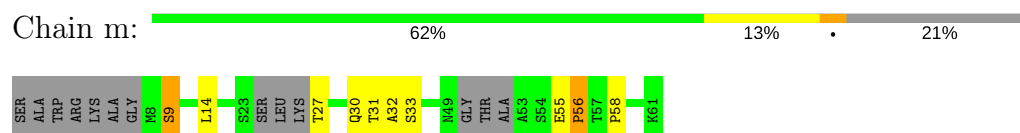
- Molecule 14: ATP synthase subunit delta, mitochondrial



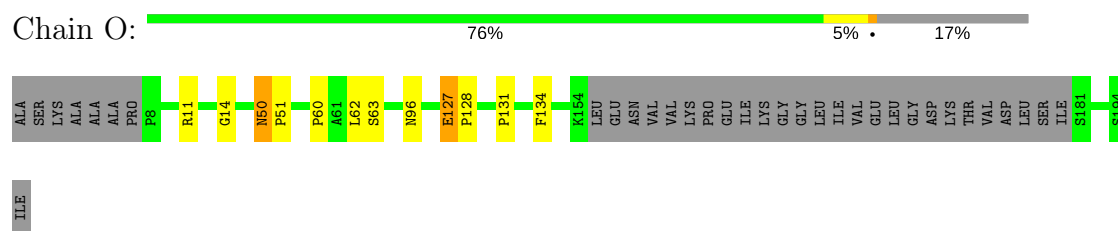
- Molecule 15: ATP synthase catalytic sector F1 epsilon subunit



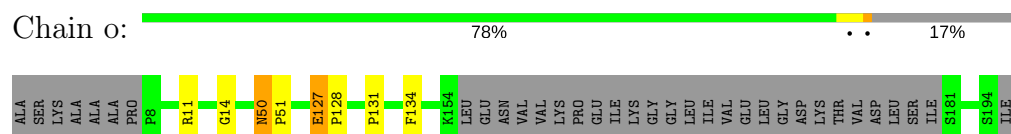
- Molecule 15: ATP synthase catalytic sector F1 epsilon subunit



- Molecule 16: ATP synthase subunit 5, mitochondrial



- Molecule 16: ATP synthase subunit 5, mitochondrial



- Molecule 17: ATP synthase subunit h



There are no outlier residues recorded for this chain.

- Molecule 17: ATP synthase subunit h



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	238848	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	71	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (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, ANP

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	0.34	0/545	0.60	0/737
1	1	0.35	0/545	0.55	0/737
1	2	0.38	0/545	0.67	1/737 (0.1%)
1	3	0.37	0/537	0.61	1/727 (0.1%)
1	4	0.34	0/545	0.61	0/737
1	5	0.32	0/545	0.58	0/737
1	6	0.33	0/537	0.60	0/727
1	7	0.31	0/529	0.56	0/716
1	8	0.32	0/545	0.56	0/737
1	9	0.32	0/537	0.57	0/727
1	J	0.34	0/545	0.61	0/737
1	L	0.35	0/545	0.55	0/737
1	M	0.38	0/545	0.67	1/737 (0.1%)
1	N	0.37	0/537	0.61	1/727 (0.1%)
1	P	0.34	0/545	0.60	0/737
1	Q	0.32	0/545	0.58	0/737
1	R	0.34	0/537	0.59	0/727
1	S	0.31	0/529	0.56	0/716
1	T	0.32	0/545	0.56	0/737
1	U	0.32	0/537	0.57	0/727
10	k	0.28	0/185	0.68	0/250
10	x	0.28	0/185	0.68	0/250
11	B	0.46	0/3753	0.62	0/5080
11	C	0.56	0/3793	0.71	2/5137 (0.0%)
11	K	0.50	0/3798	0.65	0/5143
11	W	0.46	0/3753	0.62	0/5080
11	X	0.56	0/3793	0.71	2/5137 (0.0%)
11	n	0.50	0/3798	0.65	0/5143
12	D	0.55	0/3605	0.67	0/4889
12	E	0.44	0/3592	0.59	1/4870 (0.0%)
12	F	0.52	0/3599	0.69	0/4881
12	Y	0.55	0/3605	0.67	0/4889

