



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 07:10 am GMT

PDB ID : 6TML
EMDB ID : EMD-10525
Title : Cryo-EM structure of Toxoplasma gondii mitochondrial ATP synthase hexamer, composite model
Authors : Muhleip, A.; Kock Flygaard, R.; Amunts, A.
Deposited on : 2019-12-04
Resolution : 4.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

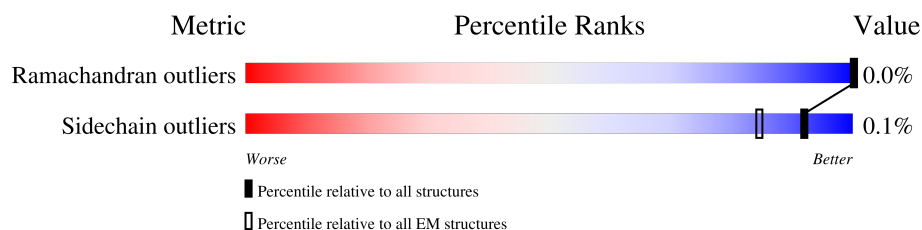
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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.
















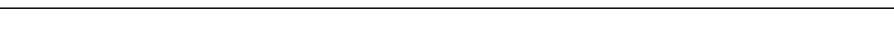
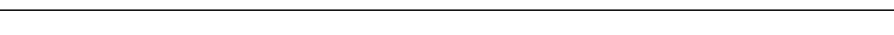
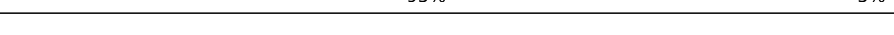
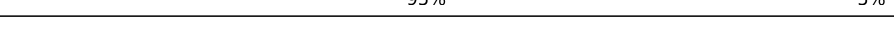
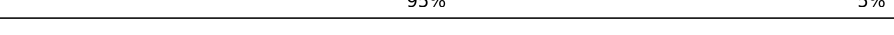
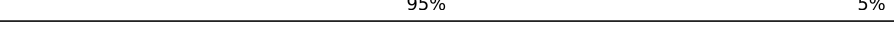
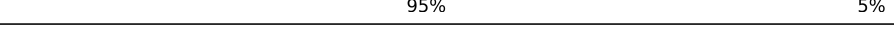
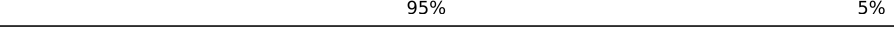




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	Q7	134	99% .
1	Q8	134	99% .
1	Q9	134	99% .
1	q7	134	99% .
1	q8	134	99% .
1	q9	134	99% .
2	I7	236	38% 62%
2	I8	236	38% 62%
2	I9	236	38% 62%
2	i7	236	38% 62%




















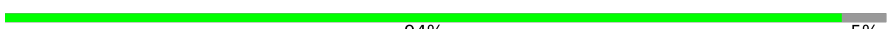
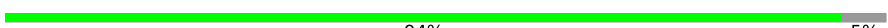

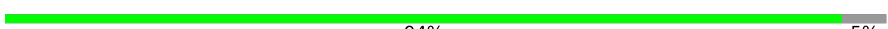


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Mol	Chain	Length	Quality of chain
2	i8	236	 38%62%
2	i9	236	 38%62%
3	T7	133	 69%31%
3	T8	133	 69%31%
3	T9	133	 69%31%
3	t7	133	 69%31%
3	t8	133	 69%31%
3	t9	133	 69%31%
4	G7	252	 44%56%
4	G8	252	 44%56%
4	G9	252	 44%56%
4	g7	252	 44%56%
4	g8	252	 44%56%
4	g9	252	 44%56%
5	O7	157	 95%5%
5	O8	157	 95%5%
5	O9	157	 95%5%
5	o7	157	 95%5%
5	o8	157	 95%5%
5	o9	157	 95%5%
6	K7	224	 52%48%
6	K8	224	 52%48%
6	K9	224	 52%48%
6	k7	224	 52%48%
6	k8	224	 52%48%




















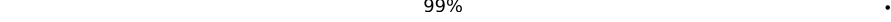
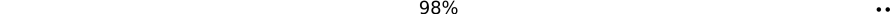
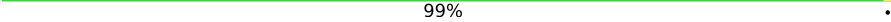
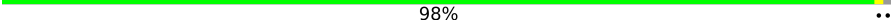

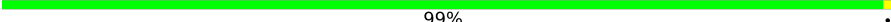
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Mol	Chain	Length	Quality of chain
6	k9	224	 52% 48%
7	J7	229	 76% 23%
7	J8	229	 76% 23%
7	J9	229	 76% 23%
7	j7	229	 76% 23%
7	j8	229	 76% 23%
7	j9	229	 76% 23%
8	S7	128	 74% 26%
8	S8	128	 74% 26%
8	S9	128	 74% 26%
8	s7	128	 74% 26%
8	s8	128	 74% 26%
8	s9	128	 74% 26%
9	U7	126	 75% 25%
9	U8	126	 75% 25%
9	U9	126	 75% 25%
9	u7	126	 75% 25%
9	u8	126	 75% 25%
9	u9	126	 75% 25%
10	H7	239	 94% 5%
10	H8	239	 94% 5%
10	H9	239	 94% 5%
10	h7	239	 94% 5%
10	h8	239	 94% 5%
10	h9	239	 94% 5%

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Mol	Chain	Length	Quality of chain
11	E7	325	 43% 57%
11	E8	325	 43% 57%
11	E9	325	 43% 57%
11	e7	325	 43% 57%
11	e8	325	 43% 57%
11	e9	325	 43% 57%
12	X7	83	 99% .
12	X8	83	 99% .
12	X9	83	 99% .
12	x7	83	 99% .
12	x8	83	 99% .
12	x9	83	 99% .
13	B7	571	 84% 15%
13	B8	571	 85% 15%
13	B9	571	 84% 15%
13	b7	571	 85% 15%
13	b8	571	 85% 15%
13	b9	571	 85% 15%
14	R7	134	 99% ..
14	R8	134	 98% ..
14	R9	134	 99% ..
14	r7	134	 98% ..
14	r8	134	 99% ..
14	r9	134	 99% ..
15	P7	138	 78% 22%












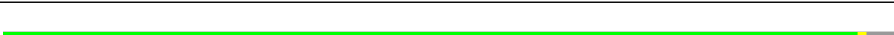

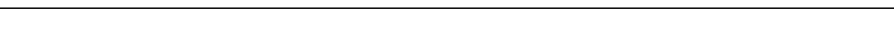
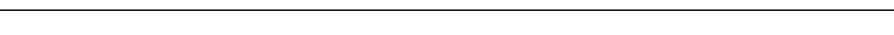
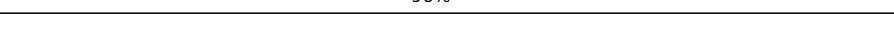
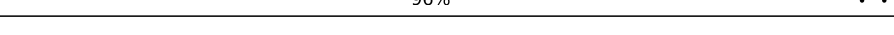
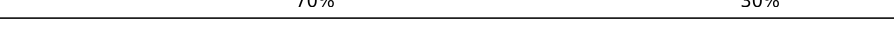







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Mol	Chain	Length	Quality of chain	
15	P8	138	<div><div></div></div>	78% 22%
15	P9	138	<div><div></div></div>	78% 22%
15	p7	138	<div><div></div></div>	78% 22%
15	p8	138	<div><div></div></div>	78% 22%
15	p9	138	<div><div></div></div>	78% 22%
16	V7	111	<div><div></div></div>	99% .
16	V8	111	<div><div></div></div>	99% .
16	V9	111	<div><div></div></div>	99% .
16	v7	111	<div><div></div></div>	99% .
16	v8	111	<div><div></div></div>	99% .
16	v9	111	<div><div></div></div>	99% .
17	L7	208	<div><div></div></div>	100%
17	L8	208	<div><div></div></div>	100%
17	L9	208	<div><div></div></div>	100%
17	l7	208	<div><div></div></div>	100%
17	l8	208	<div><div></div></div>	100%
17	l9	208	<div><div></div></div>	100%
18	C7	398	<div><div></div></div>	31% 69%
18	C8	398	<div><div></div></div>	31% 69%
18	C9	398	<div><div></div></div>	31% 69%
18	c7	398	<div><div></div></div>	31% 69%
18	c8	398	<div><div></div></div>	31% 69%
18	c9	398	<div><div></div></div>	31% 69%
19	D7	310	<div><div></div></div>	82% 18%
19	D8	310	<div><div></div></div>	82% 18%












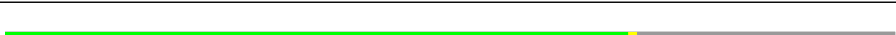

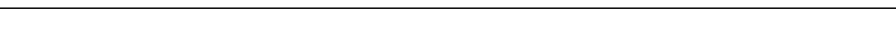
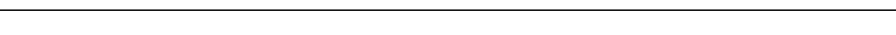
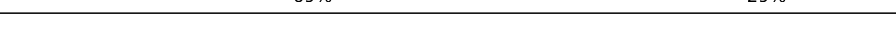

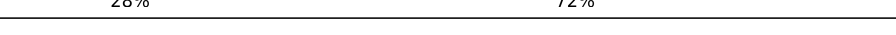







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Mol	Chain	Length	Quality of chain
19	D9	310	 82% 18%
19	d7	310	 82% 18%
19	d8	310	 82% 18%
19	d9	310	 82% 18%
20	M7	205	 47% 53%
20	M8	205	 47% 53%
20	M9	205	 47% 53%
20	m7	205	 47% 53%
20	m8	205	 47% 53%
20	m9	205	 47% 53%
21	N7	166	 96% ..
21	N8	166	 96% ..
21	N9	166	 96% ..
21	n7	166	 96% ..
21	n8	166	 96% ..
21	n9	166	 96% ..
22	F7	267	 70% 30%
22	F8	267	 70% 30%
22	F9	267	 70% 30%
22	f7	267	 70% 30%
22	f8	267	 70% 30%
22	f9	267	 70% 30%
23	W7	106	 91% 9%
23	W8	106	 91% 9%
23	W9	106	 91% 9%














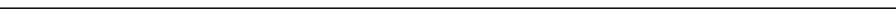











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Mol	Chain	Length	Quality of chain
23	w7	106	
23	w8	106	
23	w9	106	
24	A7	536	
24	A8	536	
24	A9	536	
24	a7	536	
24	a8	536	
24	a9	536	
25	G1	252	
25	G2	252	
25	G3	252	
25	G4	252	
25	G5	252	
25	G6	252	
26	i1	145	
26	i2	145	
26	i3	145	
26	i4	145	
26	i5	145	
26	i6	145	
27	A1	565	
27	A2	565	
27	A3	565	
27	A4	565	


























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Mol	Chain	Length	Quality of chain	
27	A5	565		91% 9%
27	A6	565		91% 9%
27	C1	565		90% 10%
27	C2	565		90% 10%
27	C3	565		90% 10%
27	C4	565		90% 10%
27	C5	565		90% 10%
27	C6	565		90% 10%
27	E1	565		90% 10%
27	E2	565		90% 10%
27	E3	565		90% 10%
27	E4	565		90% 10%
27	E5	565		90% 10%
27	E6	565		90% 10%
28	B1	560		85% 14%
28	B2	560		85% 14%
28	B3	560		85% 14%
28	B4	560		85% 14%
28	B5	560		85% 14%
28	B6	560		85% 14%
28	D1	560		85% 15%
28	D2	560		85% 15%
28	D3	560		85% 15%
28	D4	560		85% 15%
28	D5	560		85% 15%


























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Mol	Chain	Length	Quality of chain	
28	D6	560		85% 15%
28	F1	560		85% 15%
28	F2	560		85% 15%
28	F3	560		85% 15%
28	F4	560		85% 15%
28	F5	560		85% 15%
28	F6	560		85% 15%
29	g1	314		87% 13%
29	g2	314		87% 13%
29	g3	314		87% 13%
29	g4	314		87% 13%
29	g5	314		87% 13%
29	g6	314		87% 13%
30	d1	183		78% 22%
30	d2	183		78% 22%
30	d3	183		78% 22%
30	d4	183		78% 22%
30	d5	183		78% 22%
30	d6	183		78% 22%
31	e1	73		89% 11%
31	e2	73		89% 11%
31	e3	73		89% 11%
31	e4	73		89% 11%
31	e5	73		89% 11%
31	e6	73		89% 11%













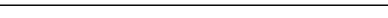


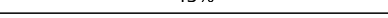
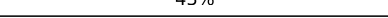
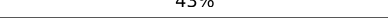
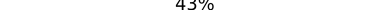
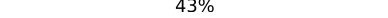
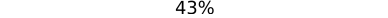
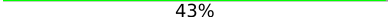
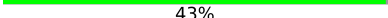
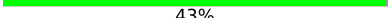

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Mol	Chain	Length	Quality of chain	
32	H1	166		
32	H2	166		
32	H3	166		
32	H4	166		
32	H5	166		
32	H6	166		
32	I1	166		
32	I2	166		
32	I3	166		
32	I4	166		
32	I5	166		
32	I6	166		
32	J1	166		
32	J2	166		
32	J3	166		
32	J4	166		
32	J5	166		
32	J6	166		
32	K1	166		
32	K2	166		
32	K3	166		
32	K4	166		
32	K5	166		
32	K6	166		
32	L1	166		

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Mol	Chain	Length	Quality of chain	
32	L2	166	 43%	57%
32	L3	166	 43%	57%
32	L4	166	 43%	57%
32	L5	166	 43%	57%
32	L6	166	 43%	57%
32	M1	166	 43%	57%
32	M2	166	 43%	57%
32	M3	166	 43%	57%
32	M4	166	 43%	57%
32	M5	166	 43%	57%
32	M6	166	 43%	57%
32	N1	166	 43%	57%
32	N2	166	 43%	57%
32	N3	166	 43%	57%
32	N4	166	 43%	57%
32	N5	166	 43%	57%
32	N6	166	 43%	57%
32	O1	166	 43%	57%
32	O2	166	 43%	57%
32	O3	166	 43%	57%
32	O4	166	 43%	57%
32	O5	166	 43%	57%
32	O6	166	 43%	57%
32	P1	166	 43%	57%
32	P2	166	 43%	57%

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Mol	Chain	Length	Quality of chain	
32	P3	166	<div><div></div></div>	43% 57%
32	P4	166	<div><div></div></div>	43% 57%
32	P5	166	<div><div></div></div>	43% 57%
32	P6	166	<div><div></div></div>	43% 57%
32	Q1	166	<div><div></div></div>	43% 57%
32	Q2	166	<div><div></div></div>	43% 57%
32	Q3	166	<div><div></div></div>	43% 57%
32	Q4	166	<div><div></div></div>	43% 57%
32	Q5	166	<div><div></div></div>	43% 57%
32	Q6	166	<div><div></div></div>	43% 57%

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 776906 atoms, of which 388256 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 ATPTG11.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	q7	133	Total	C	H	N	O	S	0	0
			2119	674	1044	194	202	5		
1	Q7	133	Total	C	H	N	O	S	0	0
			2120	674	1045	194	202	5		
1	q8	133	Total	C	H	N	O	S	0	0
			2120	674	1045	194	202	5		
1	Q8	133	Total	C	H	N	O	S	0	0
			2119	674	1044	194	202	5		
1	q9	133	Total	C	H	N	O	S	0	0
			2119	674	1044	194	202	5		
1	Q9	133	Total	C	H	N	O	S	0	0
			2120	674	1045	194	202	5		

- Molecule 2 is a protein called ATPTG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	i7	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		
2	I7	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		
2	i8	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		
2	I8	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		
2	i9	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		
2	I9	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		

- Molecule 3 is a protein called ATPTG14.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	t7	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	T7	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		
3	t8	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		
3	T8	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		
3	t9	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		
3	T9	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		

- Molecule 4 is a protein called ATPTG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	g7	112	Total	C	H	N	O	S	0	0
			1732	548	856	152	168	8		
4	G7	112	Total	C	H	N	O	S	0	0
			1731	548	855	152	168	8		
4	g8	112	Total	C	H	N	O	S	0	0
			1731	548	855	152	168	8		
4	G8	112	Total	C	H	N	O	S	0	0
			1732	548	856	152	168	8		
4	g9	112	Total	C	H	N	O	S	0	0
			1732	548	856	152	168	8		
4	G9	112	Total	C	H	N	O	S	0	0
			1731	548	855	152	168	8		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g7	51	VAL	PHE	conflict	UNP S7WD71
g7	73	CYS	SER	conflict	UNP S7WD71
g7	110	LYS	GLU	conflict	UNP S7WD71
g7	233	THR	MET	conflict	UNP S7WD71
G7	51	VAL	PHE	conflict	UNP S7WD71
G7	73	CYS	SER	conflict	UNP S7WD71
G7	110	LYS	GLU	conflict	UNP S7WD71
G7	233	THR	MET	conflict	UNP S7WD71
g8	51	VAL	PHE	conflict	UNP S7WD71
g8	73	CYS	SER	conflict	UNP S7WD71
g8	110	LYS	GLU	conflict	UNP S7WD71
g8	233	THR	MET	conflict	UNP S7WD71

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Chain	Residue	Modelled	Actual	Comment	Reference
G8	51	VAL	PHE	conflict	UNP S7WD71
G8	73	CYS	SER	conflict	UNP S7WD71
G8	110	LYS	GLU	conflict	UNP S7WD71
G8	233	THR	MET	conflict	UNP S7WD71
g9	51	VAL	PHE	conflict	UNP S7WD71
g9	73	CYS	SER	conflict	UNP S7WD71
g9	110	LYS	GLU	conflict	UNP S7WD71
g9	233	THR	MET	conflict	UNP S7WD71
G9	51	VAL	PHE	conflict	UNP S7WD71
G9	73	CYS	SER	conflict	UNP S7WD71
G9	110	LYS	GLU	conflict	UNP S7WD71
G9	233	THR	MET	conflict	UNP S7WD71

- Molecule 5 is a protein called subunit k.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	o7	149	Total	C	H	N	O	S	0	0
			2416	786	1196	210	219	5		
5	O7	149	Total	C	H	N	O	S	0	0
			2416	786	1196	210	219	5		
5	o8	149	Total	C	H	N	O	S	0	0
			2416	786	1196	210	219	5		
5	O8	149	Total	C	H	N	O	S	0	0
			2416	786	1196	210	219	5		
5	o9	149	Total	C	H	N	O	S	0	0
			2416	786	1196	210	219	5		
5	O9	149	Total	C	H	N	O	S	0	0
			2416	786	1196	210	219	5		

- Molecule 6 is a protein called subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	k7	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		
6	K7	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		
6	k8	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		
6	K8	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		
6	k9	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		

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Mol	Chain	Residues	Atoms						AltConf	Trace
6	K9	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		

- Molecule 7 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	j7	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		
7	J7	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		
7	j8	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		
7	J8	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		
7	j9	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		
7	J9	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		

- Molecule 8 is a protein called ATPTG13.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	s7	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		
8	S7	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		
8	s8	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		
8	S8	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		
8	s9	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		
8	S9	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		

- Molecule 9 is a protein called ATPTG15.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	u7	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		
9	U7	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
9	u8	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		
9	U8	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		
9	u9	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		
9	U9	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		

- Molecule 10 is a protein called ATPTG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	h7	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		
10	H7	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		
10	h8	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		
10	H8	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		
10	h9	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		
10	H9	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h7	89	ASN	HIS	conflict	UNP A0A125YL08
H7	89	ASN	HIS	conflict	UNP A0A125YL08
h8	89	ASN	HIS	conflict	UNP A0A125YL08
H8	89	ASN	HIS	conflict	UNP A0A125YL08
h9	89	ASN	HIS	conflict	UNP A0A125YL08
H9	89	ASN	HIS	conflict	UNP A0A125YL08

- Molecule 11 is a protein called ATPTG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	e7	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		
11	E7	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		

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Mol	Chain	Residues	Atoms						AltConf	Trace
11	e8	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		
11	E8	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		
11	e9	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		
11	E9	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e7	?	-	LYS	deletion	UNP A0A125YLR0
e7	63	PRO	SER	conflict	UNP A0A125YLR0
e7	99	LEU	PRO	conflict	UNP A0A125YLR0
e7	312	ALA	THR	conflict	UNP A0A125YLR0
E7	?	-	LYS	deletion	UNP A0A125YLR0
E7	63	PRO	SER	conflict	UNP A0A125YLR0
E7	99	LEU	PRO	conflict	UNP A0A125YLR0
E7	312	ALA	THR	conflict	UNP A0A125YLR0
e8	?	-	LYS	deletion	UNP A0A125YLR0
e8	63	PRO	SER	conflict	UNP A0A125YLR0
e8	99	LEU	PRO	conflict	UNP A0A125YLR0
e8	312	ALA	THR	conflict	UNP A0A125YLR0
E8	?	-	LYS	deletion	UNP A0A125YLR0
E8	63	PRO	SER	conflict	UNP A0A125YLR0
E8	99	LEU	PRO	conflict	UNP A0A125YLR0
E8	312	ALA	THR	conflict	UNP A0A125YLR0
e9	?	-	LYS	deletion	UNP A0A125YLR0
e9	63	PRO	SER	conflict	UNP A0A125YLR0
e9	99	LEU	PRO	conflict	UNP A0A125YLR0
e9	312	ALA	THR	conflict	UNP A0A125YLR0
E9	?	-	LYS	deletion	UNP A0A125YLR0
E9	63	PRO	SER	conflict	UNP A0A125YLR0
E9	99	LEU	PRO	conflict	UNP A0A125YLR0
E9	312	ALA	THR	conflict	UNP A0A125YLR0

- Molecule 12 is a protein called ATPTG17,ATPTG17,ATPTG17.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	x7	82	Total	C	H	N	O	S	0	0
			1298	420	639	116	120	3		

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Mol	Chain	Residues	Atoms						AltConf	Trace
12	X7	82	Total	C	H	N	O	S	0	0
			1298	420	639	116	120	3		
12	x8	82	Total	C	H	N	O	S	0	0
			1298	420	639	116	120	3		
12	X8	82	Total	C	H	N	O	S	0	0
			1298	420	639	116	120	3		
12	x9	82	Total	C	H	N	O	S	0	0
			1298	420	639	116	120	3		
12	X9	82	Total	C	H	N	O	S	0	0
			1298	420	639	116	120	3		

- Molecule 13 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	b7	484	Total	C	H	N	O	S	0	0
			7840	2525	3908	652	740	15		
13	B7	484	Total	C	H	N	O	S	0	0
			7839	2525	3907	652	740	15		
13	b8	484	Total	C	H	N	O	S	0	0
			7838	2525	3906	652	740	15		
13	B8	484	Total	C	H	N	O	S	0	0
			7840	2525	3908	652	740	15		
13	b9	484	Total	C	H	N	O	S	0	0
			7840	2525	3908	652	740	15		
13	B9	484	Total	C	H	N	O	S	0	0
			7839	2525	3907	652	740	15		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b7	50	LEU	SER	conflict	UNP S7V2T0
b7	474	THR	ALA	conflict	UNP S7V2T0
B7	50	LEU	SER	conflict	UNP S7V2T0
B7	474	THR	ALA	conflict	UNP S7V2T0
b8	50	LEU	SER	conflict	UNP S7V2T0
b8	474	THR	ALA	conflict	UNP S7V2T0
B8	50	LEU	SER	conflict	UNP S7V2T0
B8	474	THR	ALA	conflict	UNP S7V2T0
b9	50	LEU	SER	conflict	UNP S7V2T0
b9	474	THR	ALA	conflict	UNP S7V2T0
B9	50	LEU	SER	conflict	UNP S7V2T0
B9	474	THR	ALA	conflict	UNP S7V2T0

- Molecule 14 is a protein called ATPTG12.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	r7	133	Total	C	H	N	O	S	0	0
			2142	681	1071	182	202	6		
14	R7	133	Total	C	H	N	O	S	0	0
			2144	681	1073	182	202	6		
14	r8	133	Total	C	H	N	O	S	0	0
			2143	681	1072	182	202	6		
14	R8	133	Total	C	H	N	O	S	0	0
			2142	681	1071	182	202	6		
14	r9	133	Total	C	H	N	O	S	0	0
			2143	681	1072	182	202	6		
14	R9	133	Total	C	H	N	O	S	0	0
			2143	681	1072	182	202	6		

- Molecule 15 is a protein called ATPTG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	p7	108	Total	C	H	N	O	S	0	0
			1711	553	847	148	157	6		
15	P7	108	Total	C	H	N	O	S	0	0
			1711	553	847	148	157	6		
15	p8	108	Total	C	H	N	O	S	0	0
			1711	553	847	148	157	6		
15	P8	108	Total	C	H	N	O	S	0	0
			1711	553	847	148	157	6		
15	p9	108	Total	C	H	N	O	S	0	0
			1711	553	847	148	157	6		
15	P9	108	Total	C	H	N	O	S	0	0
			1711	553	847	148	157	6		

