wwPDB EM Validation Summary 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)

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

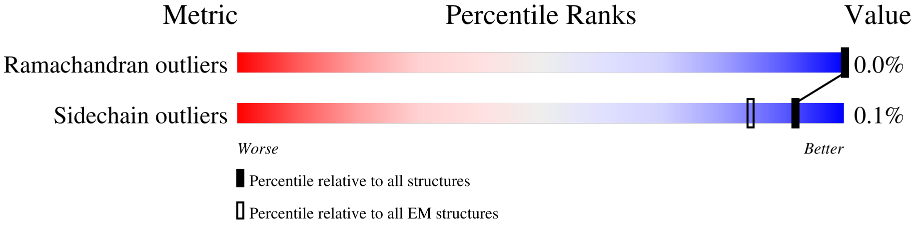
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

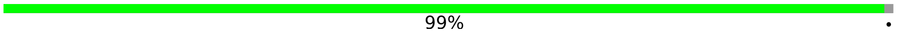
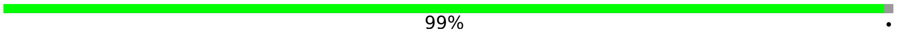
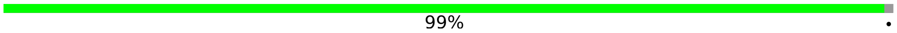
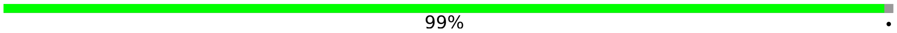
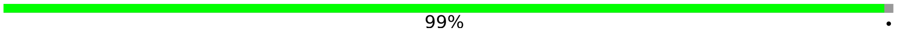
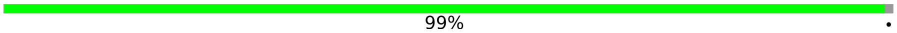
The reported resolution of this entry is 4.80 Å.

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 <=5%

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

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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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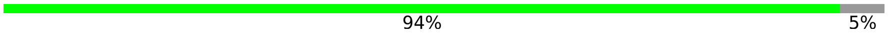
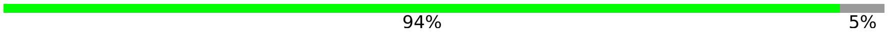
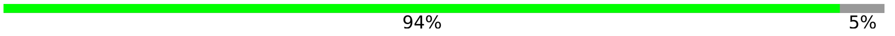
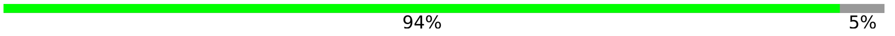
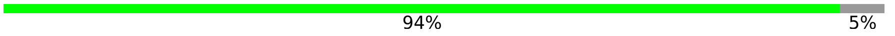
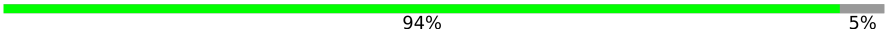
Mol	Chain	Length	Quality of chain
6	k9	224	 52% 48%
7	J7	229	 76% 23%
7	J8	229	 76% 23%
7	J9	229	 76% 23%
7	j7	229	 76% 23%
7	j8	229	 76% 23%
7	j9	229	 76% 23%
8	S7	128	 74% 26%
8	S8	128	 74% 26%
8	S9	128	 74% 26%
8	s7	128	 74% 26%
8	s8	128	 74% 26%
8	s9	128	 74% 26%
9	U7	126	 75% 25%
9	U8	126	 75% 25%
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	78% 22%
15	P9	138	78% 22%
15	p7	138	78% 22%
15	p8	138	78% 22%
15	p9	138	78% 22%
16	V7	111	99% •
16	V8	111	99% •
16	V9	111	99% •
16	v7	111	99% •
16	v8	111	99% •
16	v9	111	99% •
17	L7	208	100%
17	L8	208	100%
17	L9	208	100%
17	l7	208	100%
17	l8	208	100%
17	l9	208	100%
18	C7	398	31% 69%
18	C8	398	31% 69%
18	C9	398	31% 69%
18	c7	398	31% 69%
18	c8	398	31% 69%
18	c9	398	31% 69%
19	D7	310	82% 18%
19	D8	310	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	91% 9%
23	w8	106	91% 9%
23	w9	106	91% 9%
24	A7	536	87% 13%
24	A8	536	87% 13%
24	A9	536	87% 13%
24	a7	536	87% 13%
24	a8	536	87% 13%
24	a9	536	87% 13%
25	G1	252	69% • 29%
25	G2	252	69% • 29%
25	G3	252	70% • 29%
25	G4	252	70% • 29%
25	G5	252	69% • 29%
25	G6	252	69% • 29%
26	i1	145	28% 72%
26	i2	145	28% 72%
26	i3	145	28% 72%
26	i4	145	28% 72%
26	i5	145	28% 72%
26	i6	145	28% 72%
27	A1	565	91% 9%
27	A2	565	91% 9%
27	A3	565	91% 9%
27	A4	565	91% 9%

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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	43% 57%
32	H2	166	43% 57%
32	H3	166	43% 57%
32	H4	166	43% 57%
32	H5	166	43% 57%
32	H6	166	43% 57%
32	I1	166	42% • 57%
32	I2	166	42% • 57%
32	I3	166	42% • 57%
32	I4	166	42% • 57%
32	I5	166	42% • 57%
32	I6	166	42% • 57%
32	J1	166	43% 57%
32	J2	166	43% 57%
32	J3	166	43% 57%
32	J4	166	43% 57%
32	J5	166	43% 57%
32	J6	166	43% 57%
32	K1	166	43% 57%
32	K2	166	43% 57%
32	K3	166	43% 57%
32	K4	166	43% 57%
32	K5	166	43% 57%
32	K6	166	43% 57%
32	L1	166	43% 57%

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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	43% 57%
32	P4	166	43% 57%
32	P5	166	43% 57%
32	P6	166	43% 57%
32	Q1	166	43% 57%
32	Q2	166	43% 57%
32	Q3	166	43% 57%
32	Q4	166	43% 57%
32	Q5	166	43% 57%
32	Q6	166	43% 57%

2 Entry composition

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 2119	C 674	H 1044	N 194	O 202	S 5	0	0
1	Q7	133	Total 2120	C 674	H 1045	N 194	O 202	S 5	0	0
1	q8	133	Total 2120	C 674	H 1045	N 194	O 202	S 5	0	0
1	Q8	133	Total 2119	C 674	H 1044	N 194	O 202	S 5	0	0
1	q9	133	Total 2119	C 674	H 1044	N 194	O 202	S 5	0	0
1	Q9	133	Total 2120	C 674	H 1045	N 194	O 202	S 5	0	0

- Molecule 2 is a protein called ATPTG7.

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

- Molecule 3 is a protein called ATPTG14.

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

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

- Molecule 4 is a protein called ATPTG5.

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

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
			Total	C	H	N	O	S		
5	o7	149	2416	786	1196	210	219	5	0	0
5	O7	149	2416	786	1196	210	219	5	0	0
5	o8	149	2416	786	1196	210	219	5	0	0
5	O8	149	2416	786	1196	210	219	5	0	0
5	o9	149	2416	786	1196	210	219	5	0	0
5	O9	149	2416	786	1196	210	219	5	0	0

- Molecule 6 is a protein called subunit a.

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

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

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

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

- Molecule 8 is a protein called ATPTG13.

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

- Molecule 9 is a protein called ATPTG15.

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

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

- Molecule 10 is a protein called ATPTG6.

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

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 2179	C 719	H 1064	N 187	O 204	S 5	0	0
11	E7	140	Total 2179	C 719	H 1064	N 187	O 204	S 5	0	0

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

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 1298	C 420	H 639	N 116	O 120	S 3	0	0

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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 2142 681 1071 182 202 6	0	0
14	R7	133	Total C H N O S 2144 681 1073 182 202 6	0	0
14	r8	133	Total C H N O S 2143 681 1072 182 202 6	0	0
14	R8	133	Total C H N O S 2142 681 1071 182 202 6	0	0
14	r9	133	Total C H N O S 2143 681 1072 182 202 6	0	0
14	R9	133	Total C H N O S 2143 681 1072 182 202 6	0	0

- Molecule 15 is a protein called ATPTG10.

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

- Molecule 16 is a protein called subunit f.

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

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

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
			Total	C	H	N	O	S		
17	l7	207	3273	1013	1647	298	305	10	0	0
17	L7	207	3273	1013	1647	298	305	10	0	0
17	l8	207	3273	1013	1647	298	305	10	0	0
17	L8	207	3273	1013	1647	298	305	10	0	0
17	l9	207	3273	1013	1647	298	305	10	0	0
17	L9	207	3273	1013	1647	298	305	10	0	0

- Molecule 18 is a protein called ATPTG1.

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

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

- Molecule 19 is a protein called ATPTG2.

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

- Molecule 20 is a protein called subunit 8.

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

- Molecule 21 is a protein called ATPTG9.

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

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

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 2867	C 919	H 1425	N 245	O 274	S 4	0	0
22	F7	188	Total 2867	C 919	H 1425	N 245	O 274	S 4	0	0
22	f8	188	Total 2867	C 919	H 1425	N 245	O 274	S 4	0	0
22	F8	188	Total 2867	C 919	H 1425	N 245	O 274	S 4	0	0
22	f9	188	Total 2867	C 919	H 1425	N 245	O 274	S 4	0	0
22	F9	188	Total 2867	C 919	H 1425	N 245	O 274	S 4	0	0

- Molecule 23 is a protein called ATPTG16.

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

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

- Molecule 24 is a protein called subunit d.

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

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 2895	C 895	H 1480	N 255	O 261	S 4	0	0
25	G2	180	Total 2894	C 895	H 1479	N 255	O 261	S 4	0	0

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

- Molecule 26 is a protein called Inhibitor of F1.

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

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

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

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

- 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 7314 2293 3676 628 703 14	0	0
28	F1	475	Total C H N O S 7265 2278 3653 624 696 14	0	0
28	D1	475	Total C H N O S 7265 2278 3653 624 696 14	0	0
28	B2	479	Total C H N O S 7314 2293 3676 628 703 14	0	0
28	F2	475	Total C H N O S 7265 2278 3653 624 696 14	0	0
28	D2	475	Total C H N O S 7265 2278 3653 624 696 14	0	0
28	B3	479	Total C H N O S 7314 2293 3676 628 703 14	0	0
28	F3	475	Total C H N O S 7265 2278 3653 624 696 14	0	0

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

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

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

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

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

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

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

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

- Molecule 32 is a protein called subunit c.