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
12	Z	0.44	0/3592	0.59	1/4870 (0.0%)
12	c	0.52	0/3599	0.69	0/4881
13	G	0.44	0/2055	0.58	0/2766
13	j	0.44	0/2055	0.58	0/2766
14	H	0.46	0/759	0.59	0/1040
14	l	0.46	0/759	0.59	0/1040
15	I	0.48	0/326	0.80	2/445 (0.4%)
15	m	0.48	0/326	0.79	2/445 (0.4%)
16	O	0.61	0/793	0.99	2/1101 (0.2%)
16	o	0.62	0/793	0.99	2/1101 (0.2%)
2	A	0.50	0/422	0.77	1/570 (0.2%)
2	V	0.50	0/422	0.77	1/570 (0.2%)
3	a	0.45	0/2023	0.70	0/2758
3	p	0.45	0/2023	0.70	0/2758
4	b	0.46	0/1159	0.72	2/1599 (0.1%)
4	q	0.46	0/1159	0.72	2/1599 (0.1%)
5	d	0.56	0/936	0.81	1/1286 (0.1%)
5	r	0.56	0/936	0.81	1/1286 (0.1%)
7	f	0.40	0/624	0.64	2/845 (0.2%)
7	t	0.41	0/624	0.64	2/845 (0.2%)
9	i	0.42	0/488	0.60	0/659
9	w	0.42	0/488	0.60	0/659
All	All	0.48	0/74640	0.66	30/101276 (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
15	I	0	1
15	m	0	1
16	O	0	1
16	o	0	1
4	b	0	1
4	q	0	1
8	g	0	2
8	u	0	2
All	All	0	10

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	r	170	LEU	CA-CB-CG	7.82	133.28	115.30
5	d	170	LEU	CA-CB-CG	7.81	133.25	115.30
2	V	26	LEU	CA-CB-CG	7.74	133.09	115.30
2	A	26	LEU	CA-CB-CG	7.73	133.08	115.30
15	m	56	PRO	N-CA-CB	6.38	110.96	103.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	I	9	SER	Peptide
16	O	50	ASN	Peptide
4	b	186	ASN	Peptide
8	g	80	UNK	Mainchain,Peptide
4	q	186	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	537	0	582	5	0
1	1	537	0	582	3	0
1	2	537	0	582	5	0
1	3	529	0	570	4	0
1	4	537	0	582	5	0
1	5	537	0	582	6	0
1	6	529	0	570	7	0
1	7	522	0	570	19	0
1	8	537	0	582	10	0
1	9	529	0	570	5	0
1	J	537	0	582	5	0
1	L	537	0	582	3	0
1	M	537	0	582	6	0
1	N	529	0	570	5	0
1	P	537	0	582	6	0
1	Q	537	0	582	6	0
1	R	529	0	570	5	0
1	S	522	0	570	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	537	0	582	4	0
1	U	529	0	570	5	0
2	A	410	0	444	3	0
2	V	410	0	444	3	0
3	a	1971	0	2071	0	0
3	p	1971	0	2071	0	0
4	b	1153	0	781	0	0
4	q	1153	0	781	0	0
5	d	930	0	618	0	0
5	r	930	0	618	0	0
6	e	245	0	51	0	0
6	s	245	0	51	0	0
7	f	607	0	527	0	0
7	t	607	0	527	0	0
8	g	530	0	108	0	0
8	u	530	0	108	0	0
9	i	473	0	476	0	0
9	w	473	0	476	0	0
10	k	180	0	192	0	0
10	x	180	0	192	0	0
11	B	3700	0	3749	119	0
11	C	3739	0	3767	91	0
11	K	3745	0	3769	89	0
11	W	3700	0	3749	110	0
11	X	3739	0	3767	86	0
11	n	3745	0	3769	0	0
12	D	3549	0	3620	75	0
12	E	3536	0	3610	94	0
12	F	3543	0	3615	109	0
12	Y	3549	0	3620	69	0
12	Z	3536	0	3610	97	0
12	c	3543	0	3615	0	0
13	G	2030	0	2081	51	0
13	j	2030	0	2081	0	0
14	H	751	0	598	55	0
14	l	751	0	598	0	0
15	I	324	0	249	20	0
15	m	324	0	249	0	0
16	O	795	0	367	24	0
16	o	795	0	367	0	0
17	h	105	0	23	0	0
17	v	105	0	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	B	31	0	13	1	0
18	C	31	0	13	3	0
18	D	31	0	13	3	0
18	F	31	0	13	7	0
18	K	31	0	13	1	0
18	W	31	0	13	1	0
18	X	31	0	13	3	0
18	Y	31	0	13	3	0
18	c	31	0	13	0	0
18	n	31	0	13	0	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	D	1	0	0	0	0
19	F	1	0	0	0	0
19	K	1	0	0	0	0
19	W	1	0	0	0	0
19	X	1	0	0	0	0
19	Y	1	0	0	0	0
19	c	1	0	0	0	0
19	n	1	0	0	0	0
All	All	75614	0	73106	1086	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 10.