- Molecule 16 is a protein called subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	v7	110	Total	C	H	N	O	S	0	0
			1801	590	888	170	148	5		
16	V7	110	Total	C	H	N	O	S	0	0
			1801	590	888	170	148	5		
16	v8	110	Total	C	H	N	O	S	0	0
			1801	590	888	170	148	5		
16	V8	110	Total	C	H	N	O	S	0	0
			1801	590	888	170	148	5		
16	v9	110	Total	C	H	N	O	S	0	0
			1801	590	888	170	148	5		

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Mol	Chain	Residues	Atoms						AltConf	Trace
16	V9	110	Total	C	H	N	O	S	0	0
			1801	590	888	170	148	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v7	54	ALA	VAL	conflict	UNP S7UQT7
V7	54	ALA	VAL	conflict	UNP S7UQT7
v8	54	ALA	VAL	conflict	UNP S7UQT7
V8	54	ALA	VAL	conflict	UNP S7UQT7
v9	54	ALA	VAL	conflict	UNP S7UQT7
V9	54	ALA	VAL	conflict	UNP S7UQT7

- Molecule 17 is a protein called ATPTG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	17	207	Total	C	H	N	O	S	0	0
			3273	1013	1647	298	305	10		
17	L7	207	Total	C	H	N	O	S	0	0
			3273	1013	1647	298	305	10		
17	18	207	Total	C	H	N	O	S	0	0
			3273	1013	1647	298	305	10		
17	L8	207	Total	C	H	N	O	S	0	0
			3273	1013	1647	298	305	10		
17	19	207	Total	C	H	N	O	S	0	0
			3273	1013	1647	298	305	10		
17	L9	207	Total	C	H	N	O	S	0	0
			3273	1013	1647	298	305	10		

- Molecule 18 is a protein called ATPTG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	c7	122	Total	C	H	N	O	S	0	0
			2029	656	999	189	184	1		
18	C7	122	Total	C	H	N	O	S	0	0
			2029	656	999	189	184	1		
18	c8	122	Total	C	H	N	O	S	0	0
			2029	656	999	189	184	1		
18	C8	122	Total	C	H	N	O	S	0	0
			2029	656	999	189	184	1		
18	c9	122	Total	C	H	N	O	S	0	0
			2029	656	999	189	184	1		

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Mol	Chain	Residues	Atoms						AltConf	Trace
18	C9	122	Total	C	H	N	O	S	0	0
			2029	656	999	189	184	1		

- Molecule 19 is a protein called ATPTG2.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	d7	254	Total	C	H	N	O	S	0	0
			4046	1323	1970	365	380	8		
19	D7	254	Total	C	H	N	O	S	0	0
			4046	1323	1970	365	380	8		
19	d8	254	Total	C	H	N	O	S	0	0
			4046	1323	1970	365	380	8		
19	D8	254	Total	C	H	N	O	S	0	0
			4046	1323	1970	365	380	8		
19	d9	254	Total	C	H	N	O	S	0	0
			4046	1323	1970	365	380	8		
19	D9	254	Total	C	H	N	O	S	0	0
			4046	1323	1970	365	380	8		

- Molecule 20 is a protein called subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	m7	96	Total	C	H	N	O	S	0	0
			1509	501	744	126	131	7		
20	M7	96	Total	C	H	N	O	S	0	0
			1509	501	744	126	131	7		
20	m8	96	Total	C	H	N	O	S	0	0
			1509	501	744	126	131	7		
20	M8	96	Total	C	H	N	O	S	0	0
			1509	501	744	126	131	7		
20	m9	96	Total	C	H	N	O	S	0	0
			1509	501	744	126	131	7		
20	M9	96	Total	C	H	N	O	S	0	0
			1509	501	744	126	131	7		

- Molecule 21 is a protein called ATPTG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	n7	160	Total	C	H	N	O	S	0	0
			2449	774	1202	227	235	11		
21	N7	160	Total	C	H	N	O	S	0	0
			2449	774	1202	227	235	11		

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Mol	Chain	Residues	Atoms						AltConf	Trace
21	n8	160	Total	C	H	N	O	S	0	0
			2449	774	1202	227	235	11		
21	N8	160	Total	C	H	N	O	S	0	0
			2449	774	1202	227	235	11		
21	n9	160	Total	C	H	N	O	S	0	0
			2449	774	1202	227	235	11		
21	N9	160	Total	C	H	N	O	S	0	0
			2449	774	1202	227	235	11		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n7	140	SER	ALA	conflict	UNP A0A125YUZ2
N7	140	SER	ALA	conflict	UNP A0A125YUZ2
n8	140	SER	ALA	conflict	UNP A0A125YUZ2
N8	140	SER	ALA	conflict	UNP A0A125YUZ2
n9	140	SER	ALA	conflict	UNP A0A125YUZ2
N9	140	SER	ALA	conflict	UNP A0A125YUZ2

- Molecule 22 is a protein called ATPTG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	f7	188	Total	C	H	N	O	S	0	0
			2867	919	1425	245	274	4		
22	F7	188	Total	C	H	N	O	S	0	0
			2867	919	1425	245	274	4		
22	f8	188	Total	C	H	N	O	S	0	0
			2867	919	1425	245	274	4		
22	F8	188	Total	C	H	N	O	S	0	0
			2867	919	1425	245	274	4		
22	f9	188	Total	C	H	N	O	S	0	0
			2867	919	1425	245	274	4		
22	F9	188	Total	C	H	N	O	S	0	0
			2867	919	1425	245	274	4		

- Molecule 23 is a protein called ATPTG16.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	w7	96	Total	C	H	N	O	S	0	0
			1509	494	755	127	129	4		
23	W7	96	Total	C	H	N	O	S	0	0
			1509	494	755	127	129	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
23	w8	96	Total	C	H	N	O	S	0	0
			1509	494	755	127	129	4		
23	W8	96	Total	C	H	N	O	S	0	0
			1509	494	755	127	129	4		
23	w9	96	Total	C	H	N	O	S	0	0
			1509	494	755	127	129	4		
23	W9	96	Total	C	H	N	O	S	0	0
			1509	494	755	127	129	4		

- Molecule 24 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	a7	467	Total	C	H	N	O	S	0	0
			7391	2405	3611	656	698	21		
24	A7	467	Total	C	H	N	O	S	0	0
			7392	2405	3612	656	698	21		
24	a8	467	Total	C	H	N	O	S	0	0
			7392	2405	3612	656	698	21		
24	A8	467	Total	C	H	N	O	S	0	0
			7390	2405	3610	656	698	21		
24	a9	467	Total	C	H	N	O	S	0	0
			7391	2405	3611	656	698	21		
24	A9	467	Total	C	H	N	O	S	0	0
			7393	2405	3613	656	698	21		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a7	351	THR	ALA	conflict	UNP S7V493
A7	351	THR	ALA	conflict	UNP S7V493
a8	351	THR	ALA	conflict	UNP S7V493
A8	351	THR	ALA	conflict	UNP S7V493
a9	351	THR	ALA	conflict	UNP S7V493
A9	351	THR	ALA	conflict	UNP S7V493

- Molecule 25 is a protein called Oligomycin sensitivity conferring protein (OSCP).

Mol	Chain	Residues	Atoms						AltConf	Trace
25	G1	180	Total	C	H	N	O	S	0	0
			2895	895	1480	255	261	4		
25	G2	180	Total	C	H	N	O	S	0	0
			2894	895	1479	255	261	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
25	G3	180	Total	C	H	N	O	S	0	0
			2894	895	1479	255	261	4		
25	G4	180	Total	C	H	N	O	S	0	0
			2894	895	1479	255	261	4		
25	G5	180	Total	C	H	N	O	S	0	0
			2897	895	1482	255	261	4		
25	G6	180	Total	C	H	N	O	S	0	0
			2895	895	1480	255	261	4		

- Molecule 26 is a protein called Inhibitor of F1.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	i1	40	Total	C	H	N	O	S	0	0
			660	213	324	56	66	1		
26	i2	40	Total	C	H	N	O	S	0	0
			660	213	324	56	66	1		
26	i3	40	Total	C	H	N	O	S	0	0
			659	213	323	56	66	1		
26	i4	40	Total	C	H	N	O	S	0	0
			660	213	324	56	66	1		
26	i5	40	Total	C	H	N	O	S	0	0
			660	213	324	56	66	1		
26	i6	40	Total	C	H	N	O	S	0	0
			660	213	324	56	66	1		

- Molecule 27 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	A1	512	Total	C	H	N	O	S	0	0
			7925	2464	4003	688	751	19		
27	E1	507	Total	C	H	N	O	S	0	0
			7848	2441	3962	682	744	19		
27	C1	507	Total	C	H	N	O	S	0	0
			7849	2442	3967	682	739	19		
27	A2	512	Total	C	H	N	O	S	0	0
			7925	2464	4003	688	751	19		
27	E2	507	Total	C	H	N	O	S	0	0
			7848	2441	3962	682	744	19		
27	C2	507	Total	C	H	N	O	S	0	0
			7849	2442	3967	682	739	19		
27	A3	512	Total	C	H	N	O	S	0	0
			7925	2464	4003	688	751	19		

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Mol	Chain	Residues	Atoms						AltConf	Trace
27	E3	507	Total	C	H	N	O	S	0	0
			7848	2441	3962	682	744	19		
27	C3	507	Total	C	H	N	O	S	0	0
			7849	2442	3967	682	739	19		
27	A4	512	Total	C	H	N	O	S	0	0
			7925	2464	4003	688	751	19		
27	E4	507	Total	C	H	N	O	S	0	0
			7848	2441	3962	682	744	19		
27	C4	507	Total	C	H	N	O	S	0	0
			7849	2442	3967	682	739	19		
27	A5	512	Total	C	H	N	O	S	0	0
			7925	2464	4003	688	751	19		
27	E5	507	Total	C	H	N	O	S	0	0
			7848	2441	3962	682	744	19		
27	C5	507	Total	C	H	N	O	S	0	0
			7849	2442	3967	682	739	19		
27	A6	512	Total	C	H	N	O	S	0	0
			7925	2464	4003	688	751	19		
27	E6	507	Total	C	H	N	O	S	0	0
			7848	2441	3962	682	744	19		
27	C6	507	Total	C	H	N	O	S	0	0
			7849	2442	3967	682	739	19		

- Molecule 28 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	B1	479	Total	C	H	N	O	S	0	0
			7314	2293	3676	628	703	14		
28	F1	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
28	D1	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
28	B2	479	Total	C	H	N	O	S	0	0
			7314	2293	3676	628	703	14		
28	F2	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
28	D2	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
28	B3	479	Total	C	H	N	O	S	0	0
			7314	2293	3676	628	703	14		
28	F3	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		

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Mol	Chain	Residues	Atoms						AltConf	Trace
28	D3	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
28	B4	479	Total	C	H	N	O	S	0	0
			7314	2293	3676	628	703	14		
28	F4	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
28	D4	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
28	B5	479	Total	C	H	N	O	S	0	0
			7314	2293	3676	628	703	14		
28	F5	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
28	D5	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
28	B6	479	Total	C	H	N	O	S	0	0
			7314	2293	3676	628	703	14		
28	F6	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
28	D6	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		

- Molecule 29 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	g1	272	Total	C	H	N	O	S	0	0
			4289	1330	2173	376	394	16		
29	g2	272	Total	C	H	N	O	S	0	0
			4289	1330	2173	376	394	16		
29	g3	272	Total	C	H	N	O	S	0	0
			4289	1330	2173	376	394	16		
29	g4	272	Total	C	H	N	O	S	0	0
			4289	1330	2173	376	394	16		
29	g5	272	Total	C	H	N	O	S	0	0
			4289	1330	2173	376	394	16		
29	g6	272	Total	C	H	N	O	S	0	0
			4289	1330	2173	376	394	16		

- Molecule 30 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	d1	143	Total	C	H	N	O	S	0	0
			2145	667	1076	181	216	5		

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Mol	Chain	Residues	Atoms						AltConf	Trace
30	d2	143	Total	C	H	N	O	S	0	0
			2145	667	1076	181	216	5		
30	d3	143	Total	C	H	N	O	S	0	0
			2145	667	1076	181	216	5		
30	d4	143	Total	C	H	N	O	S	0	0
			2145	667	1076	181	216	5		
30	d5	143	Total	C	H	N	O	S	0	0
			2145	667	1076	181	216	5		
30	d6	143	Total	C	H	N	O	S	0	0
			2145	667	1076	181	216	5		

- Molecule 31 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	e1	65	Total 1077	C 337	H 539	N 99	O 98	S 4	0	0
31	e2	65	Total 1077	C 337	H 539	N 99	O 98	S 4	0	0
31	e3	65	Total 1077	C 337	H 539	N 99	O 98	S 4	0	0
31	e4	65	Total 1077	C 337	H 539	N 99	O 98	S 4	0	0
31	e5	65	Total 1077	C 337	H 539	N 99	O 98	S 4	0	0
31	e6	65	Total 1077	C 337	H 539	N 99	O 98	S 4	0	0

- Molecule 32 is a protein called subunit c.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	H1	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	I1	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	J1	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	K1	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	L1	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	M1	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
32	N1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	O1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	P1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	Q1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	H2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	I2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	J2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	K2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	L2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	M2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	N2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	O2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	P2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	Q2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	H3	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	I3	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	J3	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	K3	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	L3	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	M3	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	N3	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
32	O3	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	P3	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	Q3	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	H4	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	I4	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	J4	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	K4	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	L4	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	M4	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	N4	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	O4	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	P4	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	Q4	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	H5	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	I5	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	J5	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	K5	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	L5	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	M5	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	N5	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	O5	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
32	P5	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	Q5	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	H6	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	I6	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	J6	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	K6	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	L6	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	M6	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	N6	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	O6	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	P6	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0
32	Q6	71	Total 1028	C 328	H 527	N 77	O 92	S 4	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: ATPTG11

Chain q7:  99%



- Molecule 1: ATPTG11

Chain Q7:  99%



- Molecule 1: ATPTG11

Chain q8:  99%



- Molecule 1: ATPTG11

Chain Q8:  99%



- Molecule 1: ATPTG11

Chain q9:  99%



- Molecule 1: ATPTG11

Chain Q9:  99%



• Molecule 2: ATPTG7

Chain i7: 38% 62%

MET	PRO	SER	SER	SER	SER	GLU	ASP	ALA	GLN	GLY	GLY	ASN	ARG	PHE	GLU	CYS	VAL	SER	ASN	THR	ARG	PRO	ASP	ARG	LYS	ASN	ALA	ALA	ALA	CYS	LEU	GLN	ARG	ARG	SER	ALA	VAL	SER	GLY	PRO	GLY	ARG	GLU	ASN	ASP	VAL	LEU	CYS	ILE	THR	THR	PRO	GLN	PRO
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HIS	VAL	ARG	ARG	GLY	LYS	SER	GLY	PRO	GLY	GLY	ARG	GLY	ASN	ARG	ARG	MET	PHE	ARG	GLY	VAL	GLY	ARG	VAL	ASP	LYS	LYS	ASN	ARG	GLY	GLY	THR	GLU	GLU	ARG	GLU	THR	LYS	ARG	ALA	PRO	ASP	LYS	LYS	ASN	VAL	HIS	ILE	GLY	PRO	GLY	ASN	ALA	ASP	VAL	SER	LEU	ARG	ARG	ILE	THR	CYS	PHE	PRO	GLN	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ARG	HIS	SER	LEU	LEU	ASN	HIS	TYR	GLY	SER	LEU	LEU	SER	SER	MET	ALA	PHE	ARG	GLY	VAL	GLY	SER	ASN	THR	PRO	ASP	LYS	LYS	ASN	ARG	GLY	GLY	THR	GLU	GLU	ARG	GLU	THR	LYS	ARG	ALA	PRO	ASP	LYS	LYS	ASN	VAL	HIS	ILE	GLY	PRO	GLY	ASN	ALA	ASP	VAL	SER	LEU	ARG	ARG	ILE	THR	CYS	PHE	PRO	GLN	SER
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• Molecule 2: ATPTG7

Chain I7: 38% 62%

MET	PRO	SER	SER	SER	SER	GLU	ASP	ALA	GLN	GLY	GLY	ASN	ARG	PHE	GLU	CYS	VAL	SER	ASN	THR	ARG	PRO	ASP	ARG	LYS	ASN	ALA	ALA	ALA	CYS	LEU	GLN	ARG	ARG	SER	ALA	VAL	SER	GLY	PRO	GLY	ARG	GLU	ASN	ASP	VAL	LEU	CYS	ILE	THR	THR	PRO	GLN	PRO
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HIS	VAL	ARG	ARG	GLY	LYS	SER	GLY	PRO	GLY	GLY	ARG	GLY	ASN	ARG	ARG	MET	PHE	ARG	GLY	VAL	GLY	SER	ASN	THR	PRO	ASP	LYS	LYS	ASN	ARG	GLY	GLY	THR	GLU	GLU	ARG	GLU	THR	LYS	ARG	ALA	PRO	ASP	LYS	LYS	ASN	VAL	HIS	ILE	GLY	PRO	GLY	ASN	ALA	ASP	VAL	SER	LEU	ARG	ARG	ILE	THR	CYS	PHE	PRO	GLN	SER
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ARG	HIS	SER	LEU	LEU	ASN	HIS	TYR	GLY	SER	LEU	LEU	SER	SER	MET	ALA	PHE	ARG	GLY	VAL	GLY	SER	ASN	THR	PRO	ASP	LYS	LYS	ASN	ARG	GLY	GLY	THR	GLU	GLU	ARG	GLU	THR	LYS	ARG	ALA	PRO	ASP	LYS	LYS	ASN	VAL	HIS	ILE	GLY	PRO	GLY	ASN	ALA	ASP	VAL	SER	LEU	ARG	ARG	ILE	THR	CYS	PHE	PRO	GLN	SER
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• Molecule 2: ATPTG7

Chain i8: 38% 62%

MET	PRO	SER	SER	SER	SER	GLU	ASP	ALA	GLN	GLY	GLY	ASN	ARG	PHE	GLU	CYS	VAL	SER	ASN	THR	ARG	PRO	ASP	ARG	LYS	ASN	ALA	ALA	ALA	CYS	LEU	GLN	ARG	ARG	SER	ALA	VAL	SER	GLY	PRO	GLY	ARG	GLU	ASN	ASP	VAL	LEU	CYS	ILE	THR	THR	PRO	GLN	PRO
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HIS	VAL	ARG	ARG	GLY	LYS	SER	GLY	PRO	GLY	GLY	ARG	GLY	ASN	ARG	ARG	MET	PHE	ARG	GLY	VAL	GLY	SER	ASN	THR	PRO	ASP	LYS	LYS	ASN	ARG	GLY	GLY	THR	GLU	GLU	ARG	GLU	THR	LYS	ARG	ALA	PRO	ASP	LYS	LYS	ASN	VAL	HIS	ILE	GLY	PRO	GLY	ASN	ALA	ASP	VAL	SER	LEU	ARG	ARG	ILE	THR	CYS	PHE	PRO	GLN	SER
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ARG	HIS	SER	LEU	LEU	ASN	HIS	TYR	GLY	SER	LEU	LEU	SER	SER	MET	ALA	PHE	ARG	GLY	VAL	GLY	SER	ASN	THR	PRO	ASP	LYS	LYS	ASN	ARG	GLY	GLY	THR	GLU	GLU	ARG	GLU	THR	LYS	ARG	ALA	PRO	ASP	LYS	LYS	ASN	VAL	HIS	ILE	GLY	PRO	GLY	ASN	ALA	ASP	VAL	SER	LEU	ARG	ARG	ILE	THR	CYS	PHE	PRO	GLN	SER
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• Molecule 2: ATPTG7

Chain I8: 38% 62%

MET	PRO	SER	SER	SER	SER	GLU	ASP	ALA	GLN	GLY	GLY	ASN	ARG	PHE	GLU	CYS	VAL	SER	ASN	THR	ARG	PRO	ASP	ARG	LYS	ASN	ALA	ALA	ALA	CYS	LEU	GLN	ARG	ARG	SER	ALA	VAL	SER	GLY	PRO	GLY	ARG	GLU	ASN	ASP	VAL	LEU	CYS	ILE	THR	THR	PRO	GLN	PRO
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HIS	VAL	ARG	ARG	GLY	LYS	SER	GLY	PRO	GLY	GLY	ARG	GLY	ASN	ARG	ARG	MET	PHE	ARG	GLY	VAL	GLY	SER	ASN	THR	PRO	ASP	LYS	LYS	ASN	ARG	GLY	GLY	THR	GLU	GLU	ARG	GLU	THR	LYS	ARG	ALA	PRO	ASP	LYS	LYS	ASN	VAL	HIS	ILE	GLY	PRO	GLY	ASN	ALA	ASP	VAL	SER	LEU	ARG	ARG	ILE	THR	CYS	PHE	PRO	GLN	SER
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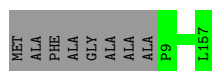
ARG	HIS	SER	LEU	LEU	ASN	HIS	TYR	GLY	SER	LEU	LEU	SER	SER	MET	ALA	PHE	ARG	GLY	VAL	GLY	SER	ASN	THR	PRO	ASP	LYS	LYS	ASN	ARG	GLY	GLY	THR	GLU	GLU	ARG	GLU	THR	LYS	ARG	ALA	PRO	ASP	LYS	LYS	ASN	VAL	HIS	ILE	GLY	PRO	GLY	ASN	ALA	ASP	VAL	SER	LEU	ARG	ARG	ILE	THR	CYS	PHE	PRO	GLN	SER
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[illegible][illegible][illegible]

MET
ALA
PHE
ALA
GLY
ALA
ALA
ALA
P9
L157

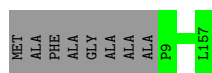
MET
ALA
PHE
ALA
GLY
ALA
ALA
ALA
P9
L157

Chain o8:  95% 5%



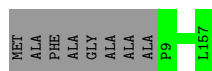
- Molecule 5: subunit k

Chain O8:  95% 5%



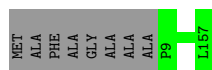
- Molecule 5: subunit k

Chain o9:  95% 5%



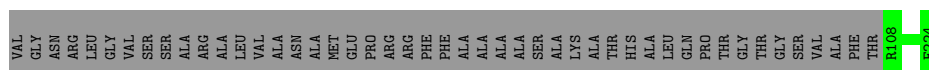
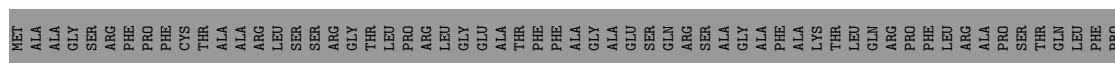
- Molecule 5: subunit k

Chain O9:  95% 5%



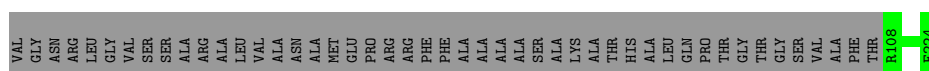
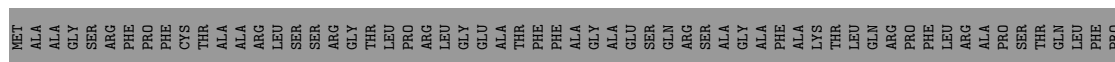
- Molecule 6: subunit a

Chain k7:  52% 48%



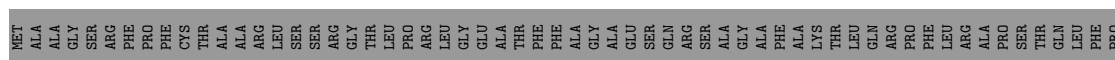
- Molecule 6: subunit a

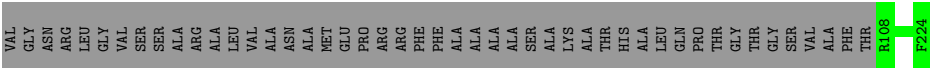
Chain K7:  52% 48%



- Molecule 6: subunit a

Chain k8:  52% 48%





• Molecule 6: subunit a



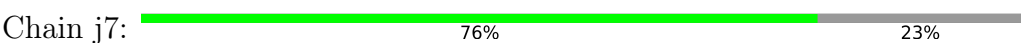
• Molecule 6: subunit a



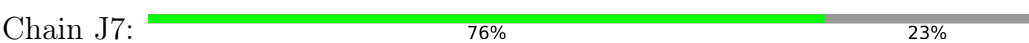
• Molecule 6: subunit a



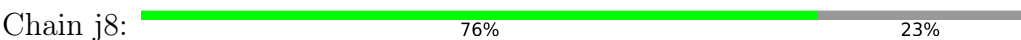
• Molecule 7: subunit i/j

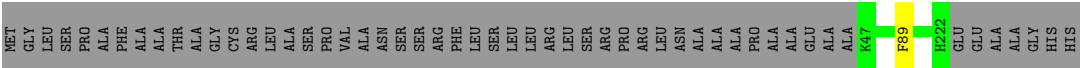


• Molecule 7: subunit i/j

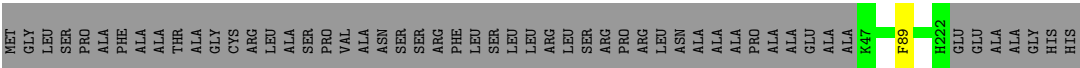
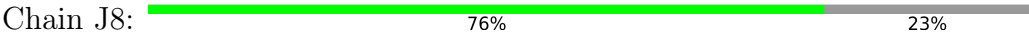