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

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

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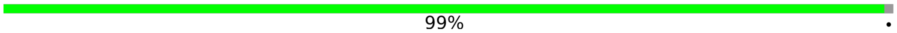
Mol	Chain	Residues	Atoms	AltConf	Trace
32	P5	71	Total C H N O S 1028 328 527 77 92 4	0	0
32	Q5	71	Total C H N O S 1028 328 527 77 92 4	0	0
32	H6	71	Total C H N O S 1028 328 527 77 92 4	0	0
32	I6	71	Total C H N O S 1028 328 527 77 92 4	0	0
32	J6	71	Total C H N O S 1028 328 527 77 92 4	0	0
32	K6	71	Total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

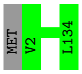
3 Residue-property plots ⓘ

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

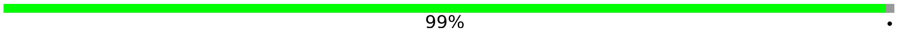
Chain q7:

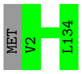




- Molecule 1: ATPTG11

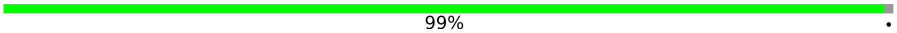
Chain Q7:

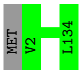




- Molecule 1: ATPTG11

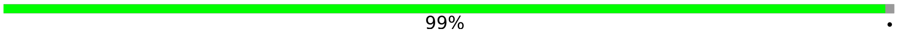
Chain q8:

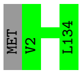




- Molecule 1: ATPTG11

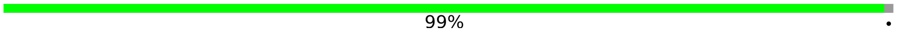
Chain Q8:

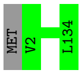




- Molecule 1: ATPTG11

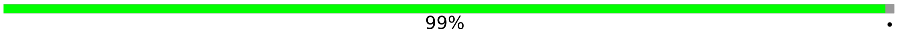
Chain q9:

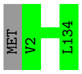




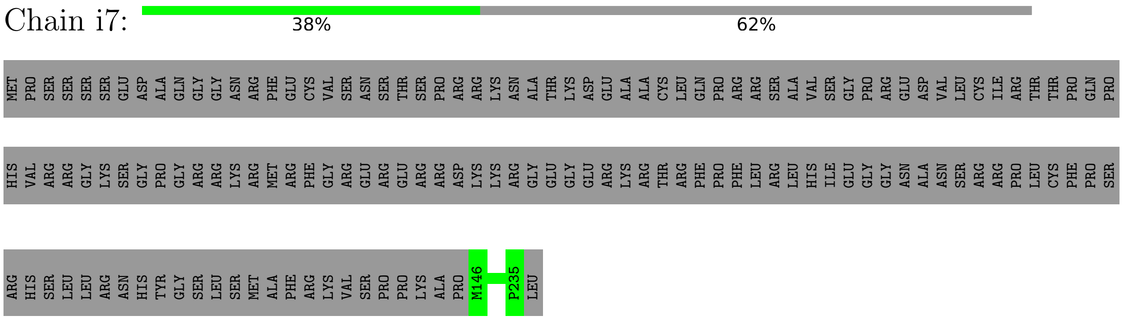
- Molecule 1: ATPTG11

Chain Q9:

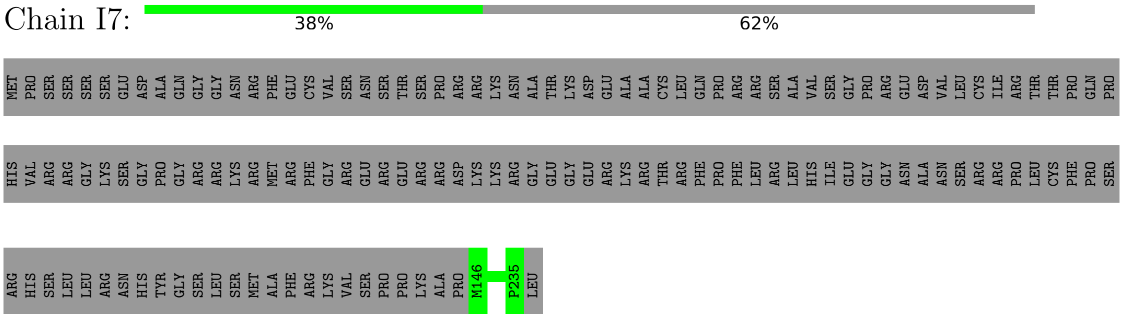




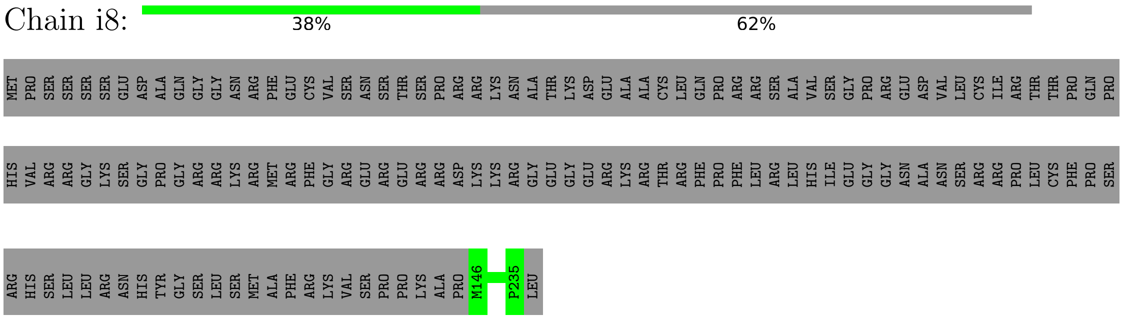
- Molecule 2: ATPTG7



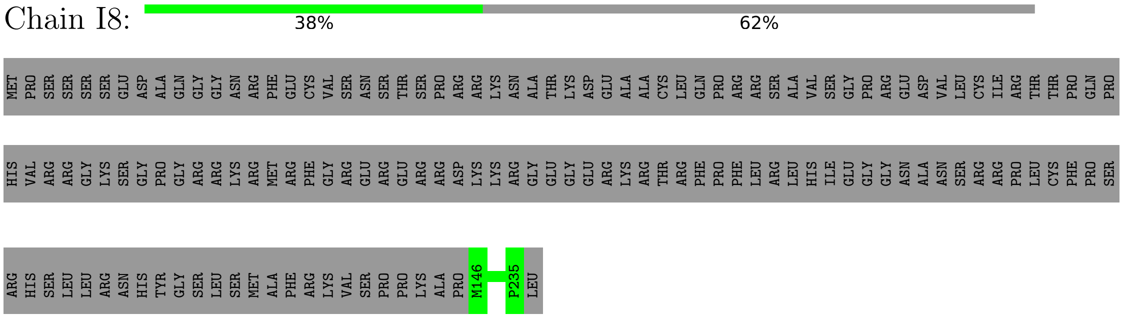
- Molecule 2: ATPTG7



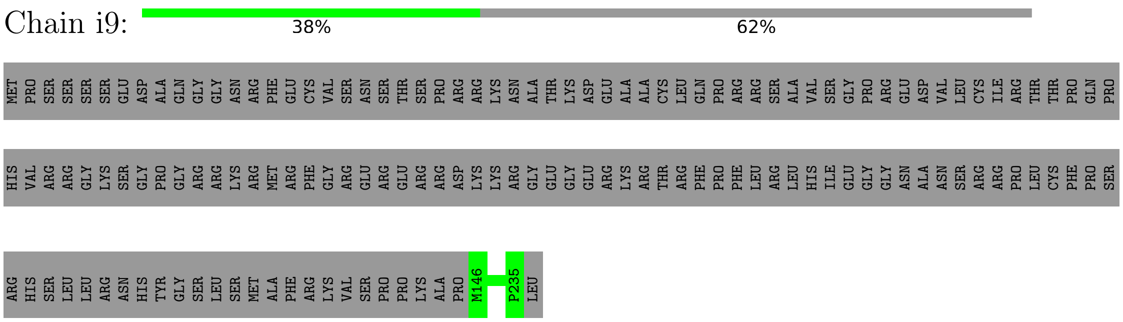
- Molecule 2: ATPTG7



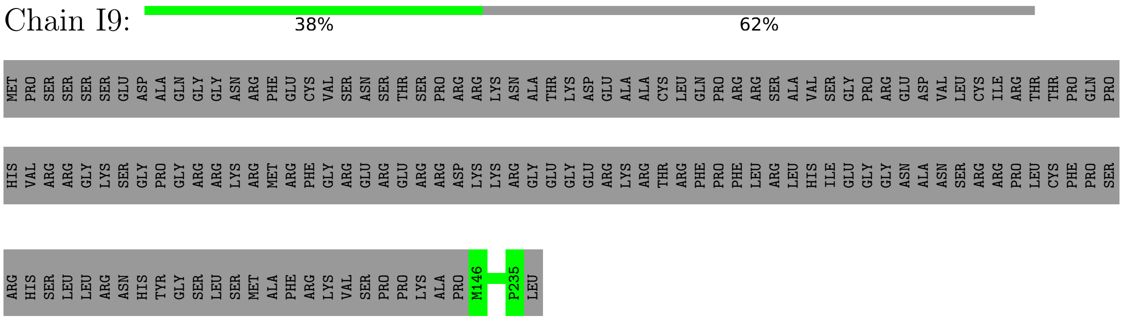
- Molecule 2: ATPTG7



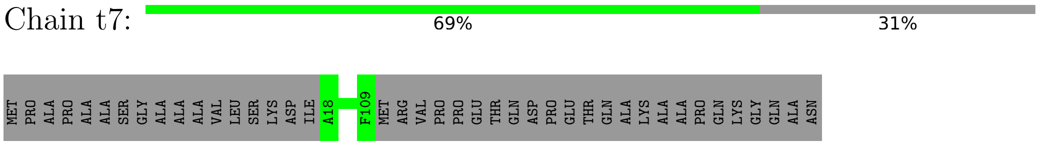
- Molecule 2: ATPTG7



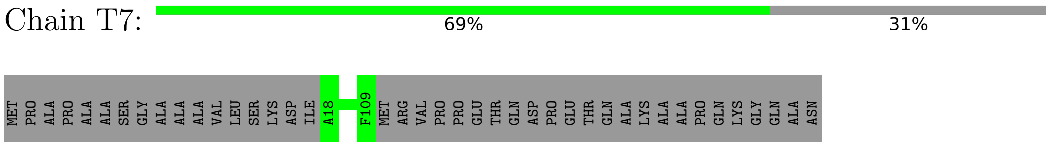
- Molecule 2: ATPTG7



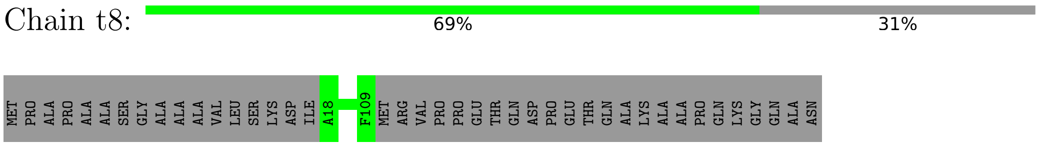
- Molecule 3: ATPTG14



- Molecule 3: ATPTG14



- Molecule 3: ATPTG14



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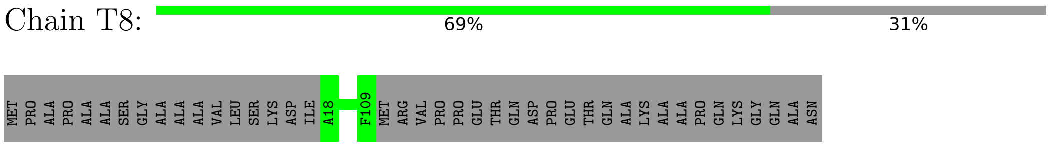