The worst 5 of 1086 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)
1:8:41:PRO:CG	14:H:42:LEU:HD11	1.46	1.42
12:E:27:GLN:NE2	16:O:63:SER:CB	1.88	1.34
1:7:40:ASN:ND2	14:H:42:LEU:HB3	1.40	1.34
16:O:63:SER:CB	12:Z:27:GLN:NE2	374.65	1.33
16:O:63:SER:CB	12:Z:27:GLN:HE21	373.89	1.26

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	73/76 (96%)	73 (100%)	0	0	100	100
1	1	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	3	72/76 (95%)	72 (100%)	0	0	100	100
1	4	73/76 (96%)	73 (100%)	0	0	100	100
1	5	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
1	6	72/76 (95%)	72 (100%)	0	0	100	100
1	7	71/76 (93%)	71 (100%)	0	0	100	100
1	8	73/76 (96%)	73 (100%)	0	0	100	100
1	9	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
1	J	73/76 (96%)	73 (100%)	0	0	100	100
1	L	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	M	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	N	72/76 (95%)	72 (100%)	0	0	100	100
1	P	73/76 (96%)	73 (100%)	0	0	100	100
1	Q	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
1	R	72/76 (95%)	72 (100%)	0	0	100	100
1	S	71/76 (93%)	71 (100%)	0	0	100	100
1	T	73/76 (96%)	73 (100%)	0	0	100	100
1	U	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
2	A	46/48 (96%)	43 (94%)	2 (4%)	1 (2%)	7	44
2	V	46/48 (96%)	43 (94%)	2 (4%)	1 (2%)	7	44
3	a	247/249 (99%)	228 (92%)	19 (8%)	0	100	100
3	p	247/249 (99%)	228 (92%)	19 (8%)	0	100	100
4	b	196/209 (94%)	186 (95%)	6 (3%)	4 (2%)	8	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	q	196/209 (94%)	186 (95%)	6 (3%)	4 (2%)	8	46
5	d	153/173 (88%)	145 (95%)	7 (5%)	1 (1%)	24	66
5	r	153/173 (88%)	145 (95%)	7 (5%)	1 (1%)	24	66
7	f	80/95 (84%)	70 (88%)	9 (11%)	1 (1%)	13	55
7	t	80/95 (84%)	70 (88%)	9 (11%)	1 (1%)	13	55
9	i	57/59 (97%)	50 (88%)	7 (12%)	0	100	100
9	w	57/59 (97%)	50 (88%)	7 (12%)	0	100	100
10	k	22/68 (32%)	19 (86%)	3 (14%)	0	100	100
10	x	22/68 (32%)	19 (86%)	3 (14%)	0	100	100
11	B	486/510 (95%)	439 (90%)	45 (9%)	2 (0%)	36	75
11	C	496/510 (97%)	449 (90%)	44 (9%)	3 (1%)	27	68
11	K	495/510 (97%)	434 (88%)	56 (11%)	5 (1%)	17	60
11	W	486/510 (95%)	439 (90%)	45 (9%)	2 (0%)	36	75
11	X	496/510 (97%)	449 (90%)	44 (9%)	3 (1%)	27	68
11	n	495/510 (97%)	434 (88%)	56 (11%)	5 (1%)	17	60
12	D	468/478 (98%)	429 (92%)	37 (8%)	2 (0%)	36	75
12	E	466/478 (98%)	424 (91%)	36 (8%)	6 (1%)	13	55
12	F	467/478 (98%)	417 (89%)	42 (9%)	8 (2%)	10	49
12	Y	468/478 (98%)	429 (92%)	37 (8%)	2 (0%)	36	75
12	Z	466/478 (98%)	424 (91%)	36 (8%)	6 (1%)	13	55
12	c	467/478 (98%)	417 (89%)	42 (9%)	8 (2%)	10	49
13	G	261/278 (94%)	229 (88%)	25 (10%)	7 (3%)	5	40
13	j	261/278 (94%)	230 (88%)	24 (9%)	7 (3%)	5	40
14	H	109/138 (79%)	89 (82%)	15 (14%)	5 (5%)	2	26
14	l	109/138 (79%)	89 (82%)	15 (14%)	5 (5%)	2	26
15	I	42/61 (69%)	27 (64%)	9 (21%)	6 (14%)	0	4
15	m	42/61 (69%)	27 (64%)	9 (21%)	6 (14%)	0	4
16	O	157/195 (80%)	126 (80%)	24 (15%)	7 (4%)	3	27
16	o	157/195 (80%)	126 (80%)	24 (15%)	7 (4%)	3	27
All	All	9946/10594 (94%)	9045 (91%)	785 (8%)	116 (1%)	19	57