• Molecule 7: subunit i/j

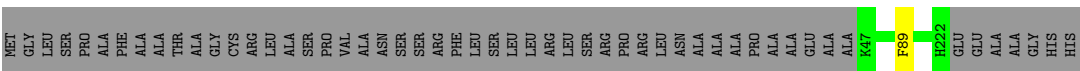
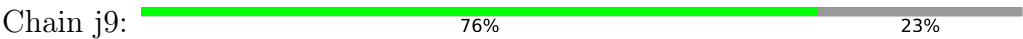




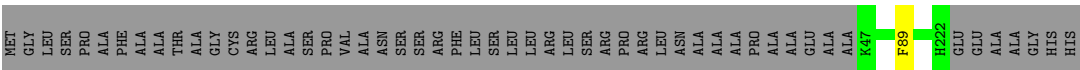
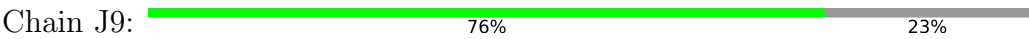
• Molecule 7: subunit i/j



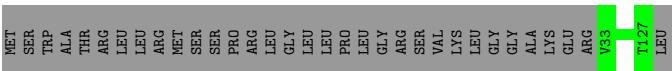
• Molecule 7: subunit i/j



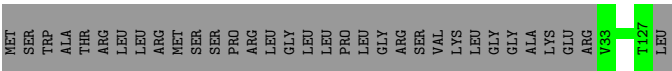
• Molecule 7: subunit i/j



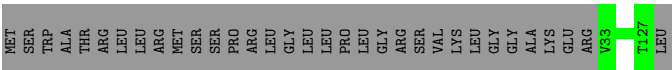
• Molecule 8: ATPTG13



• Molecule 8: ATPTG13

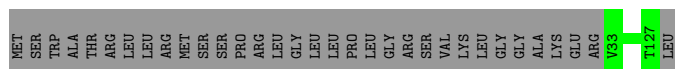


• Molecule 8: ATPTG13



• Molecule 8: ATPTG13

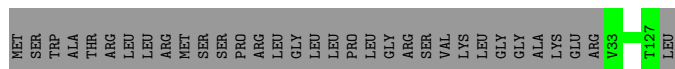




● Molecule 8: ATPTG13

Chain s9:

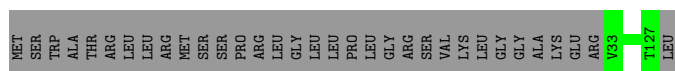
74% 26%



● Molecule 8: ATPTG13

Chain S9:

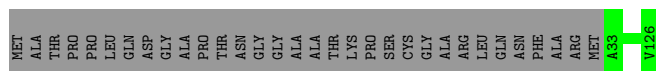
74% 26%



● Molecule 9: ATPTG15

Chain u7:

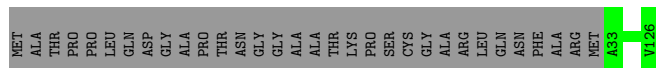
75% 25%



● Molecule 9: ATPTG15

Chain U7:

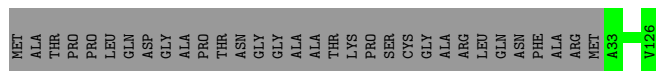
75% 25%



● Molecule 9: ATPTG15

Chain u8:

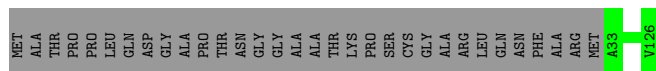
75% 25%



● Molecule 9: ATPTG15

Chain U8:

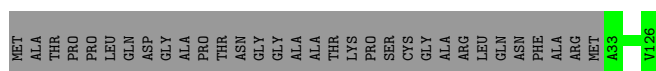
75% 25%



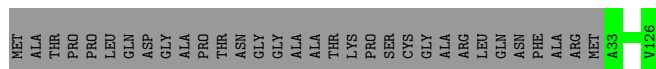
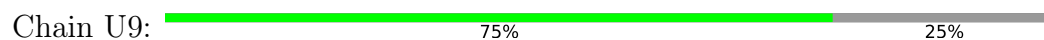
● Molecule 9: ATPTG15

Chain u9:

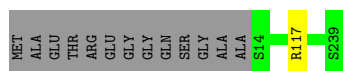
75% 25%



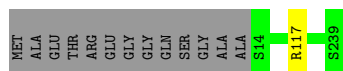
- Molecule 9: ATPTG15



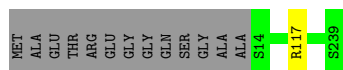
- Molecule 10: ATPTG6



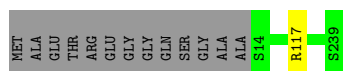
- Molecule 10: ATPTG6



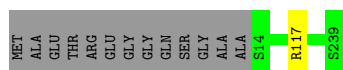
- Molecule 10: ATPTG6



- Molecule 10: ATPTG6



- Molecule 10: ATPTG6



- Molecule 10: ATPTG6







• Molecule 12: ATPTG17,ATPTG17,ATPTG17



• Molecule 12: ATPTG17,ATPTG17,ATPTG17



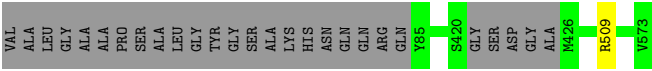
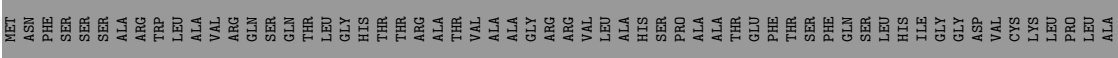
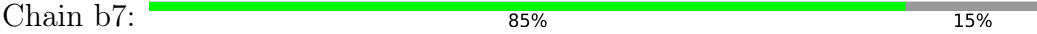
• Molecule 12: ATPTG17,ATPTG17,ATPTG17



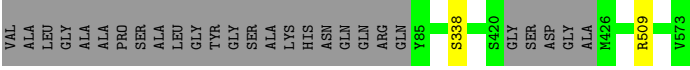
• Molecule 12: ATPTG17,ATPTG17,ATPTG17



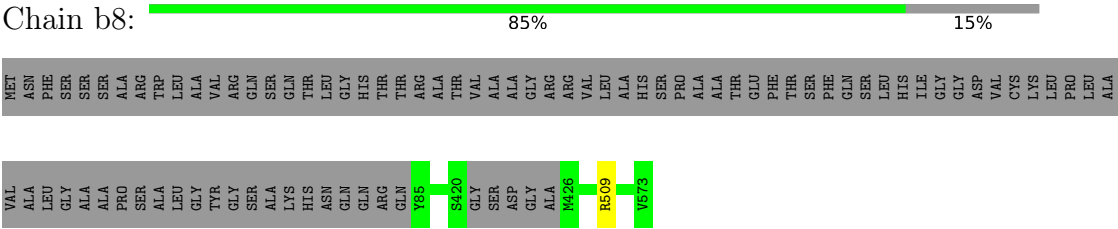
• Molecule 13: subunit b



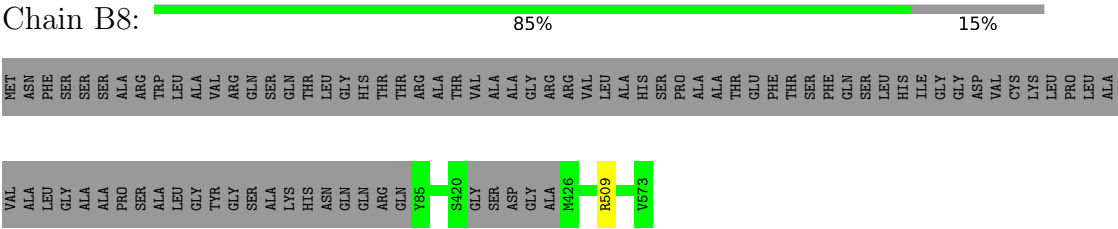
• Molecule 13: subunit b



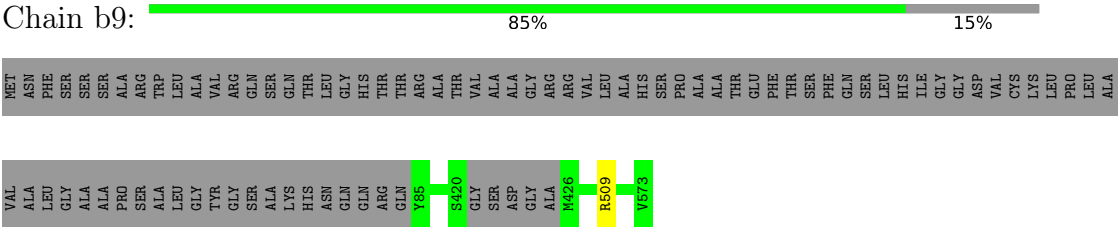
• Molecule 13: subunit b



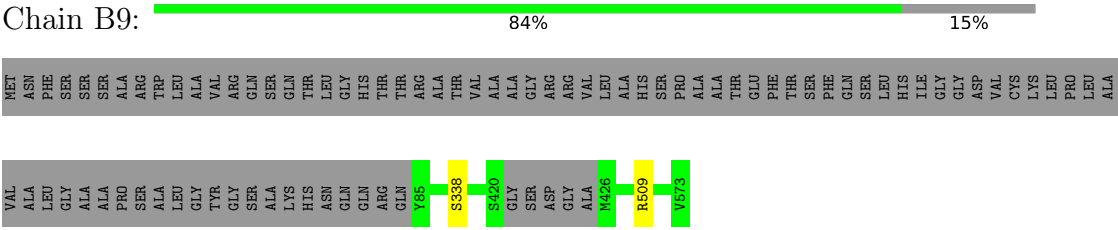
• Molecule 13: subunit b



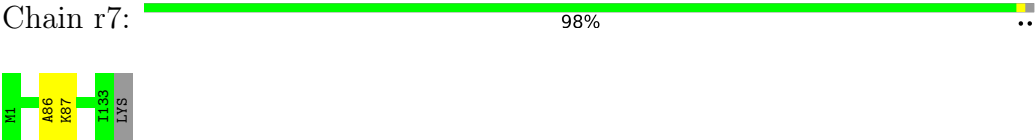
• Molecule 13: subunit b



• Molecule 13: subunit b



• Molecule 14: ATPTG12



• Molecule 14: ATPTG12



• Molecule 14: ATPTG12

Chain r8:  99% ..

• Molecule 14: ATPTG12

Chain R8:  98% ..


• Molecule 14: ATPTG12

Chain r9:  99% ..


• Molecule 14: ATPTG12

Chain R9:  99% ..


• Molecule 15: ATPTG10

Chain p7:  78% 22%


• Molecule 15: ATPTG10

Chain P7:  78% 22%

• Molecule 15: ATPTG10


Chain p8:  78% 22%

• Molecule 15: ATPTG10

Chain P8:  78% 22%




- Molecule 15: ATPTG10

Chain p9:  78% 22%



- Molecule 15: ATPTG10

Chain P9:  78% 22%



- Molecule 16: subunit f

Chain v7:  99% .



- Molecule 16: subunit f

Chain V7:  99% .



- Molecule 16: subunit f

Chain v8:  99% .



- Molecule 16: subunit f

Chain V8:  99% .



- Molecule 16: subunit f

Chain v9:  99% .



- Molecule 16: subunit f

Chain V9:  99%



- Molecule 17: ATPTG8

Chain 17:  100%



- Molecule 17: ATPTG8

Chain L7:  100%



- Molecule 17: ATPTG8

Chain l8:  100%



- Molecule 17: ATPTG8

Chain L8:  100%




- Molecule 17: ATPTG8

Chain l9:  100%



- Molecule 17: ATPTG8

Chain L9:  100%

GLY
LEU
LYS
CYS
VAL
GLY
SER
SER
ALA
TLE
TLE
GLY
THR
VAL
LEU
MET
THR
TRP
TRP
ARG
PHE
TYR
TRP
ALA
MET
TYR
ASP
PHE
GLY
LYS
LEU
LYS
TYR
LEU

• Molecule 19: ATPTG2

Chain d7: 82% 18%

MET
SER
PRO
VAL
GLY
ARG
LEU
PHE
LEU
GLY
SER
LYS
LEU
PRO
ALA
GLN
THR
TRP
GLN
SER
PHE
ARG
LEU
GLN
PRO
ALA
LEU
PRO
GLN
PHE
PHE
GLN
LYS
ARG
PHE
PHE
SER
GLY
GLY
ALA
ALA
K42
G213
THR
SER
ASP
GLY
CYS
GLY
GLU
HIS
GLY
ALA
CYS
GLY
HIS
SER
GLY
Q229

• Molecule 19: ATPTG2

Chain D7: 82% 18%

MET
SER
PRO
VAL
GLY
ARG
LEU
PHE
LEU
GLY
SER
LYS
LEU
PRO
ALA
GLN
THR
TRP
GLN
SER
PHE
ARG
LEU
GLN
PRO
ALA
LEU
PRO
GLN
PHE
PHE
GLN
LYS
ARG
PHE
PHE
SER
GLY
GLY
ALA
ALA
K42
G213
THR
SER
ASP
GLY
CYS
GLY
GLU
HIS
GLY
ALA
CYS
GLY
HIS
SER
GLY
Q229

• Molecule 19: ATPTG2

Chain d8: 82% 18%

MET
SER
PRO
VAL
GLY
ARG
LEU
PHE
LEU
GLY
SER
LYS
LEU
PRO
ALA
GLN
THR
TRP
GLN
SER
PHE
ARG
LEU
GLN
PRO
ALA
LEU
PRO
GLN
PHE
PHE
GLN
LYS
ARG
PHE
PHE
SER
GLY
GLY
ALA
ALA
K42
G213
THR
SER
ASP
GLY
CYS
GLY
GLU
HIS
GLY
ALA
CYS
GLY
HIS
SER
GLY
Q229

• Molecule 19: ATPTG2

Chain D8: 82% 18%

MET
SER
PRO
VAL
GLY
ARG
LEU
PHE
LEU
GLY
SER
LYS
LEU
PRO
ALA
GLN
THR
TRP
GLN
SER
PHE
ARG
LEU
GLN
PRO
ALA
LEU
PRO
GLN
PHE
PHE
GLN
LYS
ARG
PHE
PHE
SER
GLY
GLY
ALA
ALA
K42
G213
THR
SER
ASP
GLY
CYS
GLY
GLU
HIS
GLY
ALA
CYS
GLY
HIS
SER
GLY
Q229

• Molecule 19: ATPTG2

Chain d9: 82% 18%

MET
SER
PRO
VAL
GLY
ARG
LEU
PHE
LEU
GLY
SER
LYS
LEU
PRO
ALA
GLN
THR
TRP
GLN
SER
PHE
ARG
LEU
GLN
PRO
ALA
LEU
PRO
GLN
PHE
PHE
GLN
LYS
ARG
PHE
PHE
SER
GLY
GLY
ALA
ALA
K42
G213
THR
SER
ASP
GLY
CYS
GLY
GLU
HIS
GLY
ALA
CYS
GLY
HIS
SER
GLY
Q229

K310

• Molecule 19: ATPTG2

Chain D9: 82% 18%

MET SER PRO THR GLY ARG LEU PHE LEU GLY SER LYS LEU PRO ALA GLN THR TRP GLN SER PHE ARG LEU GLN PRO ALA ALA LEU PRO GLN PHE THR ALA GLN LYS ARG PHE PHE SER GLY GLY ALA ALA K42 Q213 THR SER ASP GLY CYS GLY GLU HIS GLY ALA CYS GLY HIS SER GLY Q229

K310

• Molecule 20: subunit 8

Chain m7: 47% 53%

MET ASN THR PHE LEU THR PRO ALA ALA ALA ALA ARG ARG VAL SER VAL ALA ALA SER PHE PHE ARG ALA ARG SER ALA ALA SER SER GLY THR GLY ARG ARG GLY PHE ALA ARG ALA SER ALA VAL GLY GLY PHE THR GLY CYS MET ARG VAL ALA ALA A96 Q191 ASP PHE PRO ALA SER GLN ARG PRO ALA THR LYS THR GLY SER THR SER ALA LYS LYS

LYS ALA HIS GLY ARG GLN SER GLY LYS LYS LYS LYS GLN SER THR GLU SER VAL GLY GLY ARG ARG GLY PHE ALA ARG ALA SER ALA VAL VAL GLY GLY PHE THR GLY CYS MET ARG VAL ALA ALA A96 Q191 ASP PHE PRO ALA SER GLN ARG PRO ALA THR LYS THR GLY SER THR SER ALA LYS LYS

• Molecule 20: subunit 8

Chain M7: 47% 53%

MET ASN THR PHE LEU THR PRO ALA ALA ALA ALA ARG ARG VAL SER VAL ALA ALA SER PHE PHE ARG ALA ARG SER ALA ALA SER SER GLY THR GLU SER VAL GLY GLY ARG ARG GLY PHE ALA ARG ALA SER ALA VAL VAL GLY GLY PHE THR GLY CYS MET ARG VAL ALA ALA A96 Q191 ASP PHE PRO ALA SER GLN ARG PRO ALA THR LYS THR GLY SER THR SER ALA LYS LYS

LYS ALA HIS GLY ARG GLN SER GLY LYS LYS LYS LYS GLN SER THR GLU SER VAL GLY GLY ARG ARG GLY PHE ALA ARG ALA SER ALA VAL VAL GLY GLY PHE THR GLY CYS MET ARG VAL ALA ALA A96 Q191 ASP PHE PRO ALA SER GLN ARG PRO ALA THR LYS THR GLY SER THR SER ALA LYS LYS

• Molecule 20: subunit 8

Chain m8: 47% 53%

MET ASN THR PHE LEU THR PRO ALA ALA ALA ALA ARG ARG VAL SER VAL ALA ALA SER PHE PHE ARG ALA ARG SER ALA ALA SER SER GLY THR GLU SER VAL GLY GLY ARG ARG GLY PHE ALA ARG ALA SER ALA VAL VAL GLY GLY PHE THR GLY CYS MET ARG VAL ALA ALA A96 Q191 ASP PHE PRO ALA SER GLN ARG PRO ALA THR LYS THR GLY SER THR SER ALA LYS LYS

LYS ALA HIS GLY ARG GLN SER GLY LYS LYS LYS LYS GLN SER THR GLU SER VAL GLY GLY ARG ARG GLY PHE ALA ARG ALA SER ALA VAL VAL GLY GLY PHE THR GLY CYS MET ARG VAL ALA ALA A96 Q191 ASP PHE PRO ALA SER GLN ARG PRO ALA THR LYS THR GLY SER THR SER ALA LYS LYS

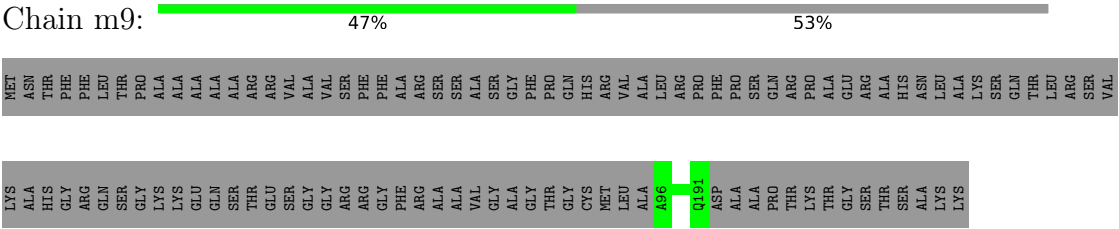
• Molecule 20: subunit 8

Chain M8: 47% 53%

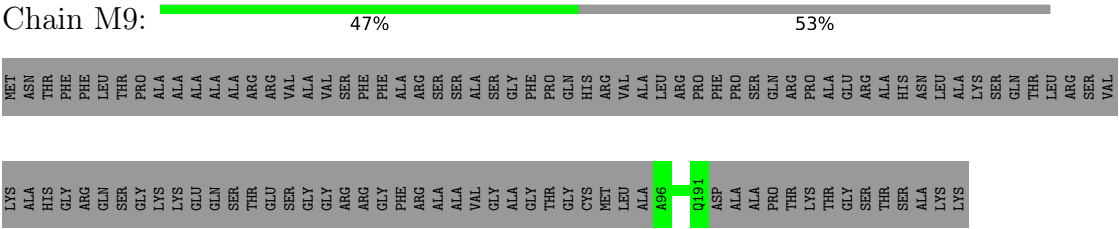
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LYS ALA HIS GLY ARG GLN SER GLY LYS LYS LYS LYS GLN SER THR GLU SER VAL GLY GLY ARG ARG GLY PHE ALA ARG ALA SER ALA VAL VAL GLY GLY PHE THR GLY CYS MET ARG VAL ALA ALA A96 Q191 ASP PHE PRO ALA SER GLN ARG PRO ALA THR LYS THR GLY SER THR SER ALA LYS LYS

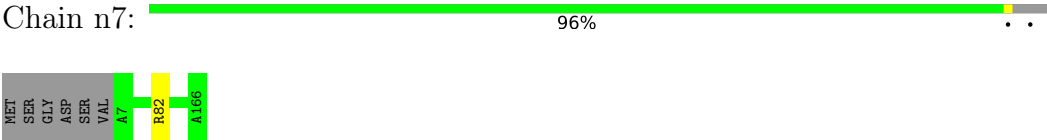
• Molecule 20: subunit 8



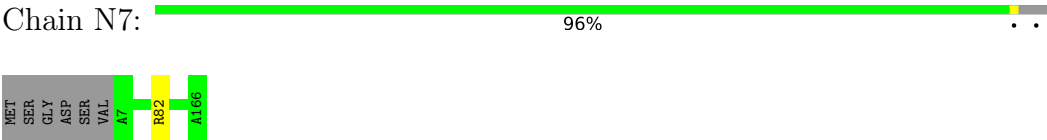
• Molecule 20: subunit 8



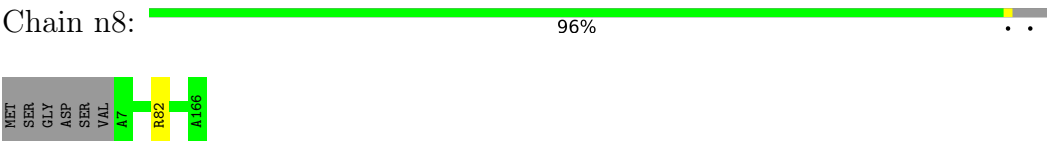
• Molecule 21: ATPTG9



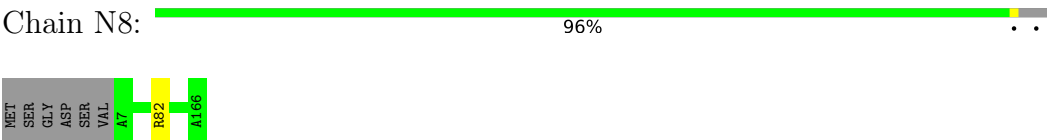
• Molecule 21: ATPTG9



• Molecule 21: ATPTG9



• Molecule 21: ATPTG9



• Molecule 21: ATPTG9

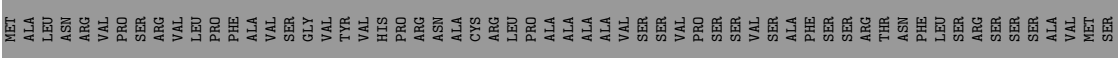




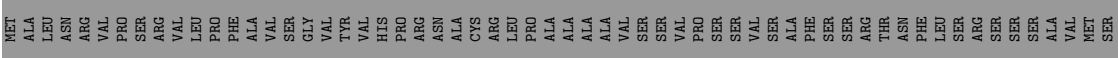
• Molecule 21: ATPTG9



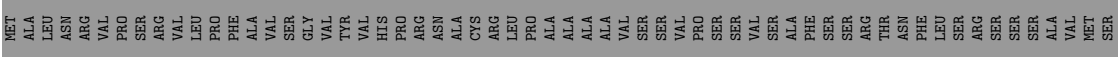
• Molecule 22: ATPTG4



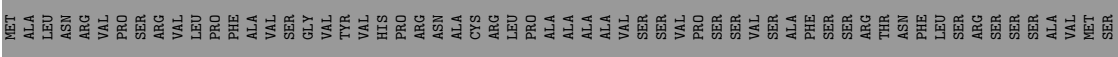
• Molecule 22: ATPTG4



• Molecule 22: ATPTG4



• Molecule 22: ATPTG4



• Molecule 22: ATPTG4



MET ALA LEU ASN ARG VAL PRO SER ARG VAL LEU PRO PHE ALA VAL SER GLY VAL TYR VAL HIS PRO ARG ASN ALA CYS ARG LEU PRO ALA ALA ALA VAL SER SER VAL PHE SER ARG THR ASN PHE LEU SER ARG SER SER ALA VAL MET SER