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	b	187	PRO
7	f	14	ASN
12	D	29	GLU
12	F	28	SER
13	G	152	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	55/56 (98%)	55 (100%)	0	100	100
1	1	55/56 (98%)	55 (100%)	0	100	100
1	2	55/56 (98%)	55 (100%)	0	100	100
1	3	54/56 (96%)	54 (100%)	0	100	100
1	4	55/56 (98%)	55 (100%)	0	100	100
1	5	55/56 (98%)	54 (98%)	1 (2%)	62	85
1	6	54/56 (96%)	54 (100%)	0	100	100
1	7	54/56 (96%)	54 (100%)	0	100	100
1	8	55/56 (98%)	55 (100%)	0	100	100
1	9	54/56 (96%)	54 (100%)	0	100	100
1	J	55/56 (98%)	55 (100%)	0	100	100
1	L	55/56 (98%)	55 (100%)	0	100	100
1	M	55/56 (98%)	55 (100%)	0	100	100
1	N	54/56 (96%)	54 (100%)	0	100	100
1	P	55/56 (98%)	55 (100%)	0	100	100
1	Q	55/56 (98%)	54 (98%)	1 (2%)	62	85
1	R	54/56 (96%)	54 (100%)	0	100	100
1	S	54/56 (96%)	54 (100%)	0	100	100
1	T	55/56 (98%)	55 (100%)	0	100	100
1	U	54/56 (96%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	47/47 (100%)	47 (100%)	0	100	100
2	V	47/47 (100%)	47 (100%)	0	100	100
3	a	217/217 (100%)	216 (100%)	1 (0%)	90	96
3	p	217/217 (100%)	216 (100%)	1 (0%)	90	96
4	b	48/182 (26%)	48 (100%)	0	100	100
4	q	48/182 (26%)	48 (100%)	0	100	100
5	d	42/158 (27%)	40 (95%)	2 (5%)	28	65
5	r	42/158 (27%)	40 (95%)	2 (5%)	28	65
7	f	46/76 (60%)	46 (100%)	0	100	100
7	t	46/76 (60%)	46 (100%)	0	100	100
9	i	49/49 (100%)	49 (100%)	0	100	100
9	w	49/49 (100%)	49 (100%)	0	100	100
10	k	18/57 (32%)	18 (100%)	0	100	100
10	x	18/57 (32%)	18 (100%)	0	100	100
11	B	384/412 (93%)	348 (91%)	36 (9%)	9	42
11	C	384/412 (93%)	356 (93%)	28 (7%)	15	51
11	K	384/412 (93%)	365 (95%)	19 (5%)	27	64
11	W	384/412 (93%)	348 (91%)	36 (9%)	9	42
11	X	384/412 (93%)	356 (93%)	28 (7%)	15	51
11	n	384/412 (93%)	365 (95%)	19 (5%)	27	64
12	D	380/384 (99%)	360 (95%)	20 (5%)	25	63
12	E	378/384 (98%)	357 (94%)	21 (6%)	23	61
12	F	379/384 (99%)	359 (95%)	20 (5%)	25	63
12	Y	380/384 (99%)	360 (95%)	20 (5%)	25	63
12	Z	378/384 (98%)	357 (94%)	21 (6%)	23	61
12	c	379/384 (99%)	359 (95%)	20 (5%)	25	63
13	G	218/236 (92%)	191 (88%)	27 (12%)	5	29
13	j	218/236 (92%)	191 (88%)	27 (12%)	5	29
14	H	54/112 (48%)	39 (72%)	15 (28%)	0	3
14	l	54/112 (48%)	39 (72%)	15 (28%)	0	3
15	I	23/48 (48%)	20 (87%)	3 (13%)	4	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	m	23/48 (48%)	20 (87%)	3 (13%)	4	27
All	All	7194/8260 (87%)	6808 (95%)	386 (5%)	29	62