HIS PRO CYS ALA THR ALA ARG HIS PHE S71 A102 SER GLY ILE ALA SER GLY THR A112 A267

- Molecule 22: ATPTG4

Chain F9:  70% 30%

MET ALA LEU ASN ARG VAL PRO SER ARG VAL LEU PRO PHE ALA VAL SER GLY VAL TYR VAL HIS PRO ARG ASN ALA CYS ARG LEU PRO ALA ALA ALA VAL SER SER VAL PHE SER ARG THR ASN PHE LEU SER ARG SER SER ALA VAL MET SER

HIS PRO CYS ALA THR ALA ARG HIS PHE S71 A102 SER GLY ILE ALA SER GLY THR A112 A267

- Molecule 23: ATPTG16

Chain w7:  91% 9%

MET P2 Q22 PRO ASN GLY LEU GLY GLY GLU ALA G31 S105 ALA

- Molecule 23: ATPTG16

Chain W7:  91% 9%

MET P2 Q22 PRO ASN GLY LEU GLY GLY GLU ALA G31 S105 ALA

- Molecule 23: ATPTG16

Chain w8:  91% 9%

MET P2 Q22 PRO ASN GLY LEU GLY GLY GLU ALA G31 S105 ALA

- Molecule 23: ATPTG16

Chain W8:  91% 9%

MET P2 Q22 PRO ASN GLY LEU GLY GLY GLU ALA G31 S105 ALA

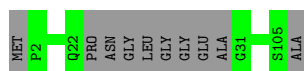
- Molecule 23: ATPTG16

Chain w9:  91% 9%


MET P2 Q22 PRO ASN GLY LEU GLY GLY GLU ALA G31 S105 ALA

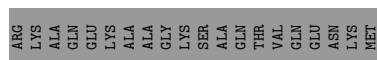
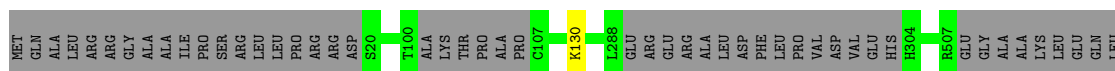
- Molecule 23: ATPTG16

Chain W9:  91% 9%



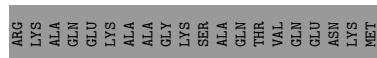
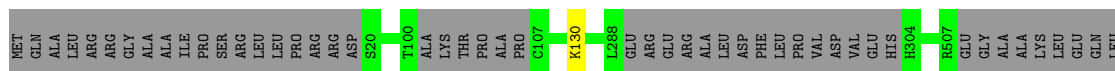
- Molecule 24: subunit d

Chain a7:  87% 13%




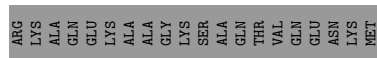
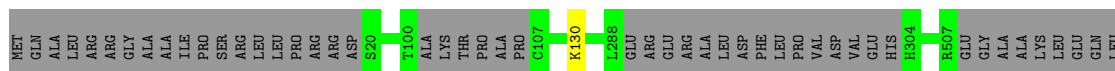
- Molecule 24: subunit d

Chain A7:  87% 13%



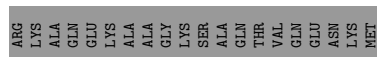
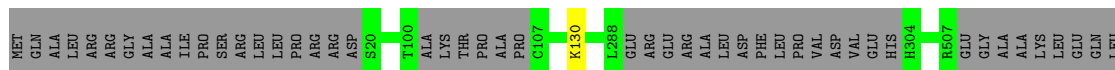
- Molecule 24: subunit d

Chain a8:  87% 13%




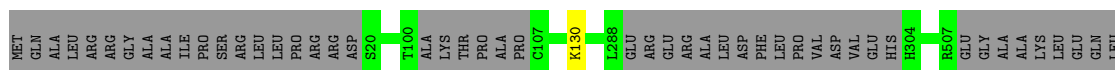
- Molecule 24: subunit d

Chain A8:  87% 13%




- Molecule 24: subunit d

Chain a9:  87% 13%



ARG
LYS
ALA
GLN
GLU
LYS
LYS
ALA
ALA
GLY
LYS
SER
SER
ALA
GLN
THR
VAL
GLN
GLU
ASN
LYS
MET

- Molecule 24: subunit d

Chain A9:  87% 13%

MET
GLN
LEU
LEU
ARG
ARG
GLY
ALA
ALA
ILE
PRO
SER
SER
ALA
GLN
THR
VAL
GLN
GLU
ASN
LYS
MET

ARG
LYS
ALA
GLN
GLU
LYS
LYS
ALA
ALA
GLY
LYS
SER
SER
ALA
GLN
THR
VAL
GLN
GLU
ASN
LYS
MET

- Molecule 25: Oligomycin sensitivity conferring protein (OSCP)

Chain G1:  69% 29%

MET
ALA
LEU
PRO
LEU
LEU
LEU
ALA
SER
ARG
ARG
ARG
LEU
PHE
SER
SER
PHE
VAL
PHE
PHE
ARG
GLY
GLN
PRO
THR
SER
SER
SER
ASN
LEU
SER
SER
LEU
VAL
ARG
ILE
GLY
GLY
LEU
HIS
GLY
GLY
SER
SER
PRO
PRO
SER
SER
ALA
THR
THR
PRO
PRO
ARG
ALA
ALA
GLN
VAL
PHE
SER
SER
ARG
ILE
ALA

PHE
SER
THR
ALA
ALA
ALA
GLU
ASP
SER
GLY
ALA
SER
Q73
Y97
M170
Y171
R172
Q207
L252

- Molecule 25: Oligomycin sensitivity conferring protein (OSCP)

Chain G2:  69% 29%

MET
ALA
LEU
PRO
LEU
LEU
LEU
ALA
SER
ARG
ARG
ARG
LEU
PHE
SER
SER
PHE
VAL
PHE
PHE
ARG
GLY
GLN
PRO
THR
SER
SER
SER
ASN
LEU
SER
SER
LEU
VAL
ARG
ILE
GLY
GLY
LEU
HIS
GLY
GLY
SER
SER
PRO
PRO
SER
SER
ALA
THR
THR
PRO
PRO
ARG
ALA
ALA
GLN
VAL
PHE
SER
SER
ARG
ILE
ALA

PHE
SER
THR
ALA
ALA
ALA
GLU
ASP
SER
GLY
ALA
SER
Q73
M169
Y171
R172
Q207
L252

- Molecule 25: Oligomycin sensitivity conferring protein (OSCP)

Chain G3:  70% 29%

MET
ALA
LEU
PRO
LEU
LEU
LEU
ALA
SER
ARG
ARG
ARG
LEU
PHE
SER
SER
PHE
VAL
PHE
PHE
ARG
GLY
GLN
PRO
THR
SER
SER
SER
ASN
LEU
SER
SER
LEU
VAL
ARG
ILE
GLY
GLY
LEU
HIS
GLY
GLY
SER
SER
PRO
PRO
SER
SER
ALA
THR
THR
PRO
PRO
ARG
ALA
ALA
GLN
VAL
PHE
SER
SER
ARG
ILE
ALA

PHE
SER
THR
ALA
ALA
ALA
GLU
ASP
SER
GLY
ALA
SER
Q73
M170
Y171
R172
Q207
L252

- Molecule 25: Oligomycin sensitivity conferring protein (OSCP)

Chain G4:  70% 29%

MET
ALA
LEU
PRO
LEU
LEU
LEU
ALA
SER
ARG
ARG
ARG
LEU
PHE
SER
SER
PHE
VAL
PHE
PHE
ARG
GLY
GLN
PRO
THR
SER
SER
SER
ASN
LEU
SER
SER
LEU
VAL
ARG
ILE
GLY
GLY
LEU
HIS
GLY
GLY
SER
SER
PRO
PRO
SER
SER
ALA
THR
THR
PRO
PRO
ARG
ALA
ALA
GLN
VAL
PHE
SER
SER
ARG
ILE
ALA

PHE
SER
THR
ALA
ALA
ALA
GLU
ASP
SER
GLY
ALA
SER
Q73
M170
Y171
R172
Q207
L252

- Chain i4: 28% 72%

ASP	HIS	MET	ASN	ALA	GLU	VAL	GLY	GLY	ILE	ALA	ARG	ASP	ILE	THR	LEU	ALA	CYS	GLN	LYS	HIS	GLY	MET	LYS	ASP	PRO	SER	ALA	ALA	PHE	MET	LYS	LEU	ILE	ILE	PHE	GLY	ALA	HIS	GLY	TYR	ALA	LYS	ASN	SER	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 26: Inhibitor of F1



ASP	HIS	MET	ASN	ALA	VAL	GLY	SER	ILE	ARG	ASP	ILE	THR	LEU	ALA	CYS	GLN	LYS	HIS	GLY	MET	LYS	ASP	PRO	SER	ALA	ALA	PHE	MET	LYS	ASP	LEU	ILE	ILE	PHE	GLY	ALA	HIS	GLY	TYR	ALA	LYS	ASN	SER	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 26: Inhibitor of F1



ASP HIS MET ASN ALA GLU VAL GLY SER ILE ARG ASP ILE THR LEU ALA CYS GLN LYS HIS GLY MET LYS ASP PRO SER ALA PHE MET LYS ASP LEU ILE ILE PHE GLY ALA HIS GLY TYR ALA LYS ASN SER LYS

- Molecule 27: ATP synthase subunit alpha



MET
THR
ILE
HIS
SER
CYS
LEU
ALA
ARG
ARG
ALA
VAl
SER
VAL
ALA
SER
GLY
GLY
ARG
ALA
PHE
ALA
ALA
SER
SER
GLY
LEU
GLY
ALA
ARG
ALA
GLN
SER
SER
ALA
ALA
VAL
VAL
GLY
ALA
LEU
LEU
HIS
THR
SER
SER
LEU
ARG
ARG
ALA
ALA
GLY
K63
K64

- Molecule 27: ATP synthase subunit alpha

[illegible]

LYS

- Molecule 27: ATP synthase subunit alpha



MET	THR	ILE	HIS	SER	CYS	LEU	ALA	ARG	ARG	VAL	ALA	VAL	SER	SER	GLY	ALA	ARG	PHE	ALA	SER	GLY	LEU	ALA	ALA	ARG	ALA	VAL	VAL	GLY	ALA	LEU	GLN	SER	ALA	ARG	LEU	LEU	HIS	THR	SER	SER	LEU	ARG	ALA	ALA	GLY	ASP	GLU	THR	THR	TRP	ILE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

E78 K564 LYS

- Molecule 27: ATP synthase subunit alpha

Chain A2:  91% 9%

MET THR ILE HIS SER CYS LEU ALA ARG ARG ALA VAL SER VAL VAL ALA ALA SER GLY GLY ALA ARG ARG PHE PHE ALA ALA SER GLY LEU GLY ALA ARG ALA VAL VAL ALA VAL GLY ALA ALA GLN SER ALA ARG LEU LEU LEU HIS THR SER SER LEU ARG ALA GLY ALA K53 K564 LYS

- Molecule 27: ATP synthase subunit alpha

Chain E2:  90% 10%

MET THR ILE HIS SER CYS LEU ALA ARG ARG ALA VAL SER VAL VAL ALA ALA SER GLY GLY ALA ARG ARG PHE PHE ALA ALA SER GLY LEU GLY ALA ARG ALA VAL VAL ALA VAL GLY ALA ALA GLN SER ALA ARG LEU LEU LEU HIS THR SER SER LEU ARG ALA GLY ALA LYS LYS ILE SER PRO SER E58 K564 LYS

- Molecule 27: ATP synthase subunit alpha

Chain C2:  90% 10%

MET THR ILE HIS SER CYS LEU ALA ARG ARG ALA VAL SER VAL VAL ALA ALA SER GLY GLY ALA ARG ARG PHE PHE ALA ALA SER GLY LEU GLY ALA ARG ALA VAL VAL ALA VAL GLY ALA ALA GLN SER ALA ARG LEU LEU LEU HIS THR SER SER LEU ARG ALA GLY ALA K52 K71 THR THR THR THR E78 K564 LYS

- Molecule 27: ATP synthase subunit alpha

Chain A3:  91% 9%

MET THR ILE HIS SER CYS LEU ALA ARG ARG ALA VAL SER VAL VAL ALA ALA SER GLY GLY ALA ARG ARG PHE PHE ALA ALA SER GLY LEU GLY ALA ARG ALA VAL VAL ALA VAL GLY ALA ALA GLN SER ALA ARG LEU LEU LEU HIS THR SER SER LEU ARG ALA GLY ALA K53 K564 LYS

- Molecule 27: ATP synthase subunit alpha

Chain E3:  90% 10%

MET THR ILE HIS SER CYS LEU ALA ARG ARG ALA VAL SER VAL VAL ALA ALA SER GLY GLY ALA ARG ARG PHE PHE ALA ALA SER GLY LEU GLY ALA ARG ALA VAL VAL ALA VAL GLY ALA ALA GLN SER ALA ARG LEU LEU LEU HIS THR SER SER LEU ARG ALA GLY ALA LYS ILE SER PRO SER E58 K564 LYS

- Molecule 27: ATP synthase subunit alpha

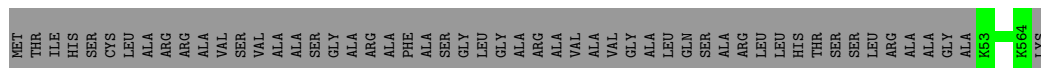
Chain C3:  90% 10%

MET THR ILE HIS SER CYS LEU ALA ARG ARG ALA VAL SER VAL VAL ALA ALA SER GLY GLY ALA ARG ARG PHE PHE ALA ALA SER GLY LEU GLY ALA ARG ALA VAL VAL ALA VAL GLY ALA ALA GLN SER ALA ARG LEU LEU LEU HIS THR SER SER LEU ARG ALA GLY ALA K52 K71 THR THR THR THR



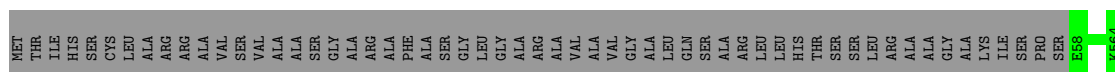
- Molecule 27: ATP synthase subunit alpha

Chain A4: 91% 9%



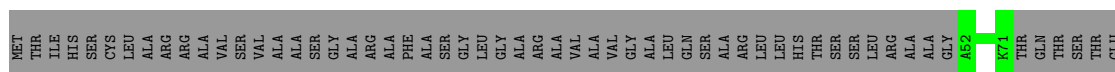
- Molecule 27: ATP synthase subunit alpha

Chain E4: 90% 10%



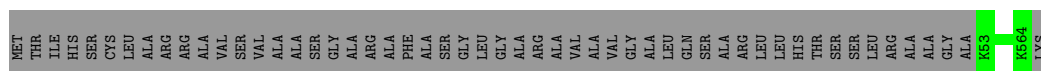
- Molecule 27: ATP synthase subunit alpha

Chain C4: 90% 10%



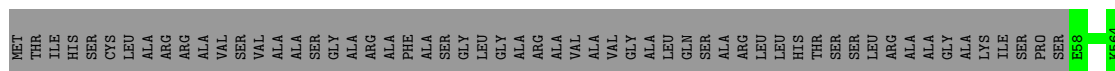
- Molecule 27: ATP synthase subunit alpha

Chain A5: 91% 9%



- Molecule 27: ATP synthase subunit alpha

Chain E5: 90% 10%

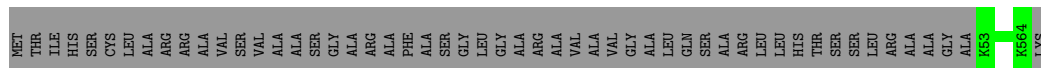


- Molecule 27: ATP synthase subunit alpha

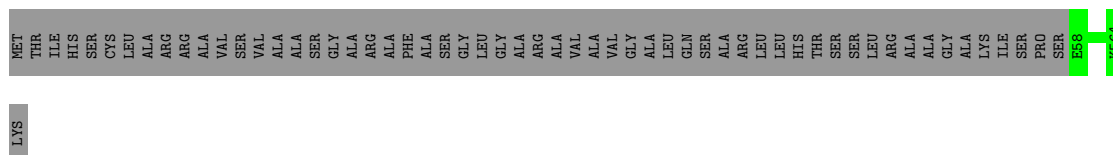
Chain C5: 90% 10%



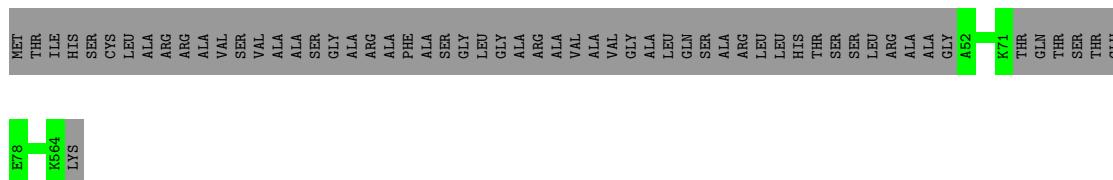
- Chain A6:  91% 9%

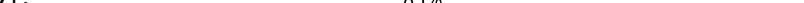


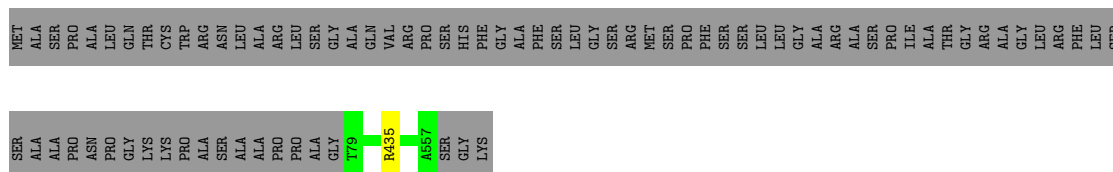
- Chain E6: 90% 10%




- Chain C6:  90% 10%

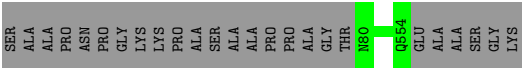


- Chain B1:  85% 14%

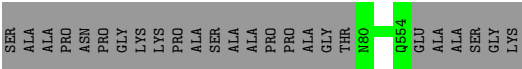
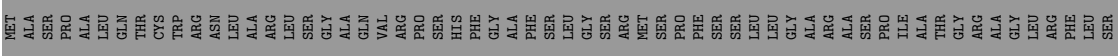
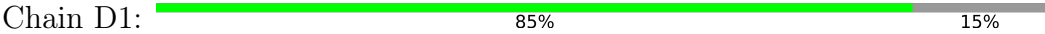


- Chain F1:  85% 15%

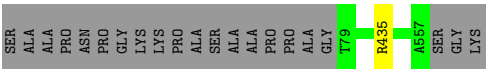
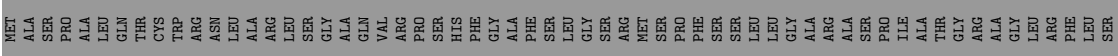
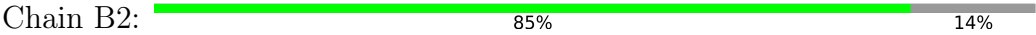




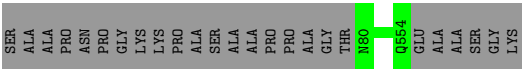
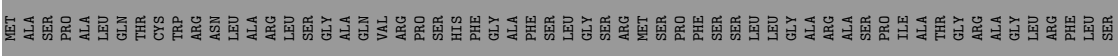
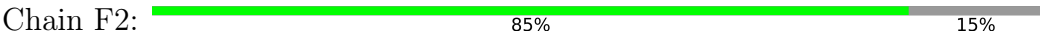
• Molecule 28: ATP synthase subunit beta



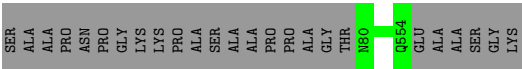
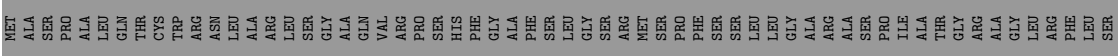
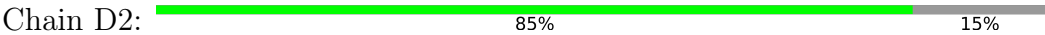
• Molecule 28: ATP synthase subunit beta



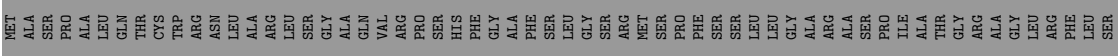
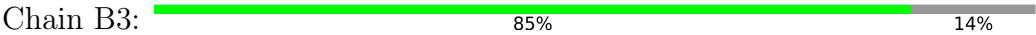
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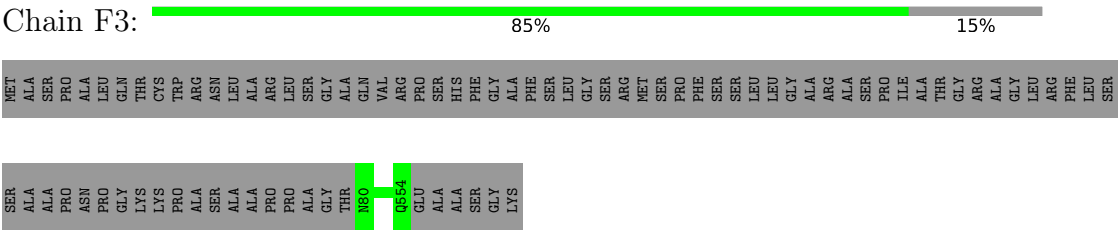
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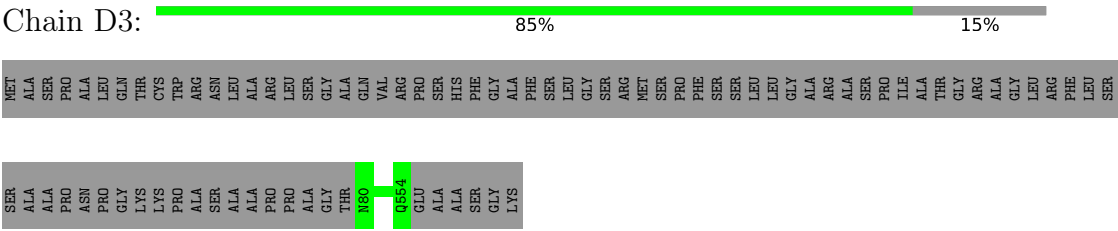
• Molecule 28: ATP synthase subunit beta



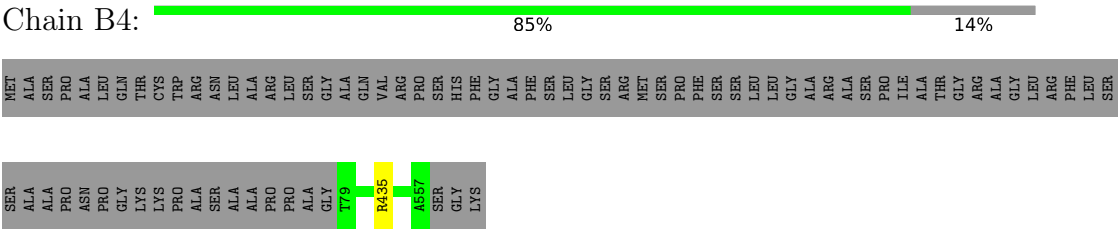
• Molecule 28: ATP synthase subunit beta



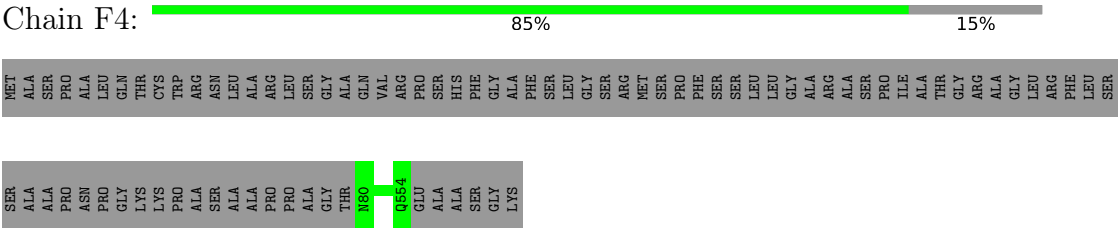
• Molecule 28: ATP synthase subunit beta



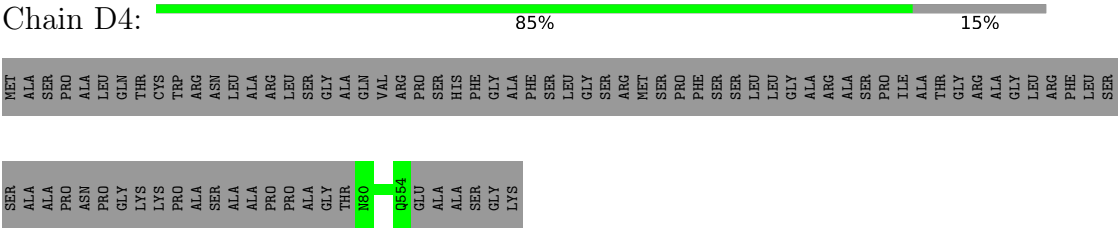
• Molecule 28: ATP synthase subunit beta




• Molecule 28: ATP synthase subunit beta



• Molecule 28: ATP synthase subunit beta




• Molecule 28: ATP synthase subunit beta

Chain B5:  85% 14%

MET ALA SER PRO PRO LEU GLN THR CYS TRP ARG ASN LEU ALA ARG LEU LEU LEU SER GLY ALA GLN VAL ARG PRO SER SER HIS PHE GLY PHE SER SER LEU LEU GLY SER ARG MET SER SER PHE SER SER LEU LEU GLY ALA ARG ALA ALA SER SER PRO ILE ALA THR GLY ARG ALA GLY LEU ARG PHE LEU SER

SER ALA ALA PRO PRO ASN PRO GLY LYS LYS CYS TRP ARG ALA ALA SER LEU ALA ALA ARG PRO PRO ALA ALA THR T79 R435 A557 SER GLY LYS


- Molecule 28: ATP synthase subunit beta

Chain F5:  85% 15%

MET ALA SER PRO PRO LEU GLN THR CYS TRP ARG ASN LEU ALA ARG LEU LEU LEU SER GLY ALA GLN VAL ARG PRO SER SER HIS PHE GLY PHE SER SER LEU LEU GLY SER ARG MET SER SER PHE SER SER LEU LEU GLY ALA ARG ALA ALA SER SER PRO ILE ALA THR GLY ARG ALA GLY LEU ARG PHE LEU SER

SER ALA ALA PRO PRO ASN PRO GLY LYS LYS CYS TRP ARG ALA ALA SER LEU ALA ALA ARG PRO PRO ALA ALA THR N80 Q554 GLU ALA ALA SER GLY LYS


- Molecule 28: ATP synthase subunit beta

Chain D5:  85% 15%

MET ALA SER PRO PRO LEU GLN THR CYS TRP ARG ASN LEU ALA ARG LEU LEU LEU SER GLY ALA GLN VAL ARG PRO SER SER HIS PHE GLY PHE SER SER LEU LEU GLY SER ARG MET SER SER PHE SER SER LEU LEU GLY ALA ARG ALA ALA SER SER PRO ILE ALA THR GLY ARG ALA GLY LEU ARG PHE LEU SER

SER ALA ALA PRO PRO ASN PRO GLY LYS LYS CYS TRP ARG ALA ALA SER LEU ALA ALA ARG PRO PRO ALA ALA THR N80 Q554 GLU ALA ALA SER GLY LYS


- Molecule 28: ATP synthase subunit beta

Chain B6:  85% 14%

MET ALA SER PRO PRO LEU GLN THR CYS TRP ARG ASN LEU ALA ARG LEU LEU LEU SER GLY ALA GLN VAL ARG PRO SER SER HIS PHE GLY PHE SER SER LEU LEU GLY SER ARG MET SER SER PHE SER SER LEU LEU GLY ALA ARG ALA ALA SER SER PRO ILE ALA THR GLY ARG ALA GLY LEU ARG PHE LEU SER

SER ALA ALA PRO PRO ASN PRO GLY LYS LYS CYS TRP ARG ALA ALA SER LEU ALA ALA ARG PRO PRO ALA ALA THR T79 R435 A557 SER GLY LYS


- Molecule 28: ATP synthase subunit beta

Chain F6:  85% 15%

MET ALA SER PRO PRO LEU GLN THR CYS TRP ARG ASN LEU ALA ARG LEU LEU LEU SER GLY ALA GLN VAL ARG PRO SER SER HIS PHE GLY PHE SER SER LEU LEU GLY SER ARG MET SER SER PHE SER SER LEU LEU GLY ALA ARG ALA ALA SER SER PRO ILE ALA THR GLY ARG ALA GLY LEU ARG PHE LEU SER

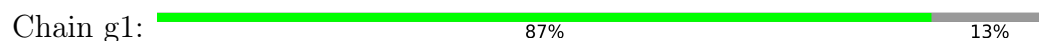
SER ALA ALA PRO PRO ASN PRO GLY LYS LYS CYS TRP ARG ALA ALA SER LEU ALA ALA ARG PRO PRO ALA ALA THR N80 Q554 GLU ALA ALA SER GLY LYS

- Molecule 28: ATP synthase subunit beta

Chain D6:  85% 15%

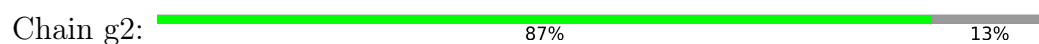
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- Molecule 29: ATP synthase subunit gamma



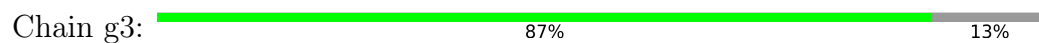
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- Molecule 29: ATP synthase subunit gamma



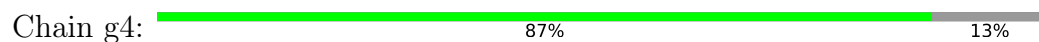
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- Molecule 29: ATP synthase subunit gamma



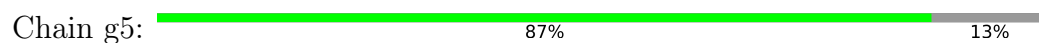
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- Molecule 29: ATP synthase subunit gamma



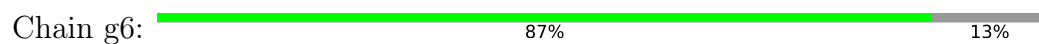
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- Molecule 29: ATP synthase subunit gamma




MET	ALA	GLY	LEU	ALA	SER	SER	SER	VAL	GLY	ALA	LEU	ARG	GLY	MET	ARG	LEU	VAL	PRO	ALA	ALA	HIS	LEU	LEU	PRO	LEU	HIS	SER	SER	ALA	PHE	GLY	GLN	THR	ARG	ASN	PHE	GLY	ALA	GLY	D42	L313	GLU
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- Molecule 29: ATP synthase subunit gamma




MET	ALA	GLY	LEU	ALA	SER	SER	SER	VAL	GLY	ALA	LEU	ARG	GLY	MET	ARG	LEU	VAL	PRO	ALA	ALA	HIS	LEU	LEU	PRO	PRO	LEU	HIS	SER	SER	ALA	ALA	PHE	GLY	GLN	GLN	THR	ARG	ASN	PHE	GLY	ALA	GLY	D42	L313	GLU
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- Molecule 30: ATP synthase subunit delta

Chain d1:  78% 22%


MET	PHE	ALA	ARG	ALA	PHE	SER	ARG	PHE	ALA	ALA	LEU	ALA	ALA	PRO	PRO	GLN	ARG	GLY	TRP	ASN	ALA	PHE	VAL	LEU	PRO	SER	ARG	HIS	PHE	ALA	THR	ALA	ALA	GLY	ALA	ASN	PRO	F41	P183
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- Molecule 30: ATP synthase subunit delta

Chain d2:  78% 22%


MET	PHE	ALA	ARG	ALA	PHE	SER	ARG	PHE	ALA	ALA	LEU	ALA	ALA	PRO	PRO	GLN	ARG	GLY	TRP	ASN	ALA	PHE	VAL	LEU	PRO	SER	ARG	HIS	PHE	ALA	THR	ALA	ALA	GLY	ALA	ASN	PRO	F41	P183
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------

- Molecule 30: ATP synthase subunit delta

Chain d3:  78% 22%


MET	PHE	ALA	ARG	ALA	PHE	SER	ARG	PHE	ALA	ALA	LEU	ALA	ALA	PRO	PRO	GLN	ARG	GLY	TRP	ASN	ALA	PHE	VAL	LEU	PRO	SER	ARG	HIS	PHE	ALA	THR	ALA	ALA	GLY	ALA	ASN	PRO	F41	P183
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------

- Molecule 30: ATP synthase subunit delta

Chain d4:  78% 22%


MET	PHE	ALA	ARG	ALA	PHE	SER	ARG	PHE	ALA	ALA	LEU	ALA	ALA	PRO	PRO	GLN	ARG	GLY	TRP	ASN	ALA	PHE	VAL	LEU	PRO	SER	ARG	HIS	PHE	ALA	THR	ALA	ALA	GLY	ALA	ASN	PRO	F41	P183
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- Molecule 30: ATP synthase subunit delta

Chain d5:  78% 22%


MET	PHE	ALA	ARG	ALA	PHE	SER	ARG	PHE	ALA	ALA	LEU	ALA	ALA	PRO	PRO	GLN	ARG	GLY	TRP	ASN	ALA	PHE	VAL	LEU	PRO	SER	ARG	HIS	PHE	ALA	THR	ALA	ALA	GLY	ALA	ASN	PRO	F41	P183
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- Molecule 30: ATP synthase subunit delta

Chain d6:  78% 22%

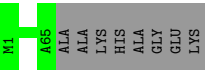
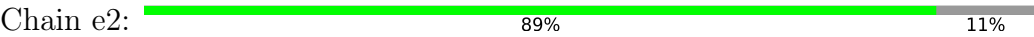
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- Molecule 31: ATP synthase subunit epsilon

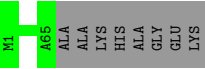
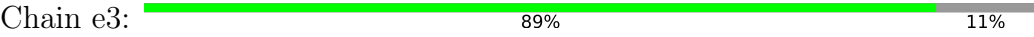
Chain e1:  89% 11%

H1	A65	ALA	LYS	HIS	ALA	GLY	GLU	LYS
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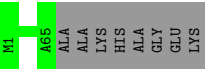
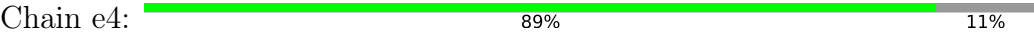
- Molecule 31: ATP synthase subunit epsilon



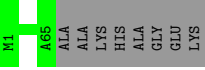
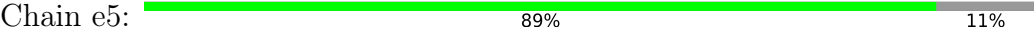
• Molecule 31: ATP synthase subunit epsilon



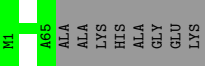
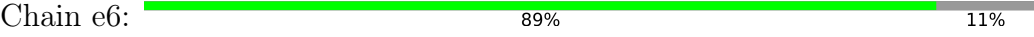
• Molecule 31: ATP synthase subunit epsilon



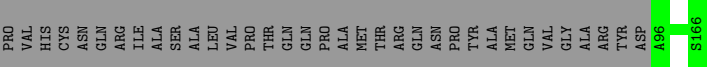
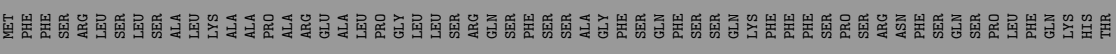
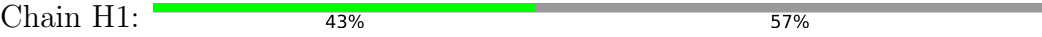
• Molecule 31: ATP synthase subunit epsilon



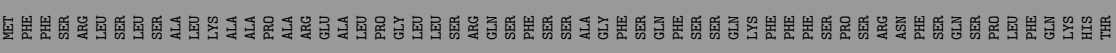
• Molecule 31: ATP synthase subunit epsilon

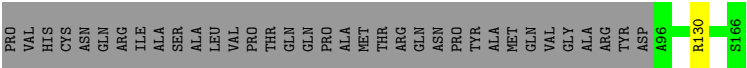


• Molecule 32: subunit c

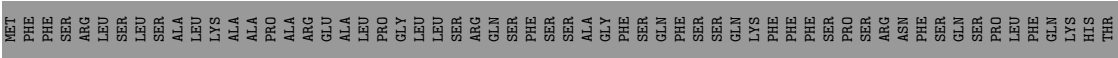


• Molecule 32: subunit c

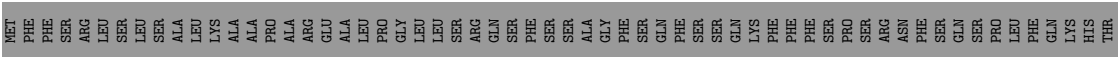




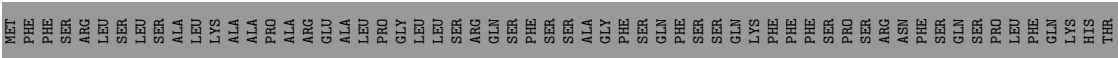
● Molecule 32: subunit c



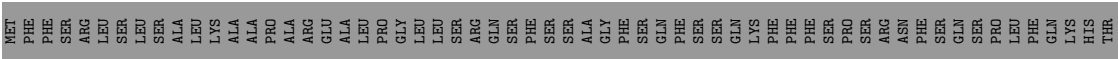
● Molecule 32: subunit c



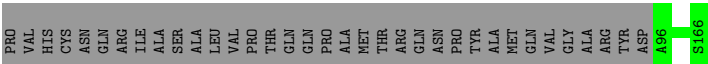
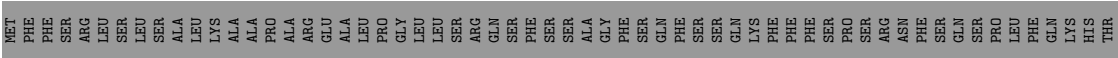
● Molecule 32: subunit c



● Molecule 32: subunit c

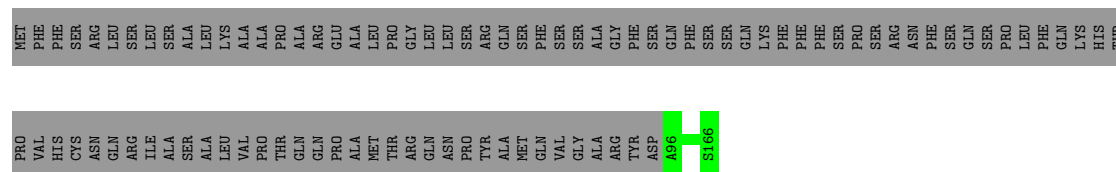


● Molecule 32: subunit c



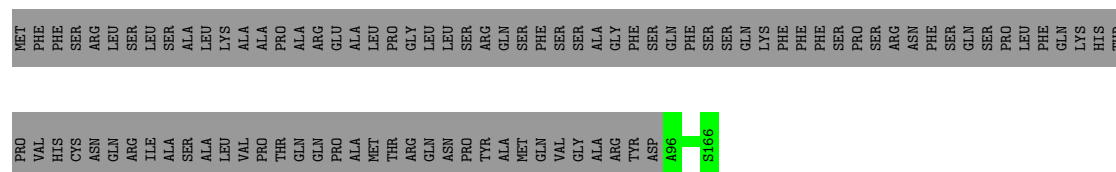
- Molecule 32: subunit c

Chain O1:  43% 57%



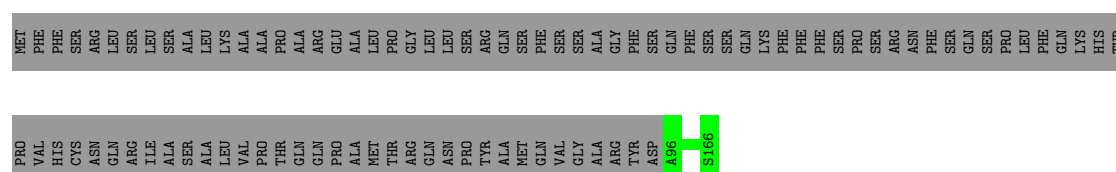
- Molecule 32: subunit c

Chain P1:



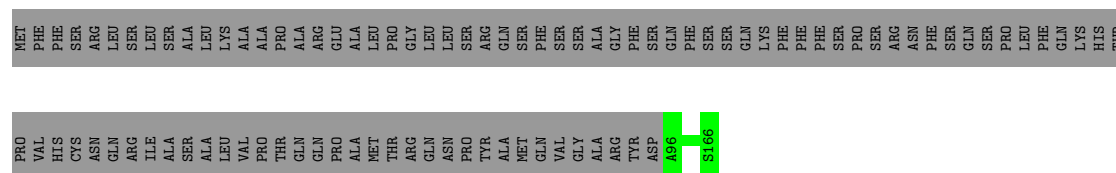
- Molecule 32: subunit c

Chain Q1: 



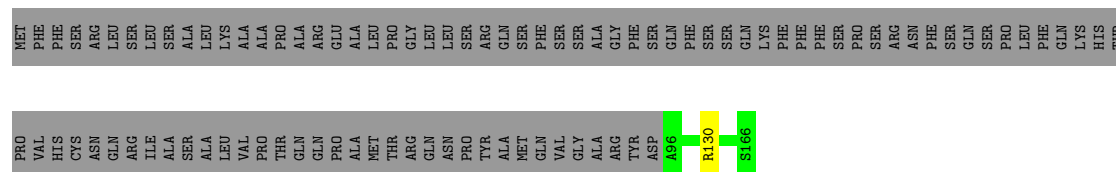
- Molecule 32: subunit c

Chain H2:  43% 57%



- Molecule 32: subunit c

Chain I2: 42% . 57%



- Molecule 32: subunit c

Chain J2:  43% 57%

MET	PHE	PHE	SER	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	GLN	ARG	GLU	ALA	LEU	PRO	GLY	LEU	LEU	LEU	ASN	PRO	TYR	ARG	GLN	SER	PHE	SER	GLY	ALA	GLY	PHE	SER	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	SER	PRO	ARG	ASN	PHE	SER	GLN	PRO	PRO	PHE	GLN	LYS	HIS	THR
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	VAL	PRO	THR	GLN	GLN	PRO	GLU	ALA	ALA	LEU	PRO	THR	ARG	GLY	LEU	LEU	ASN	PRO	TYR	ARG	GLN	SER	PHE	SER	GLY	ALA	GLY	PHE	SER	ASP	A96	S166
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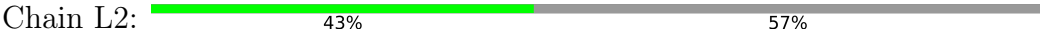
• Molecule 32: subunit c



MET	PHE	PHE	SER	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	GLN	ARG	GLU	ALA	LEU	PRO	GLY	LEU	LEU	LEU	ASN	PRO	TYR	ARG	GLN	SER	PHE	SER	GLY	ALA	GLY	PHE	SER	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	SER	PRO	ARG	ASN	PHE	SER	GLN	PRO	PRO	PHE	GLN	LYS	HIS	THR
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	VAL	PRO	THR	GLN	GLN	PRO	GLU	ALA	ALA	LEU	PRO	THR	ARG	GLY	LEU	LEU	ASN	PRO	TYR	ARG	GLN	SER	PHE	SER	GLY	ALA	GLY	PHE	SER	ASP	A96	S166
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• Molecule 32: subunit c



MET	PHE	PHE	SER	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	GLN	ARG	GLU	ALA	LEU	PRO	GLY	LEU	LEU	LEU	ASN	PRO	TYR	ARG	GLN	SER	PHE	SER	GLY	ALA	GLY	PHE	SER	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	SER	PRO	ARG	ASN	PHE	SER	GLN	PRO	PRO	PHE	GLN	LYS	HIS	THR
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	VAL	PRO	THR	GLN	GLN	PRO	GLU	ALA	ALA	LEU	PRO	THR	ARG	GLY	LEU	LEU	ASN	PRO	TYR	ARG	GLN	SER	PHE	SER	GLY	ALA	GLY	PHE	SER	ASP	A96	S166
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• Molecule 32: subunit c



MET	PHE	PHE	SER	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	GLN	ARG	GLU	ALA	LEU	PRO	GLY	LEU	LEU	LEU	ASN	PRO	TYR	ARG	GLN	SER	PHE	SER	GLY	ALA	GLY	PHE	SER	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	SER	PRO	ARG	ASN	PHE	SER	GLN	PRO	PRO	PHE	GLN	LYS	HIS	THR
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	VAL	PRO	THR	GLN	GLN	PRO	GLU	ALA	ALA	LEU	PRO	THR	ARG	GLY	LEU	LEU	ASN	PRO	TYR	ARG	GLN	SER	PHE	SER	GLY	ALA	GLY	PHE	SER	ASP	A96	S166
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• Molecule 32: subunit c



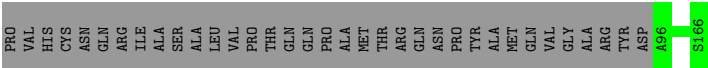
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	VAL	PRO	THR	GLN	GLN	PRO	GLU	ALA	ALA	LEU	PRO	THR	ARG	GLY	LEU	LEU	ASN	PRO	TYR	ARG	GLN	SER	PHE	SER	GLY	ALA	GLY	PHE	SER	ASP	A96	S166
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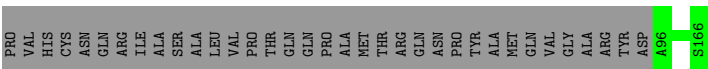
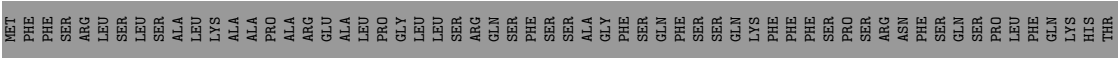
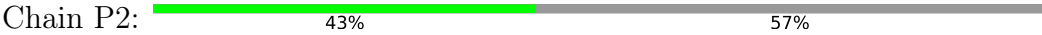
• Molecule 32: subunit c



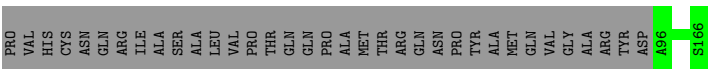
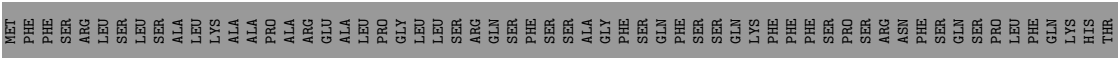
MET	PHE	PHE	SER	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	GLN	ARG	GLU	ALA	LEU	PRO	GLY	LEU	LEU	LEU	ASN	PRO	TYR	ARG	GLN	SER	PHE	SER	GLY	ALA	GLY	PHE	SER	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	SER	PRO	ARG	ASN	PHE	SER	GLN	PRO	PRO	PHE	GLN	LYS	HIS	THR
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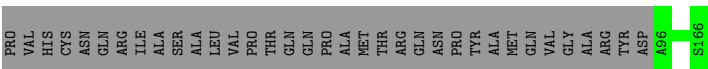
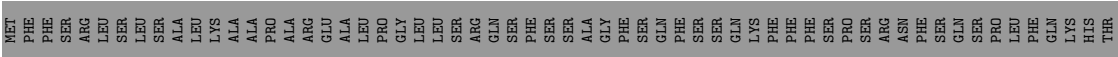
● Molecule 32: subunit c



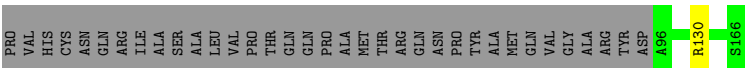
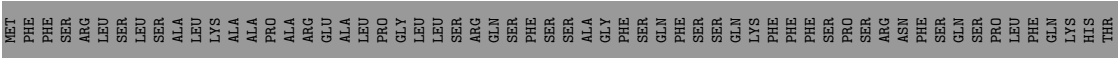
● Molecule 32: subunit c



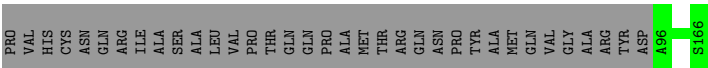
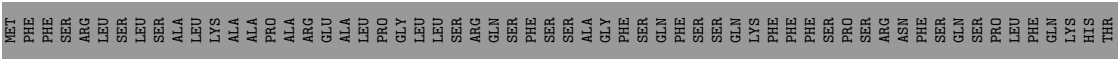
● Molecule 32: subunit c



● Molecule 32: subunit c

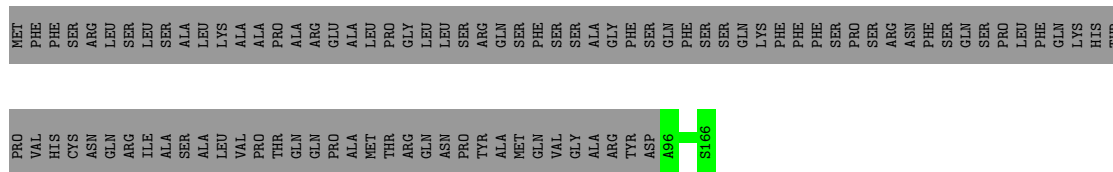


● Molecule 32: subunit c



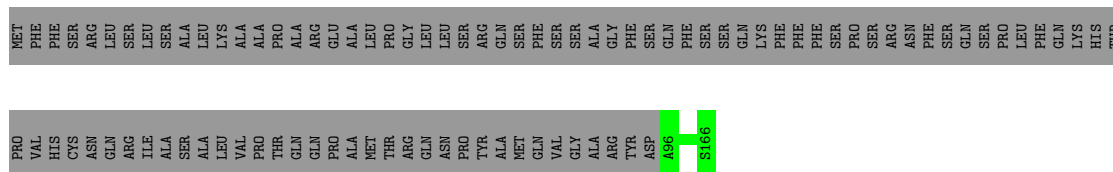
- Molecule 32: subunit c

Chain K3: 