5 of 386 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	G	276	SER
11	W	40	ILE
13	j	216	ASN
14	H	29	GLN
5	r	173	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
13	G	216	ASN
11	n	174	GLN
13	j	90	GLN
15	I	30	GLN
11	n	407	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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	ANP	B	601	19	29,33,33	3.64	7 (24%)	29,52,52	2.13	8 (27%)
18	ANP	C	601	19	29,33,33	3.45	8 (27%)	29,52,52	2.28	8 (27%)
18	ANP	D	501	19	29,33,33	3.68	8 (27%)	29,52,52	2.19	8 (27%)
18	ANP	F	501	19	29,33,33	3.59	8 (27%)	29,52,52	2.34	8 (27%)
18	ANP	K	601	19	29,33,33	3.58	7 (24%)	29,52,52	2.04	8 (27%)
18	ANP	W	601	19	29,33,33	3.64	7 (24%)	29,52,52	2.13	8 (27%)
18	ANP	X	601	19	29,33,33	3.45	8 (27%)	29,52,52	2.27	8 (27%)
18	ANP	Y	501	19	29,33,33	3.69	8 (27%)	29,52,52	2.17	8 (27%)
18	ANP	c	501	19	29,33,33	3.60	8 (27%)	29,52,52	2.34	8 (27%)
18	ANP	n	601	19	29,33,33	3.59	7 (24%)	29,52,52	2.05	8 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	ANP	B	601	19	-	1/13/38/38	0/3/3/3
18	ANP	C	601	19	-	0/13/38/38	0/3/3/3
18	ANP	D	501	19	-	0/13/38/38	0/3/3/3
18	ANP	F	501	19	-	1/13/38/38	0/3/3/3
18	ANP	K	601	19	-	0/13/38/38	0/3/3/3
18	ANP	W	601	19	-	1/13/38/38	0/3/3/3
18	ANP	X	601	19	-	0/13/38/38	0/3/3/3
18	ANP	Y	501	19	-	0/13/38/38	0/3/3/3
18	ANP	c	501	19	-	1/13/38/38	0/3/3/3
18	ANP	n	601	19	-	0/13/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	601	ANP	C8-N7	2.03	1.38	1.34
18	D	501	ANP	C8-N7	2.10	1.38	1.34
18	X	601	ANP	C8-N7	2.10	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	501	ANP	C5-C4	2.11	1.45	1.40
18	Y	501	ANP	C8-N7	2.11	1.38	1.34

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	601	ANP	N3-C2-N1	-7.35	122.58	128.86
18	W	601	ANP	N3-C2-N1	-7.33	122.59	128.86
18	F	501	ANP	N3-C2-N1	-7.19	122.71	128.86
18	c	501	ANP	N3-C2-N1	-7.16	122.74	128.86
18	C	601	ANP	N3-C2-N1	-6.92	122.94	128.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	c	501	ANP	O1B-PB-N3B-PG
18	F	501	ANP	O1B-PB-N3B-PG
18	B	601	ANP	O1B-PB-N3B-PG
18	W	601	ANP	O1B-PB-N3B-PG

There are no ring outliers.

8 monomers are involved in 22 short contacts:

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

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.