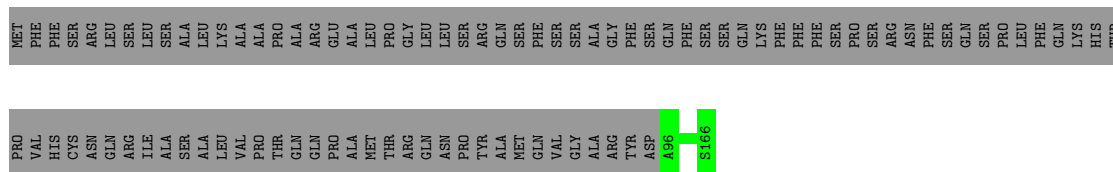
- Molecule 32: subunit c

Chain L3:



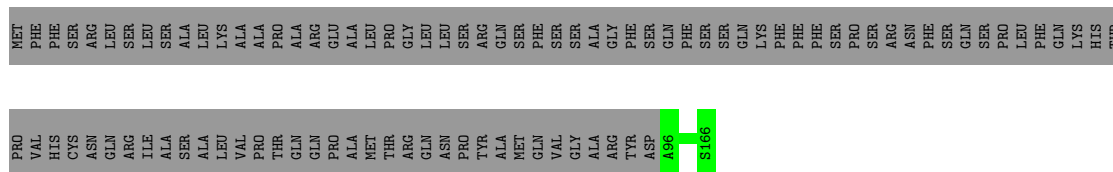
- Molecule 32: subunit c

Chain M3: 43% 57%



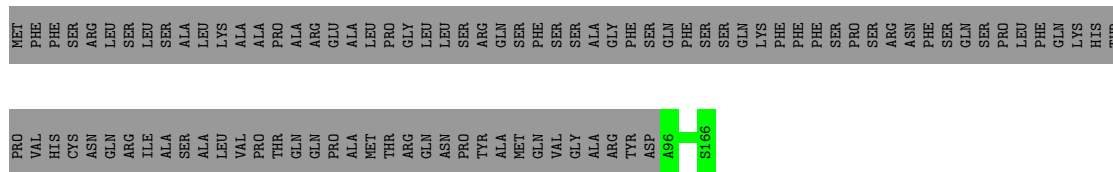
- Molecule 32: subunit c

Chain N3: 43% 57%



- Molecule 32: subunit c

Chain O3:  43% 57%



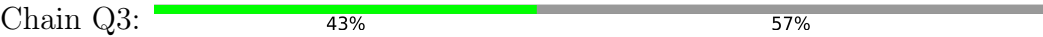
- Molecule 32: subunit c

Chain P3:

MET	PHE	PHE	PHE	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	GLN	ARG	GLU	ALA	LEU	PRO	GLY	LEU	LEU	LEU	ASN	PRO	SER	ARG	GLN	PHE	SER	VAL	GLY	ALA	GLY	PHE	TYR	ASP	SER	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	SER	SER	PRO	PRO	ARG	ASN	PHE	SER	GLN	PRO	PHE	GLN	LYS	HIS	THR
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	VAL	PRO	THR	GLN	GLN	ASN	PRO	TYR	ALA	ALA	GLN	MET	THR	ARG	GLY	LEU	LEU	ASN	PRO	TYR	ALA	ALA	GLN	MET	SER	SER	GLN	VAL	GLY	ALA	ARG	GLY	PHE	TYR	ASP	A96	S166
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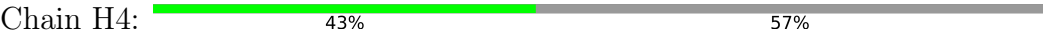
● Molecule 32: subunit c



MET	PHE	PHE	SER	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	THR	GLN	GLN	ARG	GLU	ALA	LEU	PRO	GLY	LEU	LEU	LEU	ASN	PRO	SER	ARG	GLN	PHE	SER	VAL	GLY	ALA	GLY	PHE	TYR	ASP	SER	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	SER	SER	PRO	PRO	ARG	ASN	PHE	SER	GLN	PRO	PHE	GLN	LYS	HIS	THR
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	VAL	PRO	THR	GLN	GLN	ARG	GLU	ALA	LEU	PRO	GLY	LEU	LEU	LEU	ASN	PRO	TYR	ALA	ALA	GLN	MET	SER	SER	GLN	VAL	GLY	ALA	ARG	GLY	PHE	TYR	ASP	A96	S166
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● Molecule 32: subunit c



MET	PHE	PHE	SER	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	THR	GLN	GLN	ARG	GLU	ALA	LEU	PRO	GLY	LEU	LEU	LEU	ASN	PRO	SER	ARG	GLN	PHE	SER	VAL	GLY	ALA	GLY	PHE	TYR	ASP	SER	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	SER	SER	PRO	PRO	ARG	ASN	PHE	SER	GLN	PRO	PHE	GLN	LYS	HIS	THR
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	VAL	PRO	THR	GLN	GLN	ARG	GLU	ALA	LEU	PRO	GLY	LEU	LEU	LEU	ASN	PRO	TYR	ALA	ALA	GLN	MET	SER	SER	GLN	VAL	GLY	ALA	ARG	GLY	PHE	TYR	ASP	A96	S166
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● Molecule 32: subunit c



MET	PHE	PHE	SER	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	THR	GLN	GLN	ARG	GLU	ALA	LEU	PRO	GLY	LEU	LEU	LEU	ASN	PRO	SER	ARG	GLN	PHE	SER	VAL	GLY	ALA	GLY	PHE	TYR	ASP	SER	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	SER	SER	PRO	PRO	ARG	ASN	PHE	SER	GLN	PRO	PHE	GLN	LYS	HIS	THR
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	VAL	PRO	THR	GLN	GLN	ARG	GLU	ALA	LEU	PRO	GLY	LEU	LEU	LEU	ASN	PRO	TYR	ALA	ALA	GLN	MET	SER	SER	GLN	VAL	GLY	ALA	ARG	GLY	PHE	TYR	ASP	A96	R130	S166
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● Molecule 32: subunit c



MET	PHE	PHE	SER	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	THR	GLN	GLN	ARG	GLU	ALA	LEU	PRO	GLY	LEU	LEU	LEU	ASN	PRO	SER	ARG	GLN	PHE	SER	VAL	GLY	ALA	GLY	PHE	TYR	ASP	SER	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	SER	SER	PRO	PRO	ARG	ASN	PHE	SER	GLN	PRO	PHE	GLN	LYS	HIS	THR
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	VAL	PRO	THR	GLN	GLN	ARG	GLU	ALA	LEU	PRO	GLY	LEU	LEU	LEU	ASN	PRO	TYR	ALA	ALA	GLN	MET	SER	SER	GLN	VAL	GLY	ALA	ARG	GLY	PHE	TYR	ASP	A96	S166
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● Molecule 32: subunit c

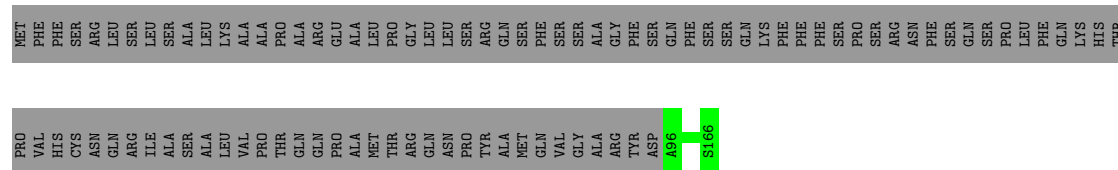


MET	PHE	PHE	SER	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	THR	GLN	GLN	ARG	GLU	ALA	LEU	PRO	GLY	LEU	LEU	LEU	ASN	PRO	SER	ARG	GLN	PHE	SER	VAL	GLY	ALA	GLY	PHE	TYR	ASP	SER	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	SER	SER	PRO	PRO	ARG	ASN	PHE	SER	GLN	PRO	PHE	GLN	LYS	HIS	THR
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	PRO	THR	GLN	PRO	ALA	MET	THR	ARG	GLN	ASN	PRO	TYR	ALA	MET	GLN	VAL	GLY	ALA	ARG	TYR	ASP	A96	S166
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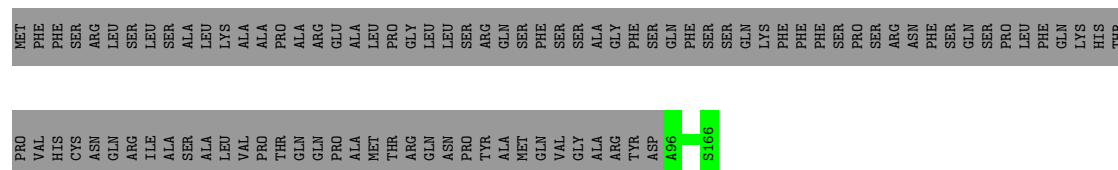
- Molecule 32: subunit c

Chain Q4: 43% 57%



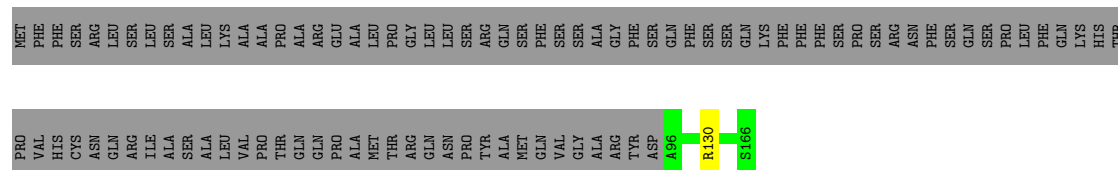
- Molecule 32: subunit c

Chain H5:  43% 57%



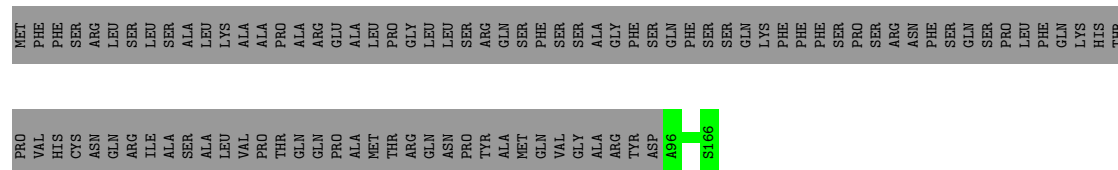
- Molecule 32: subunit c

Chain I5:  42% . 57%



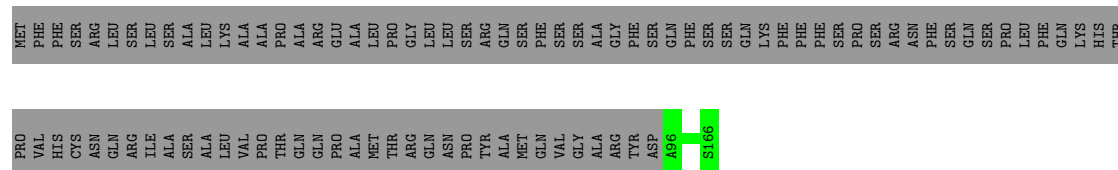
- Molecule 32: subunit c

Chain J5: 43% 57%



- Molecule 32: subunit c

Chain K5:  43% 57%



- Molecule 32: subunit c

Chain L5:  43% 57%

MET	PHE	PHE	PHE	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	ARG	GLU	GLU	ALA	LEU	PRO	PRO	GLY	LEU	LEU	LEU	SER	ARG	GLN	PHE	SER	SER	GLY	ALA	GLY	PHE	SER	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	PHE	SER	SER	PRO	PRO	PRO	LEU	PHE	GLN	LYS	HIS	THR
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	VAL	PRO	THR	GLN	GLN	ASN	PRO	TYR	ALA	MET	PRO	THR	ARG	GLY	LEU	LEU	ASN	PRO	TYR	ALA	MET	GLN	PHE	SER	VAL	GLY	ALA	ARG	TYR	ASP	A96	S166
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• Molecule 32: subunit c



MET	PHE	PHE	PHE	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	ARG	GLU	GLU	ALA	LEU	PRO	PRO	GLY	LEU	LEU	LEU	SER	ARG	GLN	PHE	SER	SER	VAL	GLY	ALA	GLY	PHE	SER	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	PHE	SER	SER	PRO	PRO	PRO	LEU	PHE	GLN	LYS	HIS	THR
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	VAL	PRO	THR	GLN	GLN	ASN	PRO	TYR	ALA	MET	PRO	THR	ARG	GLY	LEU	LEU	ASN	PRO	TYR	ALA	MET	GLN	PHE	SER	VAL	GLY	ALA	ARG	TYR	ASP	A96	S166
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• Molecule 32: subunit c



MET	PHE	PHE	PHE	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	ARG	GLU	GLU	ALA	LEU	PRO	PRO	GLY	LEU	LEU	LEU	SER	ARG	GLN	PHE	SER	SER	VAL	GLY	ALA	GLY	PHE	SER	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	PHE	SER	SER	PRO	PRO	PRO	LEU	PHE	GLN	LYS	HIS	THR
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	VAL	PRO	THR	GLN	GLN	ASN	PRO	TYR	ALA	MET	PRO	THR	ARG	GLY	LEU	LEU	ASN	PRO	TYR	ALA	MET	GLN	PHE	SER	VAL	GLY	ALA	ARG	TYR	ASP	A96	S166
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• Molecule 32: subunit c



MET	PHE	PHE	PHE	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	ARG	GLU	GLU	ALA	LEU	PRO	PRO	GLY	LEU	LEU	LEU	SER	ARG	GLN	PHE	SER	SER	VAL	GLY	ALA	GLY	PHE	SER	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	PHE	SER	SER	PRO	PRO	PRO	LEU	PHE	GLN	LYS	HIS	THR
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	VAL	PRO	THR	GLN	GLN	ASN	PRO	TYR	ALA	MET	PRO	THR	ARG	GLY	LEU	LEU	ASN	PRO	TYR	ALA	MET	GLN	PHE	SER	VAL	GLY	ALA	ARG	TYR	ASP	A96	S166
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• Molecule 32: subunit c



MET	PHE	PHE	PHE	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	ARG	GLU	GLU	ALA	LEU	PRO	PRO	GLY	LEU	LEU	LEU	SER	ARG	GLN	PHE	SER	SER	VAL	GLY	ALA	GLY	PHE	SER	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	PHE	SER	SER	PRO	PRO	PRO	LEU	PHE	GLN	LYS	HIS	THR
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PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	ALA	LEU	VAL	VAL	PRO	THR	GLN	GLN	ASN	PRO	TYR	ALA	MET	PRO	THR	ARG	GLY	LEU	LEU	ASN	PRO	TYR	ALA	MET	GLN	PHE	SER	VAL	GLY	ALA	ARG	TYR	ASP	A96	S166
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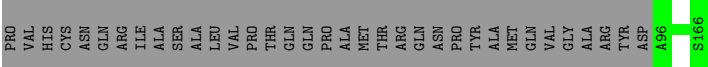
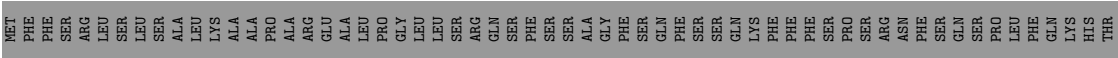
• Molecule 32: subunit c



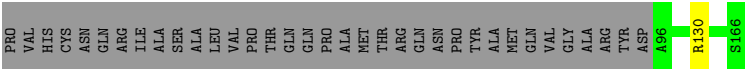
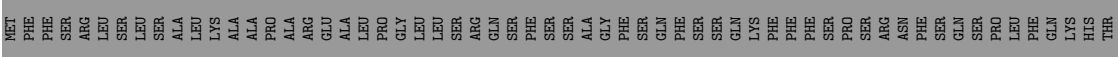
MET	PHE	PHE	PHE	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	ARG	GLU	GLU	ALA	LEU	PRO	PRO	GLY	LEU	LEU	LEU	SER	ARG	GLN	PHE	SER	SER	VAL	GLY	ALA	GLY	PHE	SER	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	PHE	SER	SER	PRO	PRO	PRO	LEU	PHE	GLN	LYS	HIS	THR
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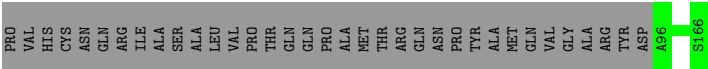
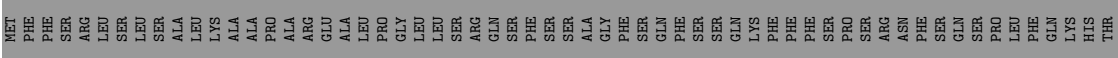
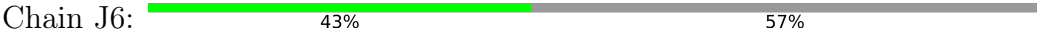
● Molecule 32: subunit c



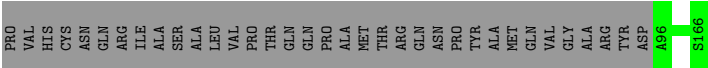
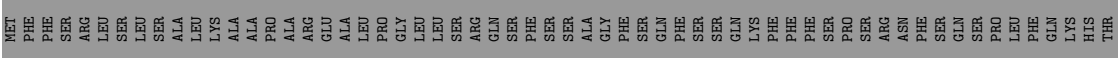
● Molecule 32: subunit c



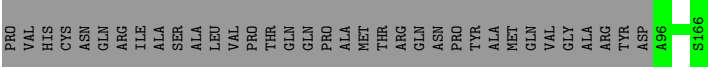
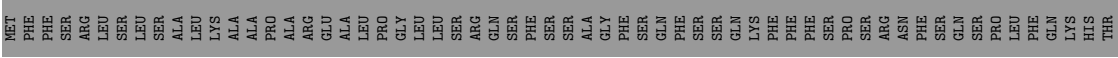
● Molecule 32: subunit c



● Molecule 32: subunit c



● Molecule 32: subunit c



- [illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	4532	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 ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	Q7	0.27	0/1103	0.42	0/1496
1	Q8	0.28	0/1103	0.44	0/1496
1	Q9	0.27	0/1103	0.41	0/1496
1	q7	0.29	0/1103	0.44	0/1496
1	q8	0.27	0/1103	0.42	0/1496
1	q9	0.28	0/1103	0.44	0/1496
2	I7	0.26	0/719	0.40	0/962
2	I8	0.27	0/719	0.40	0/962
2	I9	0.26	0/719	0.40	0/962
2	i7	0.27	0/719	0.40	0/962
2	i8	0.26	0/719	0.40	0/962
2	i9	0.27	0/719	0.40	0/962
3	T7	0.25	0/741	0.42	0/1007
3	T8	0.24	0/741	0.42	0/1007
3	T9	0.25	0/741	0.42	0/1007
3	t7	0.24	0/741	0.42	0/1007
3	t8	0.25	0/741	0.42	0/1007
3	t9	0.24	0/741	0.42	0/1007
4	G7	0.28	0/896	0.45	0/1216
4	G8	0.26	0/896	0.42	0/1216
4	G9	0.28	0/896	0.45	0/1216
4	g7	0.26	0/896	0.43	0/1216
4	g8	0.28	0/896	0.45	0/1216
4	g9	0.26	0/896	0.41	0/1216
5	O7	0.29	0/1250	0.44	0/1682
5	O8	0.26	0/1250	0.42	0/1682
5	O9	0.28	0/1250	0.43	0/1682
5	o7	0.26	0/1250	0.42	0/1682
5	o8	0.29	0/1250	0.45	0/1682
5	o9	0.26	0/1250	0.42	0/1682
6	K7	0.30	0/981	0.40	0/1321
6	K8	0.30	0/981	0.42	0/1321
6	K9	0.30	0/981	0.40	0/1321
6	k7	0.30	0/981	0.42	0/1321

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	k8	0.30	0/981	0.41	0/1321
6	k9	0.30	0/981	0.42	0/1321
7	J7	0.36	0/1573	0.45	0/2137
7	J8	0.32	0/1573	0.44	0/2137
7	J9	0.36	0/1573	0.44	0/2137
7	j7	0.32	0/1573	0.44	0/2137
7	j8	0.37	0/1573	0.45	0/2137
7	j9	0.31	0/1573	0.44	0/2137
8	S7	0.29	0/826	0.41	0/1119
8	S8	0.27	0/826	0.39	0/1119
8	S9	0.29	0/826	0.40	0/1119
8	s7	0.26	0/826	0.39	0/1119
8	s8	0.29	0/826	0.40	0/1119
8	s9	0.26	0/826	0.39	0/1119
9	U7	0.34	0/770	0.43	0/1040
9	U8	0.28	0/770	0.40	0/1040
9	U9	0.34	0/770	0.43	0/1040
9	u7	0.28	0/770	0.40	0/1040
9	u8	0.34	0/770	0.43	0/1040
9	u9	0.28	0/770	0.39	0/1040
10	H7	0.33	0/1902	0.45	0/2575
10	H8	0.29	0/1902	0.44	0/2575
10	H9	0.32	0/1902	0.44	0/2575
10	h7	0.29	0/1902	0.44	0/2575
10	h8	0.33	0/1902	0.45	0/2575
10	h9	0.28	0/1902	0.43	0/2575
11	E7	0.33	0/1154	0.45	0/1572
11	E8	0.29	0/1154	0.44	0/1572
11	E9	0.33	0/1154	0.45	0/1572
11	e7	0.29	0/1154	0.44	0/1572
11	e8	0.33	0/1154	0.46	0/1572
11	e9	0.29	0/1154	0.43	0/1572
12	X7	0.27	0/678	0.41	0/923
12	X8	0.25	0/678	0.40	0/923
12	X9	0.26	0/678	0.40	0/923
12	x7	0.25	0/678	0.40	0/923
12	x8	0.27	0/678	0.41	0/923
12	x9	0.25	0/678	0.40	0/923
13	B7	0.27	0/4016	0.42	0/5422
13	B8	0.26	0/4016	0.42	0/5422
13	B9	0.26	0/4016	0.42	0/5422
13	b7	0.26	0/4016	0.42	0/5422
13	b8	0.27	0/4016	0.42	0/5422

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
13	b9	0.26	0/4016	0.42	0/5422
14	R7	0.25	0/1092	0.41	0/1470
14	R8	0.25	0/1092	0.40	0/1470
14	R9	0.25	0/1092	0.41	0/1470
14	r7	0.25	0/1092	0.42	0/1470
14	r8	0.25	0/1092	0.41	0/1470
14	r9	0.25	0/1092	0.40	0/1470
15	P7	0.26	0/888	0.37	0/1202
15	P8	0.27	0/888	0.38	0/1202
15	P9	0.27	0/888	0.37	0/1202
15	p7	0.27	0/888	0.39	0/1202
15	p8	0.27	0/888	0.38	0/1202
15	p9	0.27	0/888	0.38	0/1202
16	V7	0.31	0/944	0.44	0/1280
16	V8	0.28	0/944	0.44	0/1280
16	V9	0.31	0/944	0.44	0/1280
16	v7	0.28	0/944	0.44	0/1280
16	v8	0.31	0/944	0.44	0/1280
16	v9	0.28	0/944	0.44	0/1280
17	L7	0.29	0/1651	0.43	0/2227
17	L8	0.26	0/1651	0.40	0/2227
17	L9	0.28	0/1651	0.43	0/2227
17	l7	0.26	0/1651	0.40	0/2227
17	l8	0.28	0/1651	0.43	0/2227
17	l9	0.26	0/1651	0.40	0/2227
18	C7	0.28	0/1057	0.42	0/1428
18	C8	0.27	0/1057	0.42	0/1428
18	C9	0.27	0/1057	0.42	0/1428
18	c7	0.27	0/1057	0.43	0/1428
18	c8	0.28	0/1057	0.43	0/1428
18	c9	0.27	0/1057	0.42	0/1428
19	D7	0.33	0/2138	0.44	0/2905
19	D8	0.28	0/2138	0.44	0/2905
19	D9	0.32	0/2138	0.44	0/2905
19	d7	0.28	0/2138	0.44	0/2905
19	d8	0.33	0/2138	0.44	0/2905
19	d9	0.28	0/2138	0.43	0/2905
20	M7	0.28	0/789	0.42	0/1065
20	M8	0.27	0/789	0.43	0/1065
20	M9	0.28	0/789	0.42	0/1065
20	m7	0.27	0/789	0.43	0/1065
20	m8	0.28	0/789	0.42	0/1065
20	m9	0.27	0/789	0.43	0/1065

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
21	N7	0.28	0/1280	0.42	0/1734
21	N8	0.26	0/1280	0.40	0/1734
21	N9	0.28	0/1280	0.42	0/1734
21	n7	0.26	0/1280	0.40	0/1734
21	n8	0.28	0/1280	0.42	0/1734
21	n9	0.25	0/1280	0.40	0/1734
22	F7	0.26	0/1475	0.42	0/2009
22	F8	0.25	0/1475	0.41	0/2009
22	F9	0.25	0/1475	0.42	0/2009
22	f7	0.25	0/1475	0.42	0/2009
22	f8	0.26	0/1475	0.42	0/2009
22	f9	0.25	0/1475	0.42	0/2009
23	W7	0.33	0/778	0.47	0/1057
23	W8	0.29	0/778	0.44	0/1057
23	W9	0.32	0/778	0.47	0/1057
23	w7	0.29	0/778	0.44	0/1057
23	w8	0.33	0/778	0.48	0/1057
23	w9	0.28	0/778	0.43	0/1057
24	A7	0.25	0/3883	0.39	0/5262
24	A8	0.25	0/3883	0.39	0/5262
24	A9	0.25	0/3883	0.39	0/5262
24	a7	0.25	0/3883	0.39	0/5262
24	a8	0.25	0/3883	0.39	0/5262
24	a9	0.25	0/3883	0.39	0/5262
25	G1	0.30	0/1431	0.67	5/1929 (0.3%)
25	G2	0.33	0/1431	0.70	6/1929 (0.3%)
25	G3	0.27	0/1431	0.56	1/1929 (0.1%)
25	G4	0.30	0/1431	0.64	3/1929 (0.2%)
25	G5	0.30	0/1431	0.65	4/1929 (0.2%)
25	G6	0.31	0/1431	0.71	7/1929 (0.4%)
26	i1	0.25	0/343	0.39	0/459
26	i2	0.25	0/343	0.38	0/459
26	i3	0.25	0/343	0.38	0/459
26	i4	0.26	0/343	0.38	0/459
26	i5	0.25	0/343	0.39	0/459
26	i6	0.25	0/343	0.38	0/459
27	A1	0.24	0/3979	0.43	0/5372
27	A2	0.24	0/3979	0.43	0/5372
27	A3	0.24	0/3979	0.43	0/5372
27	A4	0.24	0/3979	0.43	0/5372
27	A5	0.24	0/3979	0.43	0/5372
27	A6	0.24	0/3979	0.43	0/5372
27	C1	0.24	0/3938	0.43	0/5314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	C2	0.24	0/3938	0.43	0/5314
27	C3	0.24	0/3938	0.43	0/5314
27	C4	0.24	0/3938	0.43	0/5314
27	C5	0.24	0/3938	0.43	0/5314
27	C6	0.24	0/3938	0.43	0/5314
27	E1	0.24	0/3942	0.43	0/5322
27	E2	0.24	0/3942	0.42	0/5322
27	E3	0.24	0/3942	0.43	0/5322
27	E4	0.24	0/3942	0.43	0/5322
27	E5	0.24	0/3942	0.43	0/5322
27	E6	0.24	0/3942	0.43	0/5322
28	B1	0.25	0/3698	0.43	0/5016
28	B2	0.25	0/3698	0.43	0/5016
28	B3	0.25	0/3698	0.43	0/5016
28	B4	0.25	0/3698	0.43	0/5016
28	B5	0.25	0/3698	0.43	0/5016
28	B6	0.25	0/3698	0.43	0/5016
28	D1	0.25	0/3672	0.43	0/4980
28	D2	0.25	0/3672	0.43	0/4980
28	D3	0.25	0/3672	0.43	0/4980
28	D4	0.25	0/3672	0.43	0/4980
28	D5	0.25	0/3672	0.43	0/4980
28	D6	0.25	0/3672	0.43	0/4980
28	F1	0.25	0/3672	0.44	0/4980
28	F2	0.25	0/3672	0.44	0/4980
28	F3	0.25	0/3672	0.44	0/4980
28	F4	0.25	0/3672	0.44	0/4980
28	F5	0.25	0/3672	0.44	0/4980
28	F6	0.25	0/3672	0.44	0/4980
29	g1	0.24	0/2145	0.39	0/2890
29	g2	0.25	0/2145	0.39	0/2890
29	g3	0.24	0/2145	0.39	0/2890
29	g4	0.25	0/2145	0.39	0/2890
29	g5	0.24	0/2145	0.39	0/2890
29	g6	0.25	0/2145	0.39	0/2890
30	d1	0.24	0/1083	0.42	0/1466
30	d2	0.25	0/1083	0.42	0/1466
30	d3	0.24	0/1083	0.43	0/1466
30	d4	0.25	0/1083	0.42	0/1466
30	d5	0.24	0/1083	0.43	0/1466
30	d6	0.25	0/1083	0.42	0/1466
31	e1	0.26	0/547	0.43	0/733
31	e2	0.26	0/547	0.43	0/733

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
31	e3	0.26	0/547	0.43	0/733
31	e4	0.26	0/547	0.43	0/733
31	e5	0.26	0/547	0.43	0/733
31	e6	0.26	0/547	0.43	0/733
32	H1	0.26	0/507	0.38	0/686
32	H2	0.26	0/507	0.39	0/686
32	H3	0.26	0/507	0.39	0/686
32	H4	0.26	0/507	0.39	0/686
32	H5	0.26	0/507	0.38	0/686
32	H6	0.26	0/507	0.39	0/686
32	I1	0.25	0/507	0.38	0/686
32	I2	0.25	0/507	0.38	0/686
32	I3	0.25	0/507	0.38	0/686
32	I4	0.25	0/507	0.38	0/686
32	I5	0.25	0/507	0.38	0/686
32	I6	0.26	0/507	0.38	0/686
32	J1	0.26	0/507	0.39	0/686
32	J2	0.26	0/507	0.39	0/686
32	J3	0.26	0/507	0.39	0/686
32	J4	0.26	0/507	0.39	0/686
32	J5	0.26	0/507	0.39	0/686
32	J6	0.26	0/507	0.39	0/686
32	K1	0.25	0/507	0.38	0/686
32	K2	0.25	0/507	0.39	0/686
32	K3	0.25	0/507	0.39	0/686
32	K4	0.25	0/507	0.39	0/686
32	K5	0.25	0/507	0.39	0/686
32	K6	0.25	0/507	0.39	0/686
32	L1	0.25	0/507	0.41	0/686
32	L2	0.26	0/507	0.41	0/686
32	L3	0.25	0/507	0.41	0/686
32	L4	0.26	0/507	0.41	0/686
32	L5	0.25	0/507	0.41	0/686
32	L6	0.26	0/507	0.41	0/686
32	M1	0.25	0/507	0.37	0/686
32	M2	0.25	0/507	0.37	0/686
32	M3	0.25	0/507	0.37	0/686
32	M4	0.25	0/507	0.37	0/686
32	M5	0.25	0/507	0.37	0/686
32	M6	0.25	0/507	0.37	0/686
32	N1	0.24	0/507	0.38	0/686
32	N2	0.25	0/507	0.38	0/686
32	N3	0.24	0/507	0.37	0/686

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	N4	0.25	0/507	0.37	0/686
32	N5	0.24	0/507	0.37	0/686
32	N6	0.25	0/507	0.37	0/686
32	O1	0.26	0/507	0.38	0/686
32	O2	0.25	0/507	0.38	0/686
32	O3	0.26	0/507	0.38	0/686
32	O4	0.26	0/507	0.38	0/686
32	O5	0.26	0/507	0.39	0/686
32	O6	0.26	0/507	0.38	0/686
32	P1	0.26	0/507	0.42	0/686
32	P2	0.27	0/507	0.41	0/686
32	P3	0.26	0/507	0.42	0/686
32	P4	0.27	0/507	0.41	0/686
32	P5	0.26	0/507	0.42	0/686
32	P6	0.27	0/507	0.41	0/686
32	Q1	0.27	0/507	0.42	0/686
32	Q2	0.27	0/507	0.43	0/686
32	Q3	0.27	0/507	0.42	0/686
32	Q4	0.27	0/507	0.43	0/686
32	Q5	0.27	0/507	0.42	0/686
32	Q6	0.27	0/507	0.43	0/686
All	All	0.26	0/396624	0.43	26/536592 (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
7	J7	0	1
7	J8	0	1
7	J9	0	1
7	j7	0	1
7	j8	0	1
7	j9	0	1
14	R8	0	1
25	G1	0	2
25	G2	0	2
25	G3	0	3
25	G4	0	2
25	G5	0	2
25	G6	0	2
All	All	0	20

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G1	171	TYR	CA-CB-CG	11.14	134.57	113.40
25	G6	173	LYS	CD-CE-NZ	11.06	137.14	111.70
25	G5	171	TYR	CA-CB-CG	10.85	134.01	113.40
25	G6	171	TYR	CA-CB-CG	10.33	133.03	113.40
25	G4	171	TYR	CA-CB-CG	10.14	132.67	113.40
25	G1	171	TYR	N-CA-CB	8.60	126.07	110.60
25	G2	171	TYR	CA-CB-CG	8.43	129.41	113.40
25	G2	170	MET	CG-SD-CE	8.09	113.14	100.20
25	G2	170	MET	N-CA-CB	7.78	124.61	110.60
25	G1	97	TYR	CA-CB-CG	7.67	127.97	113.40
25	G2	171	TYR	N-CA-CB	7.52	124.14	110.60
25	G1	170	MET	C-N-CA	7.48	140.39	121.70
25	G5	97	TYR	CA-CB-CG	7.26	127.19	113.40
25	G2	170	MET	C-N-CA	7.05	139.34	121.70
25	G6	170	MET	C-N-CA	6.97	139.13	121.70
25	G4	170	MET	C-N-CA	6.84	138.81	121.70
25	G6	171	TYR	CB-CG-CD1	-6.59	117.04	121.00
25	G5	170	MET	C-N-CA	6.54	138.05	121.70
25	G3	170	MET	C-N-CA	6.41	137.71	121.70
25	G5	171	TYR	N-CA-CB	6.20	121.76	110.60
25	G6	97	TYR	CA-CB-CG	5.98	124.76	113.40
25	G4	171	TYR	N-CA-CB	5.64	120.75	110.60
25	G2	169	ALA	C-N-CA	-5.59	107.72	121.70
25	G6	171	TYR	N-CA-CB	5.47	120.45	110.60
25	G6	171	TYR	CB-CG-CD2	5.46	124.28	121.00
25	G1	171	TYR	CB-CG-CD1	-5.07	117.96	121.00

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	G1	171	TYR	Peptide
25	G1	172	ARG	Peptide
25	G2	171	TYR	Peptide
25	G2	172	ARG	Peptide
25	G3	171	TYR	Sidechain,Peptide
25	G3	172	ARG	Peptide
25	G4	171	TYR	Peptide
25	G4	172	ARG	Peptide
25	G5	171	TYR	Peptide

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Mol	Chain	Res	Type	Group
25	G5	172	ARG	Peptide
25	G6	171	TYR	Peptide
25	G6	172	ARG	Peptide
7	J7	89	PHE	Peptide
7	J8	89	PHE	Peptide
7	J9	89	PHE	Peptide
14	R8	87	LYS	Peptide
7	j7	89	PHE	Peptide
7	j8	89	PHE	Peptide
7	j9	89	PHE	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	Q7	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
1	Q8	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
1	Q9	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
1	q7	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
1	q8	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
1	q9	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
2	I7	88/236 (37%)	85 (97%)	3 (3%)	0	100	100
2	I8	88/236 (37%)	85 (97%)	3 (3%)	0	100	100
2	I9	88/236 (37%)	85 (97%)	3 (3%)	0	100	100
2	i7	88/236 (37%)	85 (97%)	3 (3%)	0	100	100
2	i8	88/236 (37%)	85 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	i9	88/236 (37%)	85 (97%)	3 (3%)	0	100	100
3	T7	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
3	T8	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
3	T9	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
3	t7	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
3	t8	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
3	t9	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
4	G7	110/252 (44%)	102 (93%)	8 (7%)	0	100	100
4	G8	110/252 (44%)	102 (93%)	8 (7%)	0	100	100
4	G9	110/252 (44%)	102 (93%)	8 (7%)	0	100	100
4	g7	110/252 (44%)	102 (93%)	8 (7%)	0	100	100
4	g8	110/252 (44%)	102 (93%)	8 (7%)	0	100	100
4	g9	110/252 (44%)	102 (93%)	8 (7%)	0	100	100
5	O7	147/157 (94%)	140 (95%)	7 (5%)	0	100	100
5	O8	147/157 (94%)	141 (96%)	6 (4%)	0	100	100
5	O9	147/157 (94%)	140 (95%)	7 (5%)	0	100	100
5	o7	147/157 (94%)	141 (96%)	6 (4%)	0	100	100
5	o8	147/157 (94%)	140 (95%)	7 (5%)	0	100	100
5	o9	147/157 (94%)	140 (95%)	7 (5%)	0	100	100
6	K7	115/224 (51%)	111 (96%)	4 (4%)	0	100	100
6	K8	115/224 (51%)	111 (96%)	4 (4%)	0	100	100
6	K9	115/224 (51%)	111 (96%)	4 (4%)	0	100	100
6	k7	115/224 (51%)	111 (96%)	4 (4%)	0	100	100
6	k8	115/224 (51%)	110 (96%)	5 (4%)	0	100	100
6	k9	115/224 (51%)	111 (96%)	4 (4%)	0	100	100
7	J7	174/229 (76%)	165 (95%)	9 (5%)	0	100	100
7	J8	174/229 (76%)	165 (95%)	9 (5%)	0	100	100
7	J9	174/229 (76%)	165 (95%)	9 (5%)	0	100	100
7	j7	174/229 (76%)	165 (95%)	9 (5%)	0	100	100
7	j8	174/229 (76%)	165 (95%)	9 (5%)	0	100	100
7	j9	174/229 (76%)	165 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	S7	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
8	S8	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
8	S9	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
8	s7	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
8	s8	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
8	s9	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
9	U7	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
9	U8	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
9	U9	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
9	u7	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
9	u8	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
9	u9	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
10	H7	224/239 (94%)	215 (96%)	9 (4%)	0	100	100
10	H8	224/239 (94%)	215 (96%)	9 (4%)	0	100	100
10	H9	224/239 (94%)	214 (96%)	10 (4%)	0	100	100
10	h7	224/239 (94%)	215 (96%)	9 (4%)	0	100	100
10	h8	224/239 (94%)	215 (96%)	9 (4%)	0	100	100
10	h9	224/239 (94%)	215 (96%)	9 (4%)	0	100	100
11	E7	138/325 (42%)	134 (97%)	4 (3%)	0	100	100
11	E8	138/325 (42%)	134 (97%)	4 (3%)	0	100	100
11	E9	138/325 (42%)	134 (97%)	4 (3%)	0	100	100
11	e7	138/325 (42%)	134 (97%)	4 (3%)	0	100	100
11	e8	138/325 (42%)	134 (97%)	4 (3%)	0	100	100
11	e9	138/325 (42%)	134 (97%)	4 (3%)	0	100	100
12	X7	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
12	X8	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
12	X9	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
12	x7	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
12	x8	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
12	x9	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
13	B7	480/571 (84%)	462 (96%)	17 (4%)	1 (0%)	44	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	B8	480/571 (84%)	463 (96%)	17 (4%)	0	100	100
13	B9	480/571 (84%)	461 (96%)	18 (4%)	1 (0%)	44	78
13	b7	480/571 (84%)	463 (96%)	17 (4%)	0	100	100
13	b8	480/571 (84%)	461 (96%)	19 (4%)	0	100	100
13	b9	480/571 (84%)	463 (96%)	17 (4%)	0	100	100
14	R7	131/134 (98%)	121 (92%)	9 (7%)	1 (1%)	16	53
14	R8	131/134 (98%)	118 (90%)	12 (9%)	1 (1%)	16	53
14	R9	131/134 (98%)	119 (91%)	11 (8%)	1 (1%)	16	53
14	r7	131/134 (98%)	117 (89%)	12 (9%)	2 (2%)	8	39
14	r8	131/134 (98%)	119 (91%)	11 (8%)	1 (1%)	16	53
14	r9	131/134 (98%)	120 (92%)	10 (8%)	1 (1%)	16	53
15	P7	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
15	P8	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
15	P9	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
15	p7	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
15	p8	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
15	p9	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
16	V7	108/111 (97%)	108 (100%)	0	0	100	100
16	V8	108/111 (97%)	108 (100%)	0	0	100	100
16	V9	108/111 (97%)	108 (100%)	0	0	100	100
16	v7	108/111 (97%)	108 (100%)	0	0	100	100
16	v8	108/111 (97%)	108 (100%)	0	0	100	100
16	v9	108/111 (97%)	108 (100%)	0	0	100	100
17	L7	205/208 (99%)	201 (98%)	4 (2%)	0	100	100
17	L8	205/208 (99%)	201 (98%)	4 (2%)	0	100	100
17	L9	205/208 (99%)	201 (98%)	4 (2%)	0	100	100
17	l7	205/208 (99%)	201 (98%)	4 (2%)	0	100	100
17	l8	205/208 (99%)	201 (98%)	4 (2%)	0	100	100
17	l9	205/208 (99%)	201 (98%)	4 (2%)	0	100	100
18	C7	120/398 (30%)	115 (96%)	5 (4%)	0	100	100
18	C8	120/398 (30%)	115 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	C9	120/398 (30%)	115 (96%)	5 (4%)	0	100	100
18	c7	120/398 (30%)	115 (96%)	5 (4%)	0	100	100
18	c8	120/398 (30%)	115 (96%)	5 (4%)	0	100	100
18	c9	120/398 (30%)	115 (96%)	5 (4%)	0	100	100
19	D7	250/310 (81%)	245 (98%)	5 (2%)	0	100	100
19	D8	250/310 (81%)	245 (98%)	5 (2%)	0	100	100
19	D9	250/310 (81%)	246 (98%)	4 (2%)	0	100	100
19	d7	250/310 (81%)	245 (98%)	5 (2%)	0	100	100
19	d8	250/310 (81%)	246 (98%)	4 (2%)	0	100	100
19	d9	250/310 (81%)	245 (98%)	5 (2%)	0	100	100
20	M7	94/205 (46%)	91 (97%)	3 (3%)	0	100	100
20	M8	94/205 (46%)	91 (97%)	3 (3%)	0	100	100
20	M9	94/205 (46%)	91 (97%)	3 (3%)	0	100	100
20	m7	94/205 (46%)	91 (97%)	3 (3%)	0	100	100
20	m8	94/205 (46%)	91 (97%)	3 (3%)	0	100	100
20	m9	94/205 (46%)	91 (97%)	3 (3%)	0	100	100
21	N7	158/166 (95%)	156 (99%)	2 (1%)	0	100	100
21	N8	158/166 (95%)	156 (99%)	2 (1%)	0	100	100
21	N9	158/166 (95%)	156 (99%)	2 (1%)	0	100	100
21	n7	158/166 (95%)	156 (99%)	2 (1%)	0	100	100
21	n8	158/166 (95%)	156 (99%)	2 (1%)	0	100	100
21	n9	158/166 (95%)	156 (99%)	2 (1%)	0	100	100
22	F7	184/267 (69%)	172 (94%)	12 (6%)	0	100	100
22	F8	184/267 (69%)	172 (94%)	12 (6%)	0	100	100
22	F9	184/267 (69%)	172 (94%)	12 (6%)	0	100	100
22	f7	184/267 (69%)	172 (94%)	12 (6%)	0	100	100
22	f8	184/267 (69%)	172 (94%)	12 (6%)	0	100	100
22	f9	184/267 (69%)	172 (94%)	12 (6%)	0	100	100
23	W7	92/106 (87%)	87 (95%)	5 (5%)	0	100	100
23	W8	92/106 (87%)	87 (95%)	5 (5%)	0	100	100
23	W9	92/106 (87%)	87 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	w7	92/106 (87%)	87 (95%)	5 (5%)	0	100	100
23	w8	92/106 (87%)	87 (95%)	5 (5%)	0	100	100
23	w9	92/106 (87%)	87 (95%)	5 (5%)	0	100	100
24	A7	461/536 (86%)	444 (96%)	17 (4%)	0	100	100
24	A8	461/536 (86%)	443 (96%)	18 (4%)	0	100	100
24	A9	461/536 (86%)	443 (96%)	18 (4%)	0	100	100
24	a7	461/536 (86%)	444 (96%)	17 (4%)	0	100	100
24	a8	461/536 (86%)	443 (96%)	18 (4%)	0	100	100
24	a9	461/536 (86%)	443 (96%)	18 (4%)	0	100	100
25	G1	178/252 (71%)	156 (88%)	21 (12%)	1 (1%)	22	59
25	G2	178/252 (71%)	154 (86%)	22 (12%)	2 (1%)	12	46
25	G3	178/252 (71%)	156 (88%)	21 (12%)	1 (1%)	22	59
25	G4	178/252 (71%)	154 (86%)	22 (12%)	2 (1%)	12	46
25	G5	178/252 (71%)	157 (88%)	20 (11%)	1 (1%)	22	59
25	G6	178/252 (71%)	154 (86%)	22 (12%)	2 (1%)	12	46
26	i1	38/145 (26%)	37 (97%)	1 (3%)	0	100	100
26	i2	38/145 (26%)	37 (97%)	1 (3%)	0	100	100
26	i3	38/145 (26%)	37 (97%)	1 (3%)	0	100	100
26	i4	38/145 (26%)	37 (97%)	1 (3%)	0	100	100
26	i5	38/145 (26%)	37 (97%)	1 (3%)	0	100	100
26	i6	38/145 (26%)	37 (97%)	1 (3%)	0	100	100
27	A1	510/565 (90%)	484 (95%)	26 (5%)	0	100	100
27	A2	510/565 (90%)	485 (95%)	25 (5%)	0	100	100
27	A3	510/565 (90%)	484 (95%)	26 (5%)	0	100	100
27	A4	510/565 (90%)	483 (95%)	27 (5%)	0	100	100
27	A5	510/565 (90%)	482 (94%)	28 (6%)	0	100	100
27	A6	510/565 (90%)	484 (95%)	26 (5%)	0	100	100
27	C1	503/565 (89%)	482 (96%)	21 (4%)	0	100	100
27	C2	503/565 (89%)	482 (96%)	21 (4%)	0	100	100
27	C3	503/565 (89%)	483 (96%)	20 (4%)	0	100	100
27	C4	503/565 (89%)	482 (96%)	21 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	C5	503/565 (89%)	483 (96%)	20 (4%)	0	100	100
27	C6	503/565 (89%)	482 (96%)	21 (4%)	0	100	100
27	E1	505/565 (89%)	473 (94%)	32 (6%)	0	100	100
27	E2	505/565 (89%)	473 (94%)	32 (6%)	0	100	100
27	E3	505/565 (89%)	473 (94%)	32 (6%)	0	100	100
27	E4	505/565 (89%)	473 (94%)	32 (6%)	0	100	100
27	E5	505/565 (89%)	472 (94%)	33 (6%)	0	100	100
27	E6	505/565 (89%)	473 (94%)	32 (6%)	0	100	100
28	B1	477/560 (85%)	448 (94%)	29 (6%)	0	100	100
28	B2	477/560 (85%)	448 (94%)	29 (6%)	0	100	100
28	B3	477/560 (85%)	448 (94%)	29 (6%)	0	100	100
28	B4	477/560 (85%)	448 (94%)	29 (6%)	0	100	100
28	B5	477/560 (85%)	448 (94%)	29 (6%)	0	100	100
28	B6	477/560 (85%)	448 (94%)	29 (6%)	0	100	100
28	D1	473/560 (84%)	450 (95%)	23 (5%)	0	100	100
28	D2	473/560 (84%)	450 (95%)	23 (5%)	0	100	100
28	D3	473/560 (84%)	450 (95%)	23 (5%)	0	100	100
28	D4	473/560 (84%)	450 (95%)	23 (5%)	0	100	100
28	D5	473/560 (84%)	450 (95%)	23 (5%)	0	100	100
28	D6	473/560 (84%)	451 (95%)	22 (5%)	0	100	100
28	F1	473/560 (84%)	447 (94%)	26 (6%)	0	100	100
28	F2	473/560 (84%)	448 (95%)	25 (5%)	0	100	100
28	F3	473/560 (84%)	447 (94%)	26 (6%)	0	100	100
28	F4	473/560 (84%)	446 (94%)	27 (6%)	0	100	100
28	F5	473/560 (84%)	447 (94%)	26 (6%)	0	100	100
28	F6	473/560 (84%)	447 (94%)	26 (6%)	0	100	100
29	g1	270/314 (86%)	259 (96%)	11 (4%)	0	100	100
29	g2	270/314 (86%)	259 (96%)	11 (4%)	0	100	100
29	g3	270/314 (86%)	259 (96%)	11 (4%)	0	100	100
29	g4	270/314 (86%)	259 (96%)	11 (4%)	0	100	100
29	g5	270/314 (86%)	259 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	g6	270/314 (86%)	259 (96%)	11 (4%)	0	100	100
30	d1	141/183 (77%)	135 (96%)	6 (4%)	0	100	100
30	d2	141/183 (77%)	134 (95%)	7 (5%)	0	100	100
30	d3	141/183 (77%)	135 (96%)	6 (4%)	0	100	100
30	d4	141/183 (77%)	135 (96%)	6 (4%)	0	100	100
30	d5	141/183 (77%)	135 (96%)	6 (4%)	0	100	100
30	d6	141/183 (77%)	135 (96%)	6 (4%)	0	100	100
31	e1	63/73 (86%)	59 (94%)	4 (6%)	0	100	100
31	e2	63/73 (86%)	59 (94%)	4 (6%)	0	100	100
31	e3	63/73 (86%)	59 (94%)	4 (6%)	0	100	100
31	e4	63/73 (86%)	59 (94%)	4 (6%)	0	100	100
31	e5	63/73 (86%)	59 (94%)	4 (6%)	0	100	100
31	e6	63/73 (86%)	59 (94%)	4 (6%)	0	100	100
32	H1	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	H2	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	H3	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	H4	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	H5	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	H6	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	I1	69/166 (42%)	69 (100%)	0	0	100	100
32	I2	69/166 (42%)	69 (100%)	0	0	100	100
32	I3	69/166 (42%)	69 (100%)	0	0	100	100
32	I4	69/166 (42%)	69 (100%)	0	0	100	100
32	I5	69/166 (42%)	69 (100%)	0	0	100	100
32	I6	69/166 (42%)	69 (100%)	0	0	100	100
32	J1	69/166 (42%)	64 (93%)	5 (7%)	0	100	100
32	J2	69/166 (42%)	64 (93%)	5 (7%)	0	100	100
32	J3	69/166 (42%)	64 (93%)	5 (7%)	0	100	100
32	J4	69/166 (42%)	65 (94%)	4 (6%)	0	100	100
32	J5	69/166 (42%)	64 (93%)	5 (7%)	0	100	100
32	J6	69/166 (42%)	64 (93%)	5 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	K1	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	K2	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	K3	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	K4	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	K5	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	K6	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	L1	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	L2	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	L3	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	L4	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	L5	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	L6	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	M1	69/166 (42%)	64 (93%)	5 (7%)	0	100	100
32	M2	69/166 (42%)	64 (93%)	5 (7%)	0	100	100
32	M3	69/166 (42%)	64 (93%)	5 (7%)	0	100	100
32	M4	69/166 (42%)	64 (93%)	5 (7%)	0	100	100
32	M5	69/166 (42%)	64 (93%)	5 (7%)	0	100	100
32	M6	69/166 (42%)	64 (93%)	5 (7%)	0	100	100
32	N1	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	N2	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	N3	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	N4	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	N5	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	N6	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	O1	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	O2	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	O3	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	O4	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	O5	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	O6	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	P1	69/166 (42%)	66 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	P2	69/166 (42%)	66 (96%)	3 (4%)	0	100	100
32	P3	69/166 (42%)	66 (96%)	3 (4%)	0	100	100
32	P4	69/166 (42%)	66 (96%)	3 (4%)	0	100	100
32	P5	69/166 (42%)	66 (96%)	3 (4%)	0	100	100
32	P6	69/166 (42%)	66 (96%)	3 (4%)	0	100	100
32	Q1	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	Q2	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	Q3	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	Q4	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	Q5	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	Q6	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
All	All	49152/68508 (72%)	46938 (96%)	2196 (4%)	18 (0%)	100	100

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	r7	87	LYS
14	R7	91	SER
25	G1	171	TYR
25	G2	171	TYR
14	r8	89	ALA
14	R8	88	SER
25	G3	171	TYR
25	G4	171	TYR
14	R9	89	ALA
25	G5	171	TYR
25	G6	171	TYR
13	B7	338	SER
25	G4	172	ARG
14	r9	89	ALA
13	B9	338	SER
25	G2	172	ARG
25	G6	172	ARG
14	r7	86	ALA

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	Q7	119/120 (99%)	119 (100%)	0	100	100
1	Q8	119/120 (99%)	119 (100%)	0	100	100
1	Q9	119/120 (99%)	119 (100%)	0	100	100
1	q7	119/120 (99%)	119 (100%)	0	100	100
1	q8	119/120 (99%)	119 (100%)	0	100	100
1	q9	119/120 (99%)	119 (100%)	0	100	100
2	I7	71/197 (36%)	71 (100%)	0	100	100
2	I8	71/197 (36%)	71 (100%)	0	100	100
2	I9	71/197 (36%)	71 (100%)	0	100	100
2	i7	71/197 (36%)	71 (100%)	0	100	100
2	i8	71/197 (36%)	71 (100%)	0	100	100
2	i9	71/197 (36%)	71 (100%)	0	100	100
3	T7	77/106 (73%)	77 (100%)	0	100	100
3	T8	77/106 (73%)	77 (100%)	0	100	100
3	T9	77/106 (73%)	77 (100%)	0	100	100
3	t7	77/106 (73%)	77 (100%)	0	100	100
3	t8	77/106 (73%)	77 (100%)	0	100	100
3	t9	77/106 (73%)	77 (100%)	0	100	100
4	G7	93/214 (44%)	93 (100%)	0	100	100
4	G8	93/214 (44%)	93 (100%)	0	100	100
4	G9	93/214 (44%)	93 (100%)	0	100	100
4	g7	93/214 (44%)	93 (100%)	0	100	100
4	g8	93/214 (44%)	93 (100%)	0	100	100
4	g9	93/214 (44%)	93 (100%)	0	100	100
5	O7	127/129 (98%)	127 (100%)	0	100	100
5	O8	127/129 (98%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	O9	127/129 (98%)	127 (100%)	0	100	100
5	o7	127/129 (98%)	127 (100%)	0	100	100
5	o8	127/129 (98%)	127 (100%)	0	100	100
5	o9	127/129 (98%)	127 (100%)	0	100	100
6	K7	100/175 (57%)	100 (100%)	0	100	100
6	K8	100/175 (57%)	100 (100%)	0	100	100
6	K9	100/175 (57%)	100 (100%)	0	100	100
6	k7	100/175 (57%)	100 (100%)	0	100	100
6	k8	100/175 (57%)	100 (100%)	0	100	100
6	k9	100/175 (57%)	100 (100%)	0	100	100
7	J7	160/195 (82%)	160 (100%)	0	100	100
7	J8	160/195 (82%)	160 (100%)	0	100	100
7	J9	160/195 (82%)	160 (100%)	0	100	100
7	j7	160/195 (82%)	160 (100%)	0	100	100
7	j8	160/195 (82%)	160 (100%)	0	100	100
7	j9	160/195 (82%)	160 (100%)	0	100	100
8	S7	86/113 (76%)	86 (100%)	0	100	100
8	S8	86/113 (76%)	86 (100%)	0	100	100
8	S9	86/113 (76%)	86 (100%)	0	100	100
8	s7	86/113 (76%)	86 (100%)	0	100	100
8	s8	86/113 (76%)	86 (100%)	0	100	100
8	s9	86/113 (76%)	86 (100%)	0	100	100
9	U7	76/98 (78%)	76 (100%)	0	100	100
9	U8	76/98 (78%)	76 (100%)	0	100	100
9	U9	76/98 (78%)	76 (100%)	0	100	100
9	u7	76/98 (78%)	76 (100%)	0	100	100
9	u8	76/98 (78%)	76 (100%)	0	100	100
9	u9	76/98 (78%)	76 (100%)	0	100	100
10	H7	197/204 (97%)	196 (100%)	1 (0%)	86	90
10	H8	197/204 (97%)	196 (100%)	1 (0%)	86	90
10	H9	197/204 (97%)	196 (100%)	1 (0%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	h7	197/204 (97%)	196 (100%)	1 (0%)	86	90
10	h8	197/204 (97%)	196 (100%)	1 (0%)	86	90
10	h9	197/204 (97%)	196 (100%)	1 (0%)	86	90
11	E7	118/258 (46%)	118 (100%)	0	100	100
11	E8	118/258 (46%)	118 (100%)	0	100	100
11	E9	118/258 (46%)	118 (100%)	0	100	100
11	e7	118/258 (46%)	118 (100%)	0	100	100
11	e8	118/258 (46%)	118 (100%)	0	100	100
11	e9	118/258 (46%)	118 (100%)	0	100	100
12	X7	70/71 (99%)	70 (100%)	0	100	100
12	X8	70/71 (99%)	70 (100%)	0	100	100
12	X9	70/71 (99%)	70 (100%)	0	100	100
12	x7	70/71 (99%)	70 (100%)	0	100	100
12	x8	70/71 (99%)	70 (100%)	0	100	100
12	x9	70/71 (99%)	70 (100%)	0	100	100
13	B7	428/491 (87%)	427 (100%)	1 (0%)	92	94
13	B8	428/491 (87%)	427 (100%)	1 (0%)	92	94
13	B9	428/491 (87%)	427 (100%)	1 (0%)	92	94
13	b7	428/491 (87%)	427 (100%)	1 (0%)	92	94
13	b8	428/491 (87%)	427 (100%)	1 (0%)	92	94
13	b9	428/491 (87%)	427 (100%)	1 (0%)	92	94
14	R7	116/117 (99%)	116 (100%)	0	100	100
14	R8	116/117 (99%)	116 (100%)	0	100	100
14	R9	116/117 (99%)	116 (100%)	0	100	100
14	r7	116/117 (99%)	116 (100%)	0	100	100
14	r8	116/117 (99%)	116 (100%)	0	100	100
14	r9	116/117 (99%)	116 (100%)	0	100	100
15	P7	91/113 (80%)	91 (100%)	0	100	100
15	P8	91/113 (80%)	91 (100%)	0	100	100
15	P9	91/113 (80%)	91 (100%)	0	100	100
15	p7	91/113 (80%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	p8	91/113 (80%)	91 (100%)	0	100	100
15	p9	91/113 (80%)	91 (100%)	0	100	100
16	V7	86/87 (99%)	86 (100%)	0	100	100
16	V8	86/87 (99%)	86 (100%)	0	100	100
16	V9	86/87 (99%)	86 (100%)	0	100	100
16	v7	86/87 (99%)	86 (100%)	0	100	100
16	v8	86/87 (99%)	86 (100%)	0	100	100
16	v9	86/87 (99%)	86 (100%)	0	100	100
17	L7	177/178 (99%)	177 (100%)	0	100	100
17	L8	177/178 (99%)	177 (100%)	0	100	100
17	L9	177/178 (99%)	177 (100%)	0	100	100
17	l7	177/178 (99%)	177 (100%)	0	100	100
17	l8	177/178 (99%)	177 (100%)	0	100	100
17	l9	177/178 (99%)	177 (100%)	0	100	100
18	C7	107/338 (32%)	107 (100%)	0	100	100
18	C8	107/338 (32%)	107 (100%)	0	100	100
18	C9	107/338 (32%)	107 (100%)	0	100	100
18	c7	107/338 (32%)	107 (100%)	0	100	100
18	c8	107/338 (32%)	107 (100%)	0	100	100
18	c9	107/338 (32%)	107 (100%)	0	100	100
19	D7	218/259 (84%)	218 (100%)	0	100	100
19	D8	218/259 (84%)	218 (100%)	0	100	100
19	D9	218/259 (84%)	218 (100%)	0	100	100
19	d7	218/259 (84%)	218 (100%)	0	100	100
19	d8	218/259 (84%)	218 (100%)	0	100	100
19	d9	218/259 (84%)	218 (100%)	0	100	100
20	M7	77/156 (49%)	77 (100%)	0	100	100
20	M8	77/156 (49%)	77 (100%)	0	100	100
20	M9	77/156 (49%)	77 (100%)	0	100	100
20	m7	77/156 (49%)	77 (100%)	0	100	100
20	m8	77/156 (49%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	m9	77/156 (49%)	77 (100%)	0	100	100
21	N7	138/144 (96%)	137 (99%)	1 (1%)	81	87
21	N8	138/144 (96%)	137 (99%)	1 (1%)	81	87
21	N9	138/144 (96%)	137 (99%)	1 (1%)	81	87
21	n7	138/144 (96%)	137 (99%)	1 (1%)	81	87
21	n8	138/144 (96%)	137 (99%)	1 (1%)	81	87
21	n9	138/144 (96%)	137 (99%)	1 (1%)	81	87
22	F7	155/218 (71%)	155 (100%)	0	100	100
22	F8	155/218 (71%)	155 (100%)	0	100	100
22	F9	155/218 (71%)	155 (100%)	0	100	100
22	f7	155/218 (71%)	155 (100%)	0	100	100
22	f8	155/218 (71%)	155 (100%)	0	100	100
22	f9	155/218 (71%)	155 (100%)	0	100	100
23	W7	84/89 (94%)	84 (100%)	0	100	100
23	W8	84/89 (94%)	84 (100%)	0	100	100
23	W9	84/89 (94%)	84 (100%)	0	100	100
23	w7	84/89 (94%)	84 (100%)	0	100	100
23	w8	84/89 (94%)	84 (100%)	0	100	100
23	w9	84/89 (94%)	84 (100%)	0	100	100
24	A7	392/447 (88%)	391 (100%)	1 (0%)	91	92
24	A8	392/447 (88%)	391 (100%)	1 (0%)	91	92
24	A9	392/447 (88%)	391 (100%)	1 (0%)	91	92
24	a7	392/447 (88%)	391 (100%)	1 (0%)	91	92
24	a8	392/447 (88%)	391 (100%)	1 (0%)	91	92
24	a9	392/447 (88%)	391 (100%)	1 (0%)	91	92
25	G1	154/212 (73%)	152 (99%)	2 (1%)	65	77
25	G2	154/212 (73%)	152 (99%)	2 (1%)	65	77
25	G3	154/212 (73%)	153 (99%)	1 (1%)	84	88
25	G4	154/212 (73%)	152 (99%)	2 (1%)	65	77
25	G5	154/212 (73%)	152 (99%)	2 (1%)	65	77
25	G6	154/212 (73%)	152 (99%)	2 (1%)	65	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	i1	37/125 (30%)	37 (100%)	0	100	100
26	i2	37/125 (30%)	37 (100%)	0	100	100
26	i3	37/125 (30%)	37 (100%)	0	100	100
26	i4	37/125 (30%)	37 (100%)	0	100	100
26	i5	37/125 (30%)	37 (100%)	0	100	100
26	i6	37/125 (30%)	37 (100%)	0	100	100
27	A1	421/454 (93%)	421 (100%)	0	100	100
27	A2	421/454 (93%)	421 (100%)	0	100	100
27	A3	421/454 (93%)	421 (100%)	0	100	100
27	A4	421/454 (93%)	421 (100%)	0	100	100
27	A5	421/454 (93%)	421 (100%)	0	100	100
27	A6	421/454 (93%)	421 (100%)	0	100	100
27	C1	415/454 (91%)	415 (100%)	0	100	100
27	C2	415/454 (91%)	415 (100%)	0	100	100
27	C3	415/454 (91%)	415 (100%)	0	100	100
27	C4	415/454 (91%)	415 (100%)	0	100	100
27	C5	415/454 (91%)	415 (100%)	0	100	100
27	C6	415/454 (91%)	415 (100%)	0	100	100
27	E1	416/454 (92%)	416 (100%)	0	100	100
27	E2	416/454 (92%)	416 (100%)	0	100	100
27	E3	416/454 (92%)	416 (100%)	0	100	100
27	E4	416/454 (92%)	416 (100%)	0	100	100
27	E5	416/454 (92%)	416 (100%)	0	100	100
27	E6	416/454 (92%)	416 (100%)	0	100	100
28	B1	390/447 (87%)	389 (100%)	1 (0%)	91	92
28	B2	390/447 (87%)	389 (100%)	1 (0%)	91	92
28	B3	390/447 (87%)	389 (100%)	1 (0%)	91	92
28	B4	390/447 (87%)	389 (100%)	1 (0%)	91	92
28	B5	390/447 (87%)	389 (100%)	1 (0%)	91	92
28	B6	390/447 (87%)	389 (100%)	1 (0%)	91	92
28	D1	388/447 (87%)	388 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	D2	388/447 (87%)	388 (100%)	0	100	100
28	D3	388/447 (87%)	388 (100%)	0	100	100
28	D4	388/447 (87%)	388 (100%)	0	100	100
28	D5	388/447 (87%)	388 (100%)	0	100	100
28	D6	388/447 (87%)	388 (100%)	0	100	100
28	F1	388/447 (87%)	388 (100%)	0	100	100
28	F2	388/447 (87%)	388 (100%)	0	100	100
28	F3	388/447 (87%)	388 (100%)	0	100	100
28	F4	388/447 (87%)	388 (100%)	0	100	100
28	F5	388/447 (87%)	388 (100%)	0	100	100
28	F6	388/447 (87%)	388 (100%)	0	100	100
29	g1	228/257 (89%)	228 (100%)	0	100	100
29	g2	228/257 (89%)	228 (100%)	0	100	100
29	g3	228/257 (89%)	228 (100%)	0	100	100
29	g4	228/257 (89%)	228 (100%)	0	100	100
29	g5	228/257 (89%)	228 (100%)	0	100	100
29	g6	228/257 (89%)	228 (100%)	0	100	100
30	d1	118/144 (82%)	118 (100%)	0	100	100
30	d2	118/144 (82%)	118 (100%)	0	100	100
30	d3	118/144 (82%)	118 (100%)	0	100	100
30	d4	118/144 (82%)	118 (100%)	0	100	100
30	d5	118/144 (82%)	118 (100%)	0	100	100
30	d6	118/144 (82%)	118 (100%)	0	100	100
31	e1	57/61 (93%)	57 (100%)	0	100	100
31	e2	57/61 (93%)	57 (100%)	0	100	100
31	e3	57/61 (93%)	57 (100%)	0	100	100
31	e4	57/61 (93%)	57 (100%)	0	100	100
31	e5	57/61 (93%)	57 (100%)	0	100	100
31	e6	57/61 (93%)	57 (100%)	0	100	100
32	H1	52/133 (39%)	52 (100%)	0	100	100
32	H2	52/133 (39%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	H3	52/133 (39%)	52 (100%)	0	100	100
32	H4	52/133 (39%)	52 (100%)	0	100	100
32	H5	52/133 (39%)	52 (100%)	0	100	100
32	H6	52/133 (39%)	52 (100%)	0	100	100
32	I1	52/133 (39%)	51 (98%)	1 (2%)	52	70
32	I2	52/133 (39%)	51 (98%)	1 (2%)	52	70
32	I3	52/133 (39%)	51 (98%)	1 (2%)	52	70
32	I4	52/133 (39%)	51 (98%)	1 (2%)	52	70
32	I5	52/133 (39%)	51 (98%)	1 (2%)	52	70
32	I6	52/133 (39%)	51 (98%)	1 (2%)	52	70
32	J1	52/133 (39%)	52 (100%)	0	100	100
32	J2	52/133 (39%)	52 (100%)	0	100	100
32	J3	52/133 (39%)	52 (100%)	0	100	100
32	J4	52/133 (39%)	52 (100%)	0	100	100
32	J5	52/133 (39%)	52 (100%)	0	100	100
32	J6	52/133 (39%)	52 (100%)	0	100	100
32	K1	52/133 (39%)	52 (100%)	0	100	100
32	K2	52/133 (39%)	52 (100%)	0	100	100
32	K3	52/133 (39%)	52 (100%)	0	100	100
32	K4	52/133 (39%)	52 (100%)	0	100	100
32	K5	52/133 (39%)	52 (100%)	0	100	100
32	K6	52/133 (39%)	52 (100%)	0	100	100
32	L1	52/133 (39%)	52 (100%)	0	100	100
32	L2	52/133 (39%)	52 (100%)	0	100	100
32	L3	52/133 (39%)	52 (100%)	0	100	100
32	L4	52/133 (39%)	52 (100%)	0	100	100
32	L5	52/133 (39%)	52 (100%)	0	100	100
32	L6	52/133 (39%)	52 (100%)	0	100	100
32	M1	52/133 (39%)	52 (100%)	0	100	100
32	M2	52/133 (39%)	52 (100%)	0	100	100
32	M3	52/133 (39%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	M4	52/133 (39%)	52 (100%)	0	100	100
32	M5	52/133 (39%)	52 (100%)	0	100	100
32	M6	52/133 (39%)	52 (100%)	0	100	100
32	N1	52/133 (39%)	52 (100%)	0	100	100
32	N2	52/133 (39%)	52 (100%)	0	100	100
32	N3	52/133 (39%)	52 (100%)	0	100	100
32	N4	52/133 (39%)	52 (100%)	0	100	100
32	N5	52/133 (39%)	52 (100%)	0	100	100
32	N6	52/133 (39%)	52 (100%)	0	100	100
32	O1	52/133 (39%)	52 (100%)	0	100	100
32	O2	52/133 (39%)	52 (100%)	0	100	100
32	O3	52/133 (39%)	52 (100%)	0	100	100
32	O4	52/133 (39%)	52 (100%)	0	100	100
32	O5	52/133 (39%)	52 (100%)	0	100	100
32	O6	52/133 (39%)	52 (100%)	0	100	100
32	P1	52/133 (39%)	52 (100%)	0	100	100
32	P2	52/133 (39%)	52 (100%)	0	100	100
32	P3	52/133 (39%)	52 (100%)	0	100	100
32	P4	52/133 (39%)	52 (100%)	0	100	100
32	P5	52/133 (39%)	52 (100%)	0	100	100
32	P6	52/133 (39%)	52 (100%)	0	100	100
32	Q1	52/133 (39%)	52 (100%)	0	100	100
32	Q2	52/133 (39%)	52 (100%)	0	100	100
32	Q3	52/133 (39%)	52 (100%)	0	100	100
32	Q4	52/133 (39%)	52 (100%)	0	100	100
32	Q5	52/133 (39%)	52 (100%)	0	100	100
32	Q6	52/133 (39%)	52 (100%)	0	100	100
All	All	41370/56094 (74%)	41323 (100%)	47 (0%)	92	94

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	h7	117	ARG

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Mol	Chain	Res	Type
13	b7	509	ARG
21	n7	82	ARG
24	a7	130	LYS
10	H7	117	ARG
13	B7	509	ARG
21	N7	82	ARG
24	A7	130	LYS
25	G1	171	TYR
25	G1	207	GLN
25	G2	171	TYR
25	G2	207	GLN
28	B1	435	ARG
32	I1	130	ARG
28	B2	435	ARG
32	I2	130	ARG
10	h8	117	ARG
13	b8	509	ARG
21	n8	82	ARG
24	a8	130	LYS
10	H8	117	ARG
13	B8	509	ARG
21	N8	82	ARG
24	A8	130	LYS
25	G3	207	GLN
25	G4	171	TYR
25	G4	207	GLN
28	B3	435	ARG
32	I3	130	ARG
28	B4	435	ARG
32	I4	130	ARG
10	h9	117	ARG
13	b9	509	ARG
21	n9	82	ARG
24	a9	130	LYS
10	H9	117	ARG
13	B9	509	ARG
21	N9	82	ARG
24	A9	130	LYS
25	G5	171	TYR
25	G5	207	GLN
25	G6	171	TYR
25	G6	207	GLN

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Mol	Chain	Res	Type
28	B5	435	ARG
32	I5	130	ARG
28	B6	435	ARG
32	I6	130	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
2	i7	202	GLN
7	j7	210	HIS
10	h7	209	GLN
13	b7	163	ASN
13	b7	185	ASN
13	b7	347	GLN
14	r7	22	GLN
15	p7	67	ASN
18	c7	55	GLN
18	c7	59	GLN
4	G7	175	GLN
10	H7	209	GLN
11	E7	243	HIS
13	B7	185	ASN
13	B7	347	GLN
13	B7	570	HIS
14	R7	22	GLN
15	P7	67	ASN
18	C7	59	GLN
25	G1	201	GLN
27	E1	527	ASN
28	B1	80	ASN
28	B1	197	GLN
28	F1	372	GLN
28	D1	154	GLN
28	D1	269	HIS
28	D1	342	GLN
28	D1	361	GLN
27	E2	527	ASN
28	F2	370	GLN
28	F2	372	GLN
28	D2	154	GLN
28	D2	269	HIS
28	D2	342	GLN

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Mol	Chain	Res	Type
28	D2	361	GLN
29	g2	246	GLN
2	i8	202	GLN
4	g8	169	GLN
4	g8	175	GLN
10	h8	209	GLN
11	e8	243	HIS
13	b8	163	ASN
13	b8	185	ASN
13	b8	347	GLN
13	b8	570	HIS
14	r8	22	GLN
15	p8	67	ASN
18	c8	59	GLN
7	J8	210	HIS
10	H8	209	GLN
13	B8	163	ASN
13	B8	185	ASN
13	B8	347	GLN
14	R8	22	GLN
18	C8	55	GLN
18	C8	59	GLN
25	G3	201	GLN
25	G4	201	GLN
27	E3	527	ASN
28	B3	80	ASN
28	B3	197	GLN
28	F3	372	GLN
28	D3	154	GLN
28	D3	269	HIS
28	D3	342	GLN
28	D3	361	GLN
27	E4	527	ASN
28	F4	372	GLN
28	D4	154	GLN
28	D4	269	HIS
28	D4	342	GLN
28	D4	361	GLN
7	j9	210	HIS
10	h9	209	GLN
13	b9	163	ASN
13	b9	185	ASN

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Mol	Chain	Res	Type
13	b9	347	GLN
14	r9	22	GLN
15	p9	67	ASN
18	c9	55	GLN
18	c9	59	GLN
4	G9	175	GLN
10	H9	209	GLN
11	E9	243	HIS
13	B9	185	ASN
13	B9	347	GLN
13	B9	570	HIS
14	R9	22	GLN
15	P9	67	ASN
18	C9	59	GLN
21	N9	48	ASN
25	G6	201	GLN
27	E5	527	ASN
28	B5	80	ASN
28	B5	197	GLN
28	F5	372	GLN
28	D5	269	HIS
28	D5	342	GLN
28	D5	361	GLN
27	E6	527	ASN
28	F6	372	GLN
28	D6	154	GLN
28	D6	269	HIS
28	D6	342	GLN
28	D6	361	GLN
29	g6	246	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.