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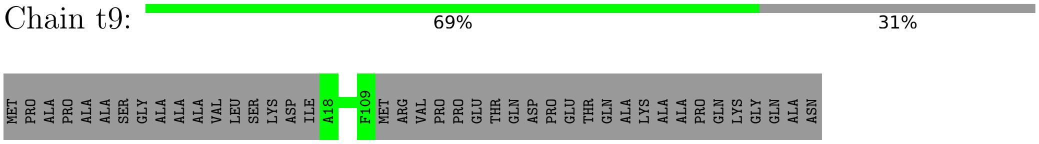

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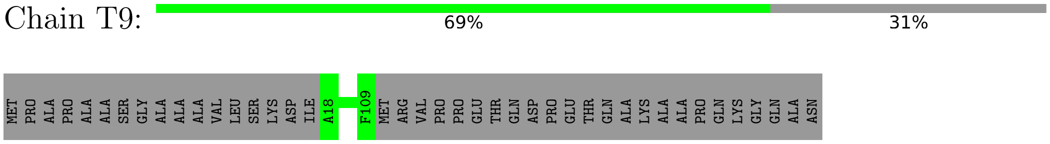
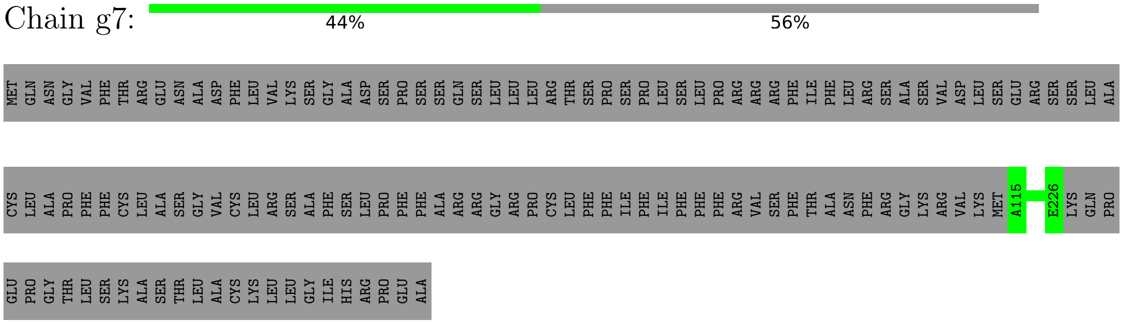
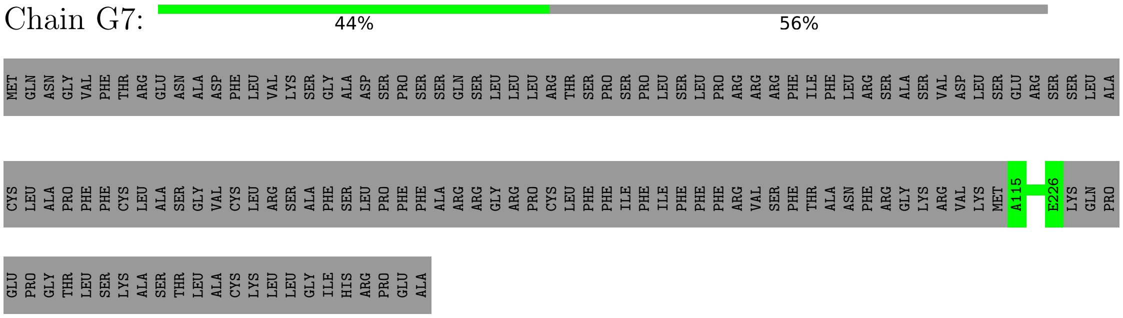


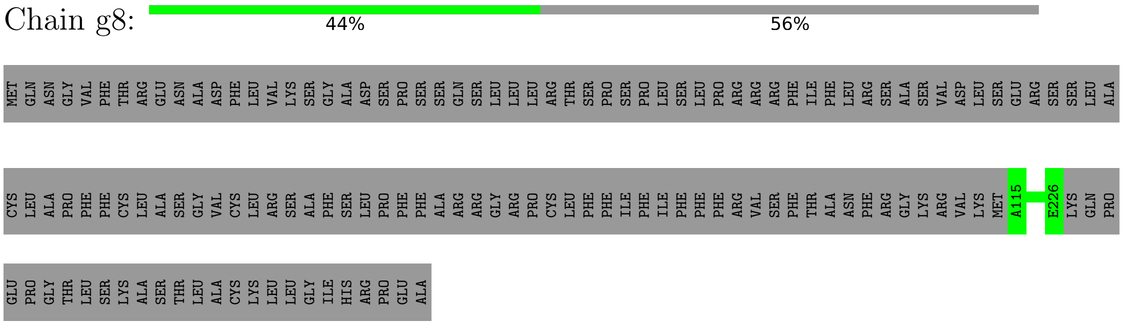
- Molecule 4: ATPTG5



- Molecule 4: ATPTG5

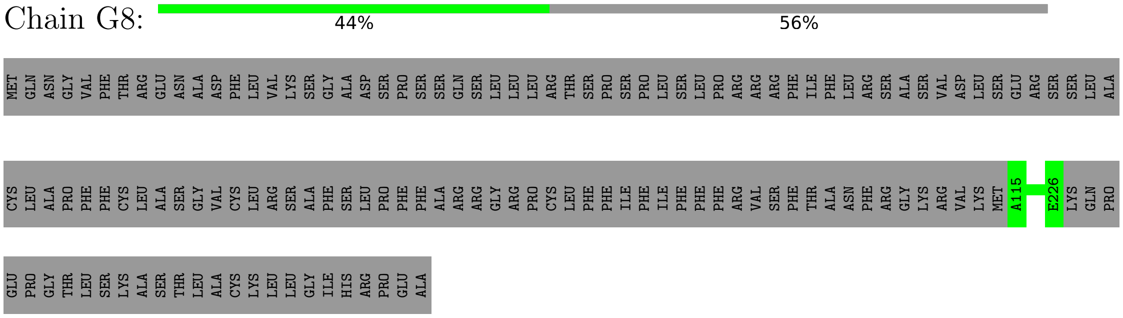


- Molecule 4: ATPTG5



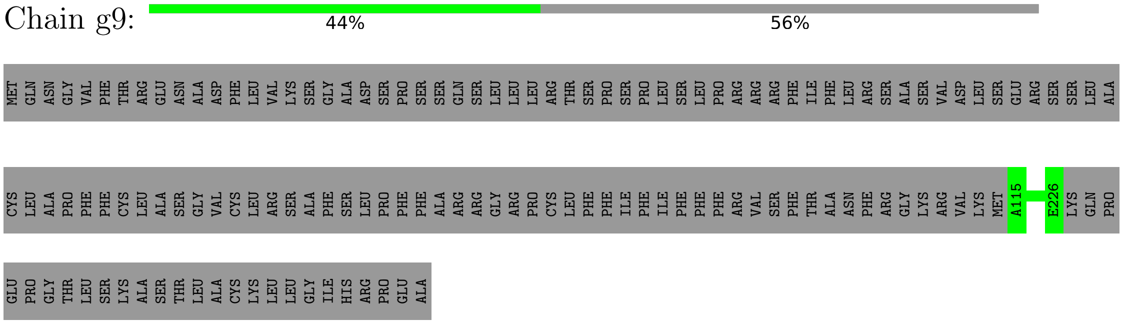
- Molecule 4: ATPTG5

Chain G8:



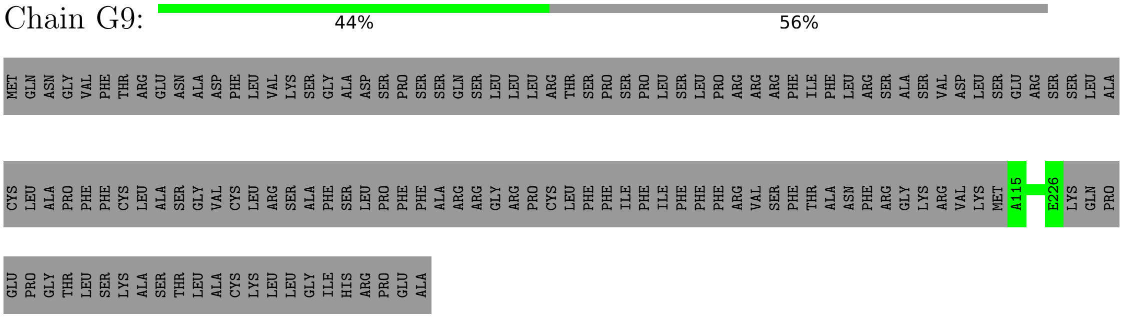
- Molecule 4: ATPTG5

Chain g9:



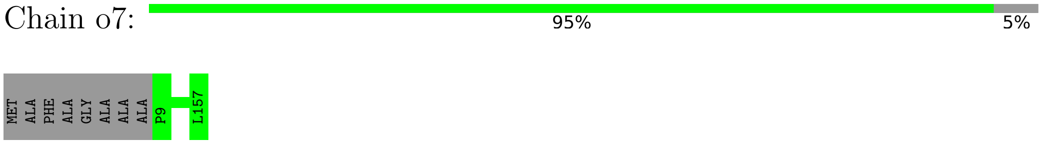
- Molecule 4: ATPTG5

Chain G9:



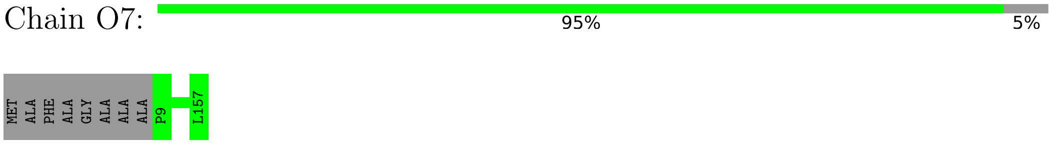
- Molecule 5: subunit k

Chain o7:



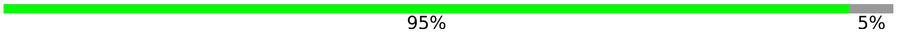
- Molecule 5: subunit k

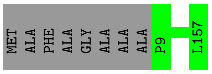
Chain O7:



- Molecule 5: subunit k

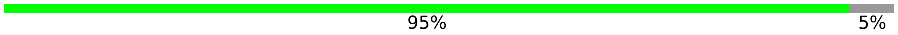
Chain o8:

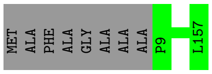




- Molecule 5: subunit k

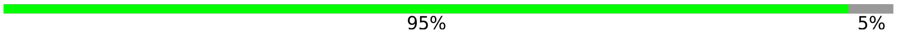
Chain O8:

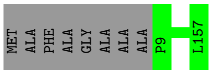




- Molecule 5: subunit k

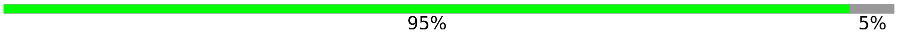
Chain o9:

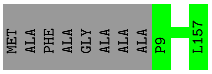




- Molecule 5: subunit k

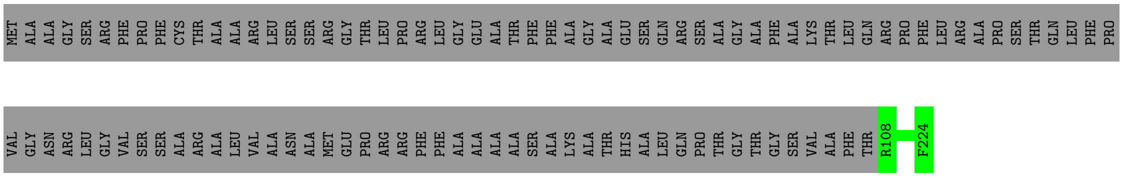
Chain O9:





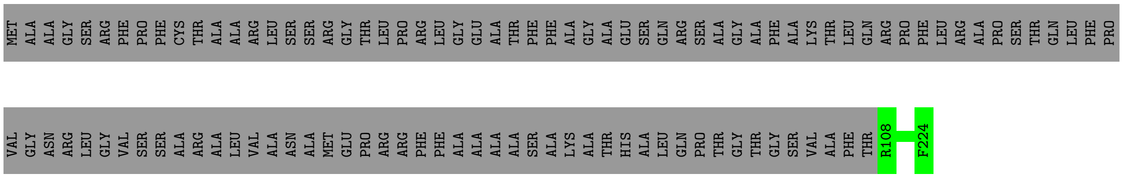
- Molecule 6: subunit a

Chain k7:



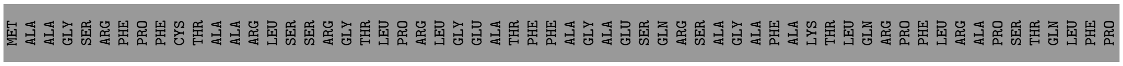
- Molecule 6: subunit a

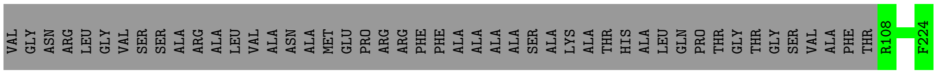
Chain K7:



- Molecule 6: subunit a

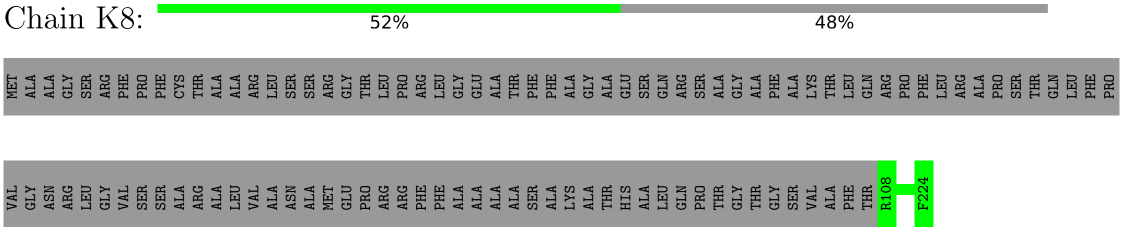
Chain k8:





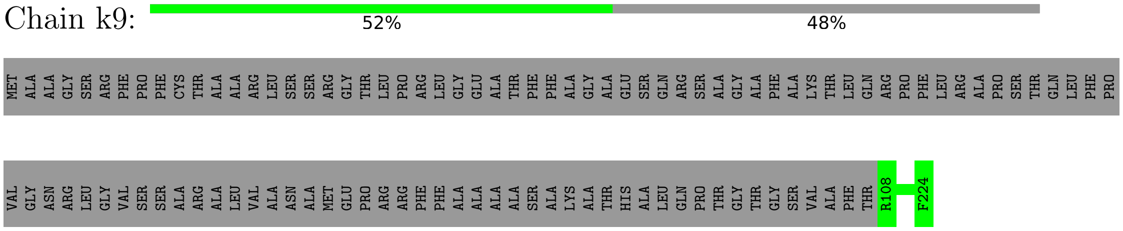
- Molecule 6: subunit a

Chain K8:



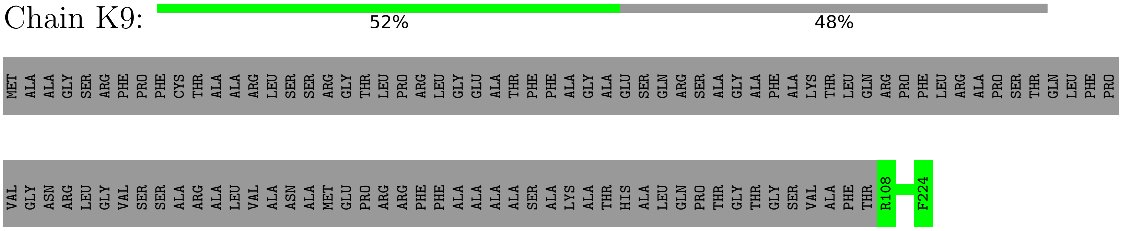
- Molecule 6: subunit a

Chain k9:



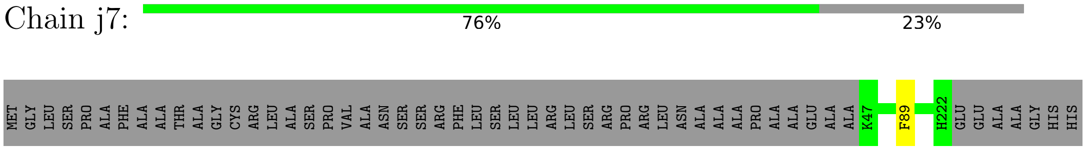
- Molecule 6: subunit a

Chain K9:



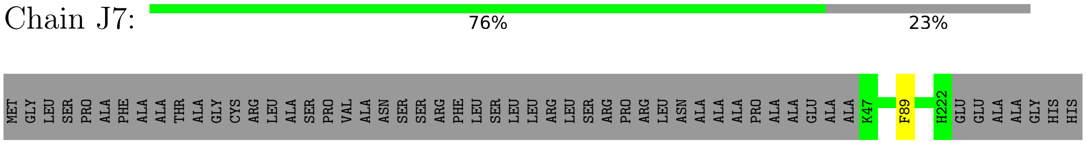
- Molecule 7: subunit i/j

Chain j7:



- Molecule 7: subunit i/j

Chain J7:



- Molecule 7: subunit i/j

Chain j8:

- Molecule 7: subunit i/j

Chain J8:


- Molecule 7: subunit i/j

Chain j9:


- Molecule 7: subunit i/j

Chain J9:


- Molecule 8: ATPTG13

Chain s7:


- Molecule 8: ATPTG13

Chain S7:


- Molecule 8: ATPTG13

Chain s8:


- Molecule 8: ATPTG13

Chain S8:


- Molecule 8: ATPTG13

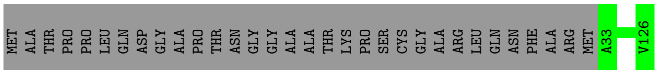
Chain s9:

- Molecule 8: ATPTG13

Chain S9:

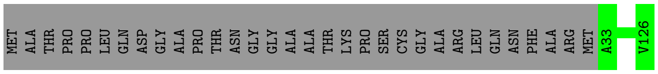
- Molecule 9: ATPTG15

Chain u7:



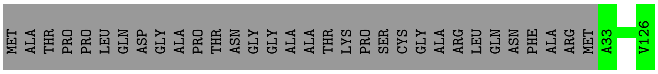
- Molecule 9: ATPTG15

Chain U7:



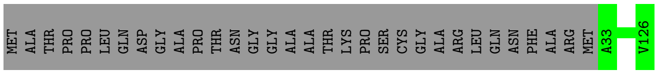
- Molecule 9: ATPTG15

Chain u8:



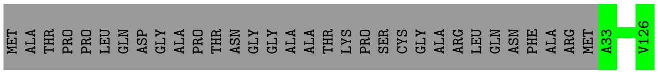
- Molecule 9: ATPTG15

Chain U8:



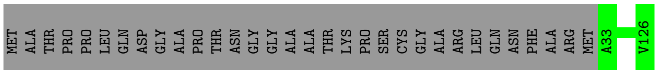
- Molecule 9: ATPTG15

Chain u9:



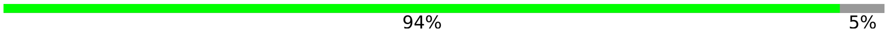
- Molecule 9: ATPTG15

Chain U9:



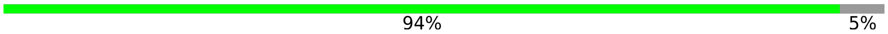
- Molecule 10: ATPTG6

Chain h7:



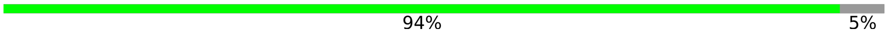
- Molecule 10: ATPTG6

Chain H7:



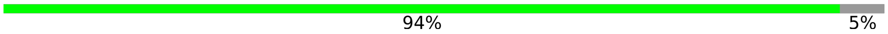
- Molecule 10: ATPTG6

Chain h8:



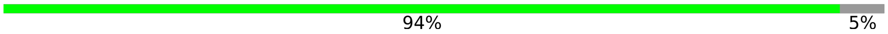
- Molecule 10: ATPTG6

Chain H8:



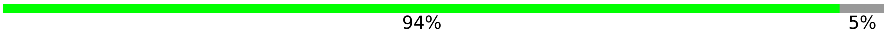
- Molecule 10: ATPTG6

Chain h9:

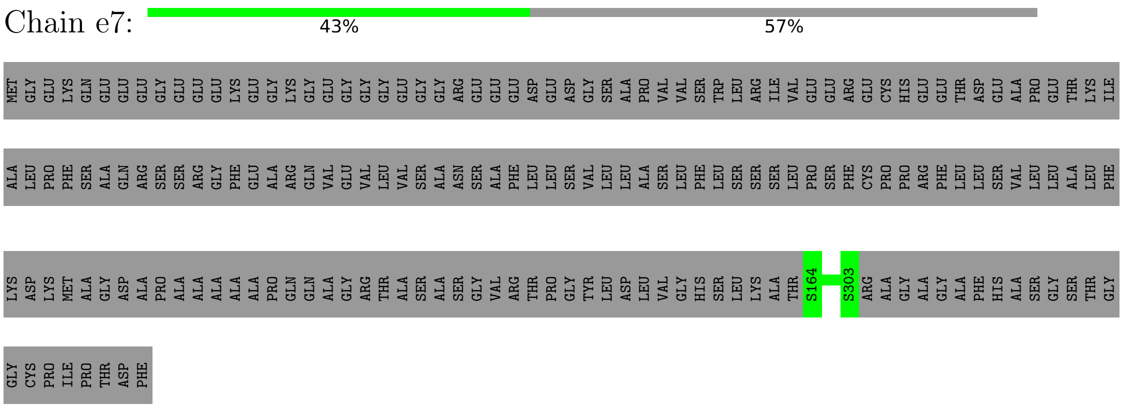


- Molecule 10: ATPTG6

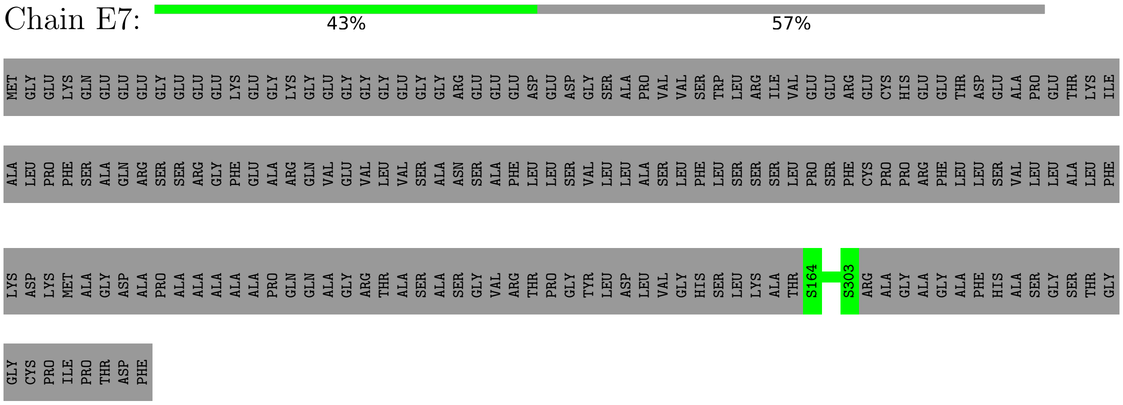
Chain H9:



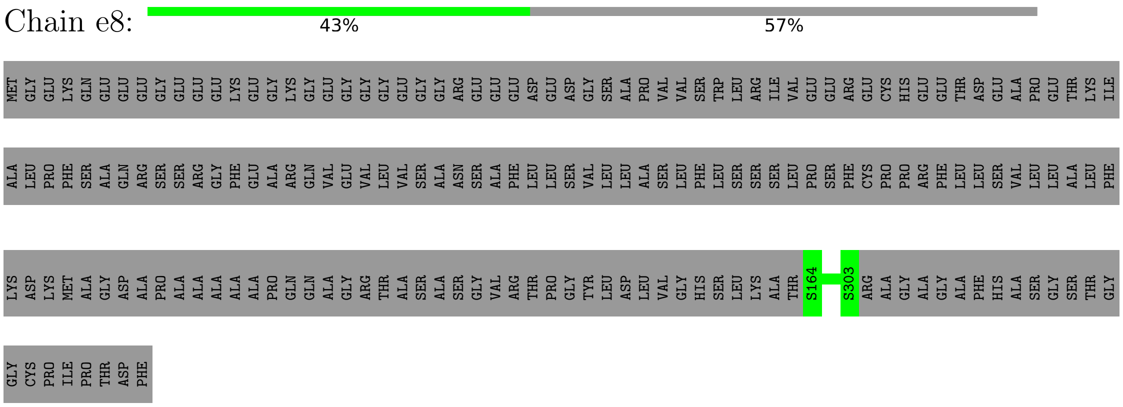
- Molecule 11: ATPTG3



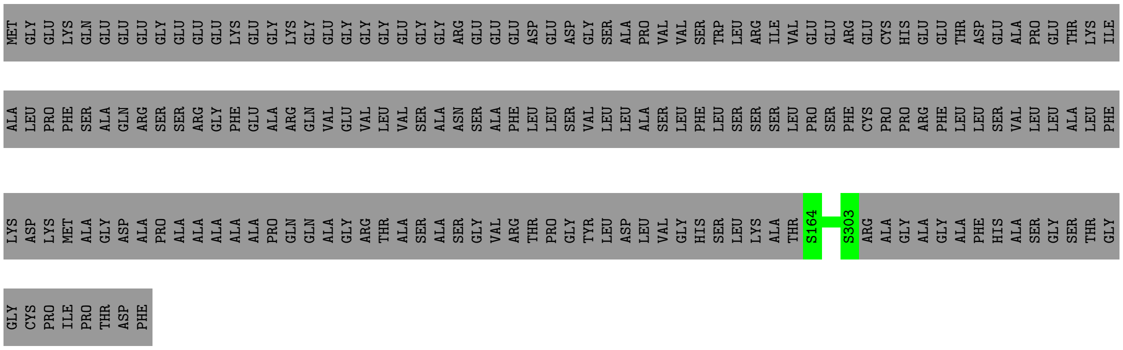
- Molecule 11: ATPTG3



- Molecule 11: ATPTG3

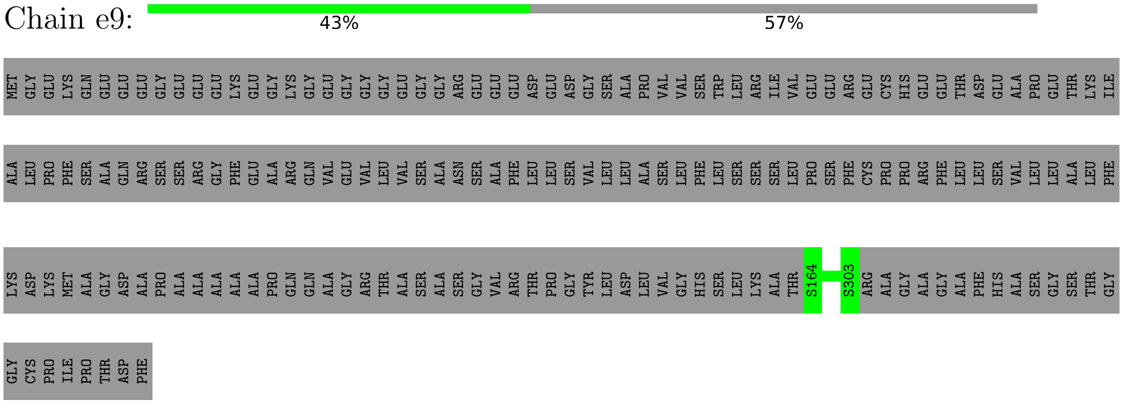


- Molecule 11: ATPTG3



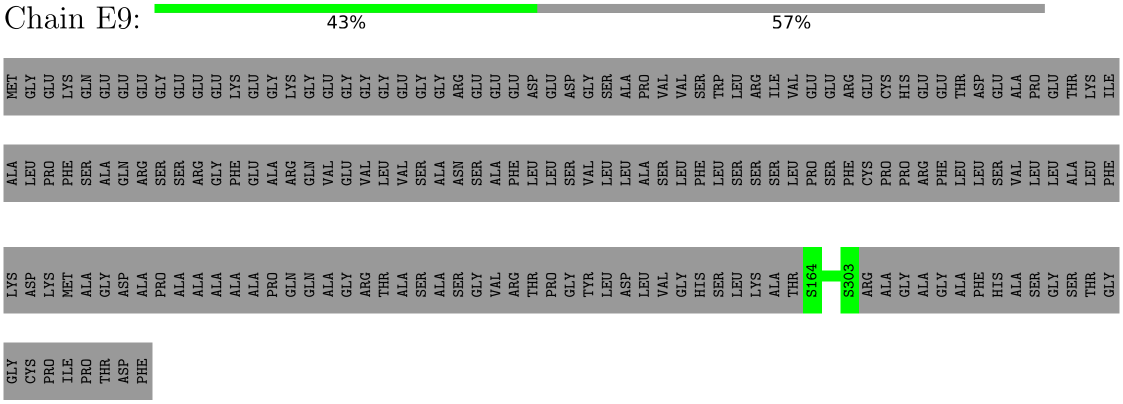
- Molecule 11: ATPTG3

Chain e9:



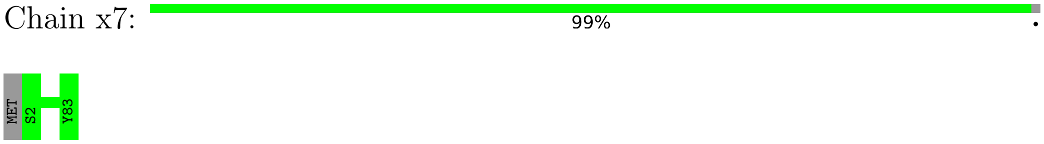
- Molecule 11: ATPTG3

Chain E9:



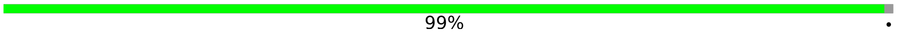
- Molecule 12: ATPTG17,ATPTG17,ATPTG17

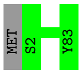
Chain x7:



- Molecule 12: ATPTG17,ATPTG17,ATPTG17

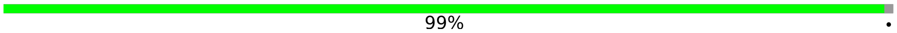
Chain X7:

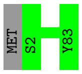




- Molecule 12: ATPTG17,ATPTG17,ATPTG17

Chain x8:





- Molecule 12: ATPTG17,ATPTG17,ATPTG17

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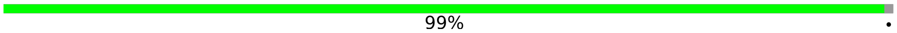
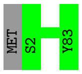
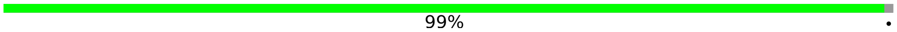
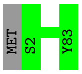




- Molecule 12: ATPTG17,ATPTG17,ATPTG17

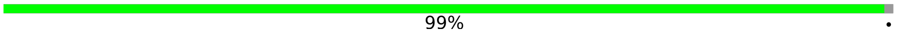
Chain x9:

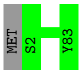




- Molecule 12: ATPTG17,ATPTG17,ATPTG17

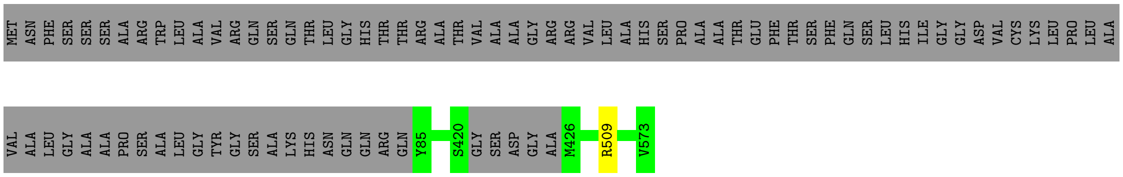
Chain X9:





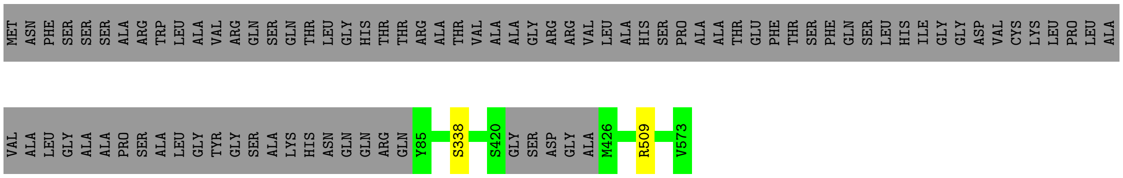
- Molecule 13: subunit b

Chain b7:



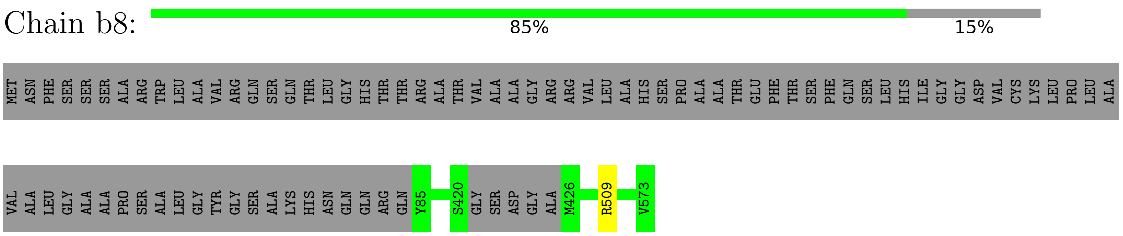
- Molecule 13: subunit b

Chain B7:



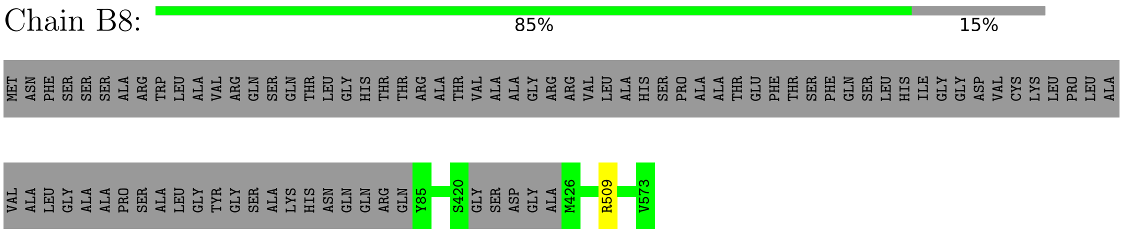
- Molecule 13: subunit b

Chain b8:



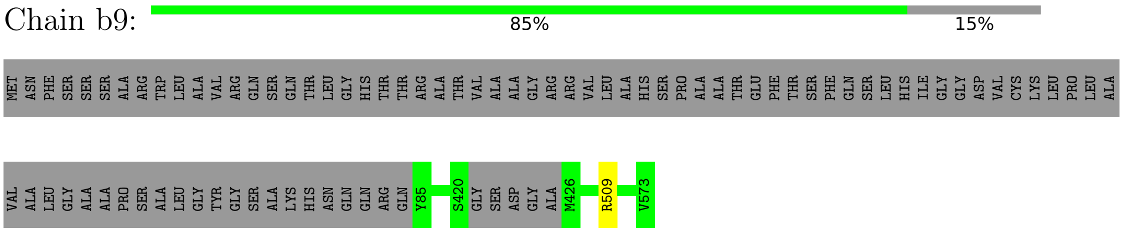
- Molecule 13: subunit b

Chain B8:



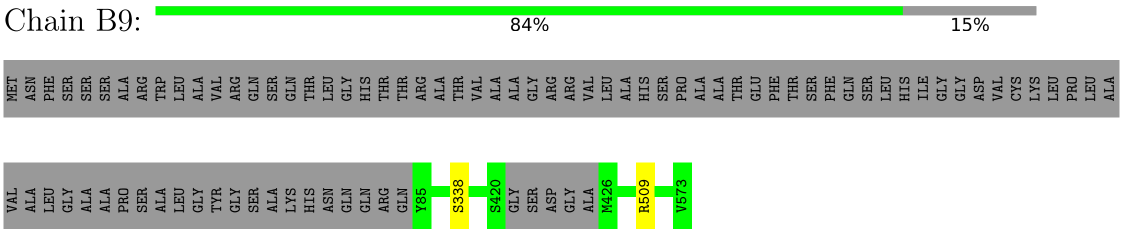
- Molecule 13: subunit b

Chain b9:



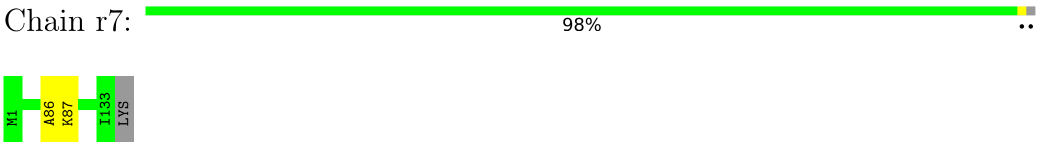
- Molecule 13: subunit b

Chain B9:



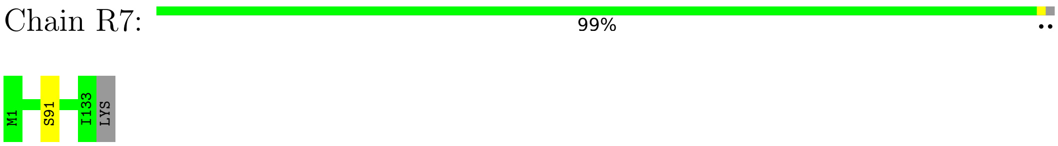
- Molecule 14: ATPTG12

Chain r7:



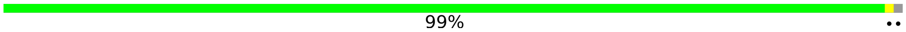
- Molecule 14: ATPTG12

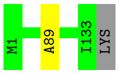
Chain R7:



- Molecule 14: ATPTG12

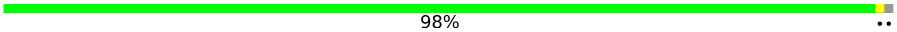
Chain r8:

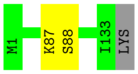




- Molecule 14: ATPTG12

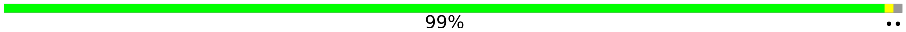
Chain R8:

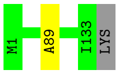




- Molecule 14: ATPTG12

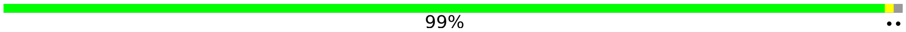
Chain r9:

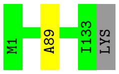




- Molecule 14: ATPTG12

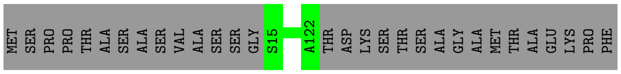
Chain R9:





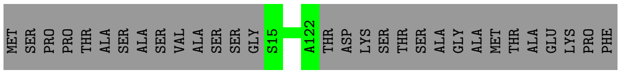
- Molecule 15: ATPTG10

Chain p7:



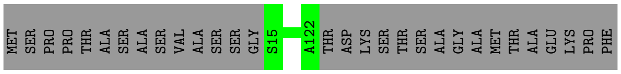
- Molecule 15: ATPTG10

Chain P7:



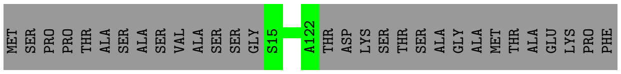
- Molecule 15: ATPTG10

Chain p8:



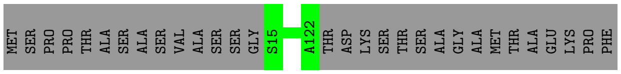
- Molecule 15: ATPTG10

Chain P8:



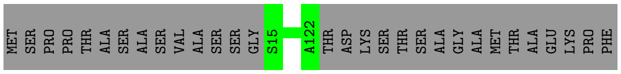
- Molecule 15: ATPTG10

Chain p9:



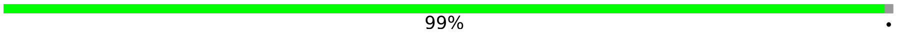
- Molecule 15: ATPTG10

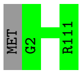
Chain P9:



- Molecule 16: subunit f

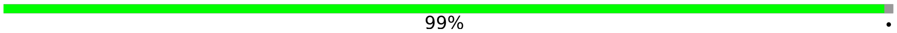
Chain v7:

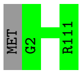




- Molecule 16: subunit f

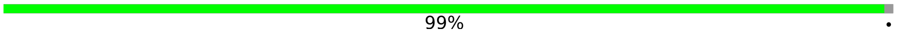
Chain V7:

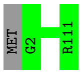




- Molecule 16: subunit f

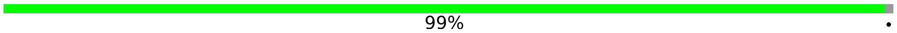
Chain v8:

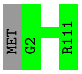




- Molecule 16: subunit f

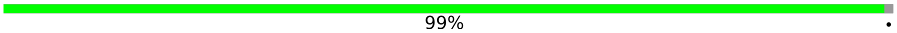
Chain V8:

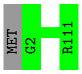




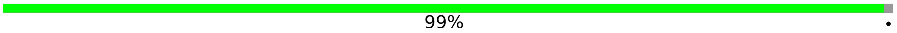
- Molecule 16: subunit f

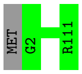
Chain v9:



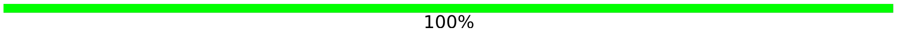


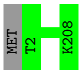
- Molecule 16: subunit f

Chain V9:




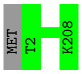
- Molecule 17: ATPTG8

Chain l7:




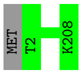
- Molecule 17: ATPTG8

Chain L7:

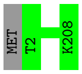
- Molecule 17: ATPTG8

Chain l8:

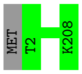
- Molecule 17: ATPTG8

Chain L8:

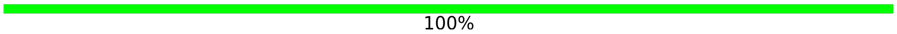



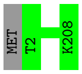
- Molecule 17: ATPTG8

Chain l9:

- Molecule 17: ATPTG8

Chain L9:




- Molecule 18: ATPTG1

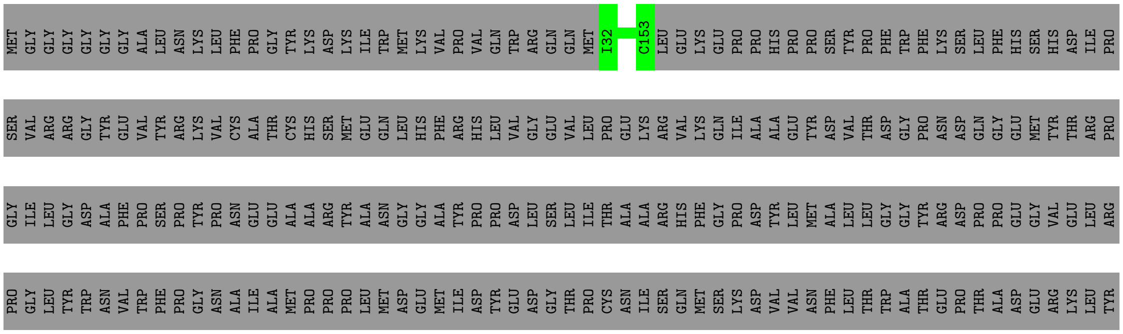
Chain c7:

- Molecule 18: ATPTG1

Chain C7:

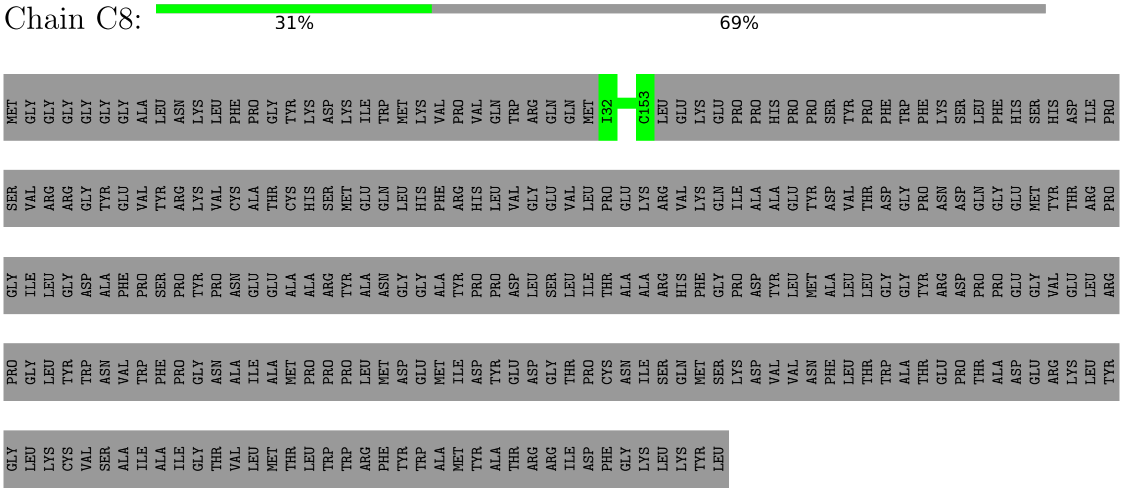
- Molecule 18: ATPTG1

Chain c8:



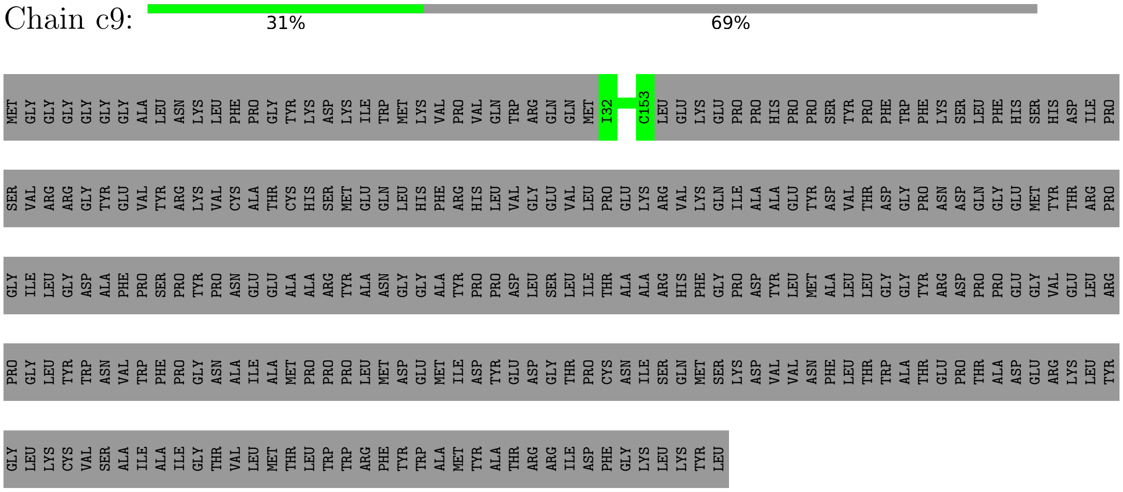
- Molecule 18: ATPTG1

Chain C8:



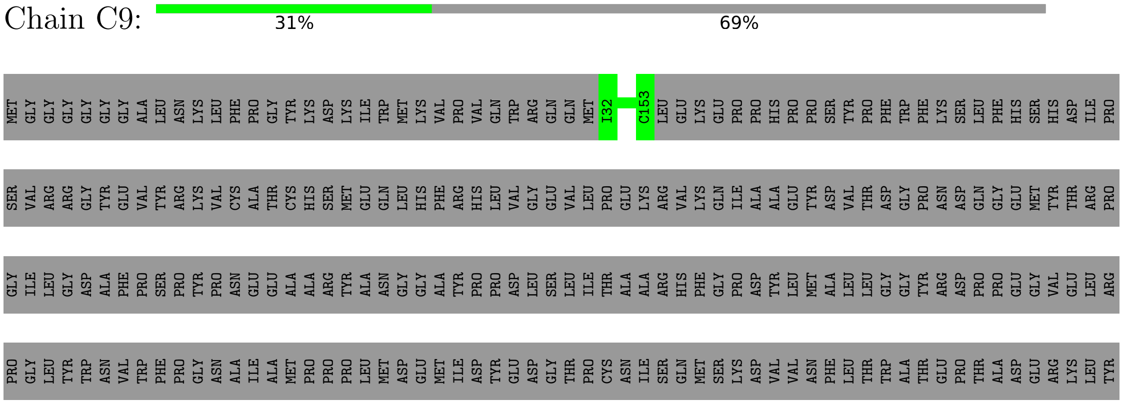
- Molecule 18: ATPTG1

Chain c9:



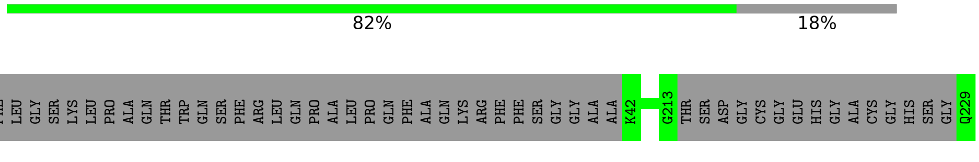
- Molecule 18: ATPTG1

Chain C9:



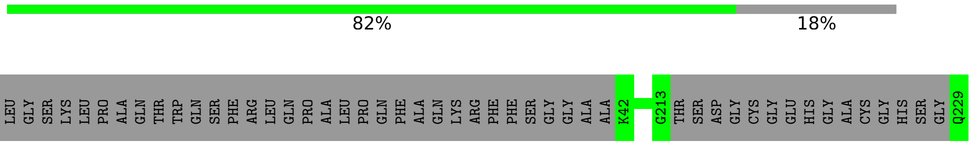
- Molecule 19: ATPTG2

Chain d7:



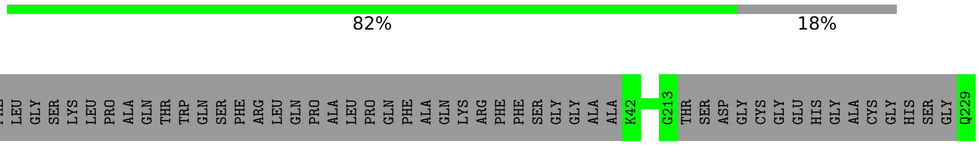
- Molecule 19: ATPTG2

Chain D7:



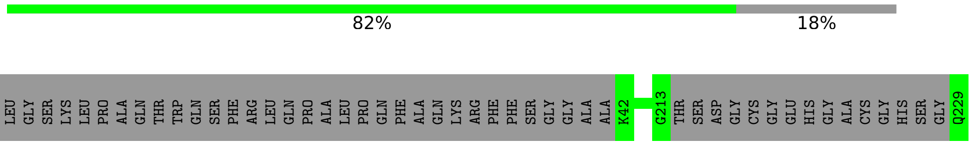
- Molecule 19: ATPTG2

Chain d8:



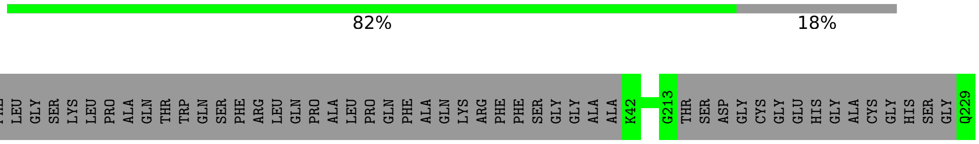
- Molecule 19: ATPTG2

Chain D8:



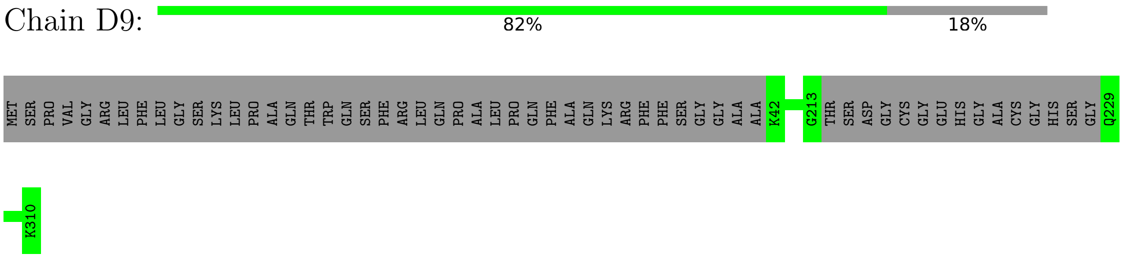
- Molecule 19: ATPTG2

Chain d9:



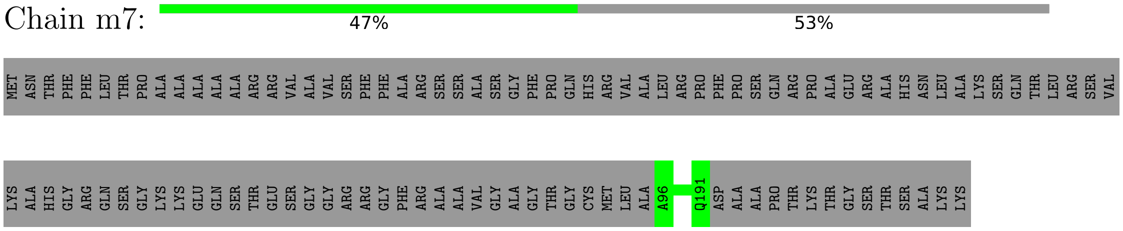
- Molecule 19: ATPTG2

Chain D9:



- Molecule 20: subunit 8

Chain m7:



- Molecule 20: subunit 8

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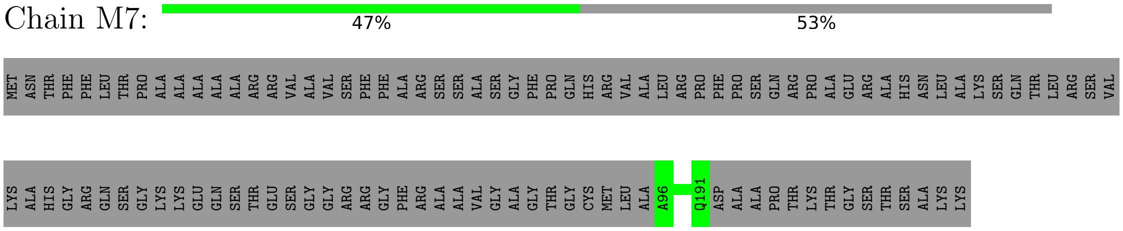

- Molecule 20: subunit 8

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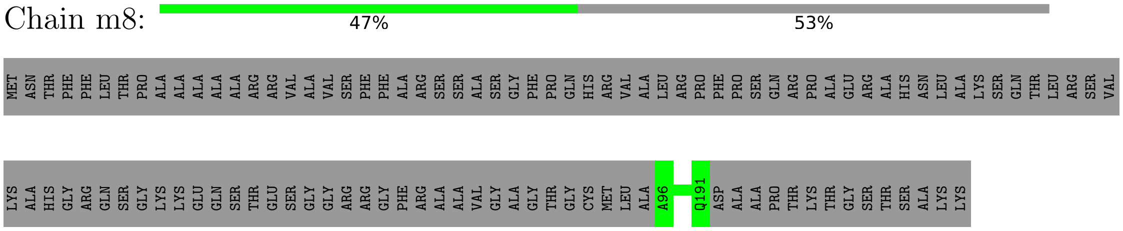

- Molecule 20: subunit 8

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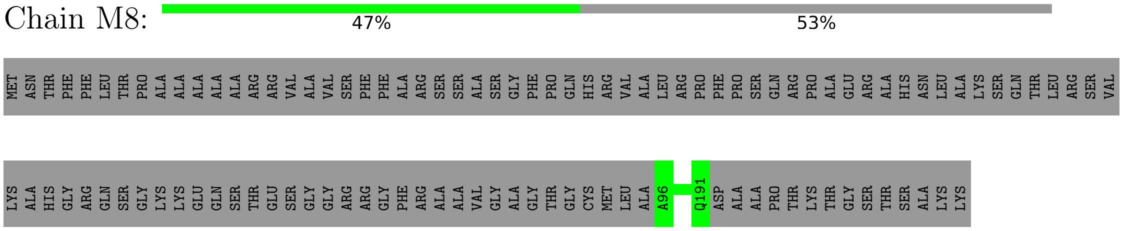
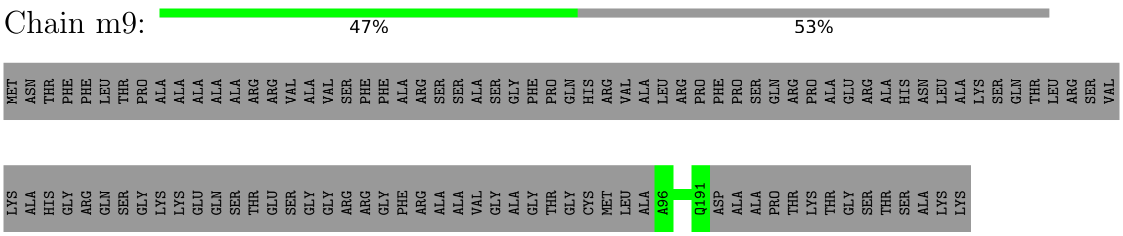
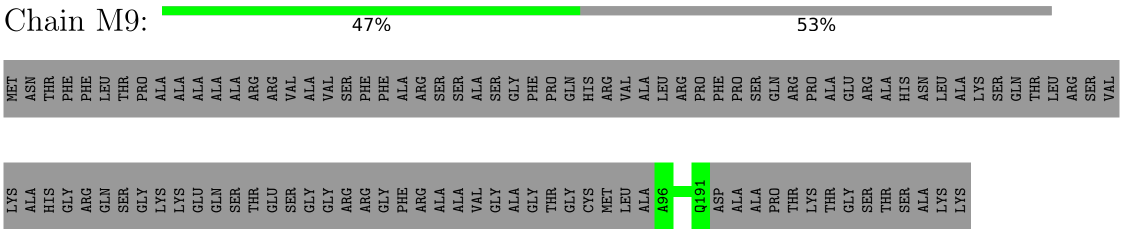


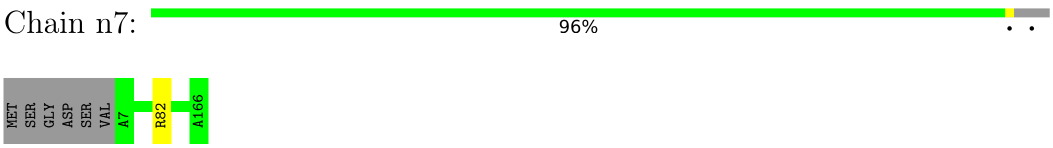
- Molecule 20: subunit 8



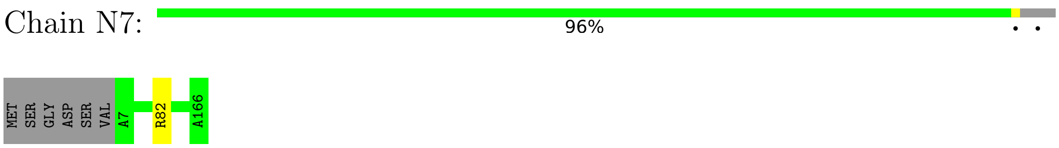
- Molecule 20: subunit 8



- Molecule 21: ATPTG9



- Molecule 21: ATPTG9



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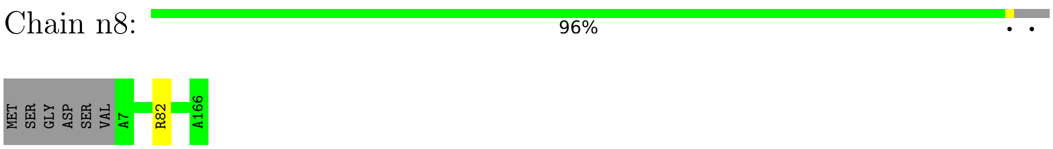
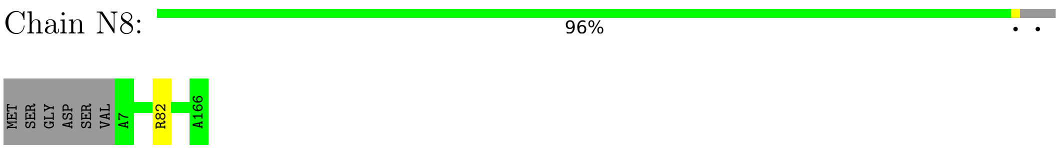
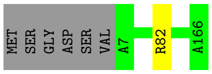


- Molecule 21: ATPTG9

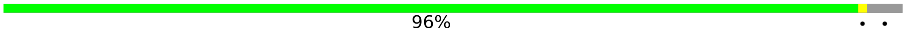


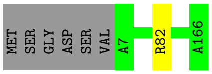
- Molecule 21: ATPTG9



- Molecule 21: ATPTG9

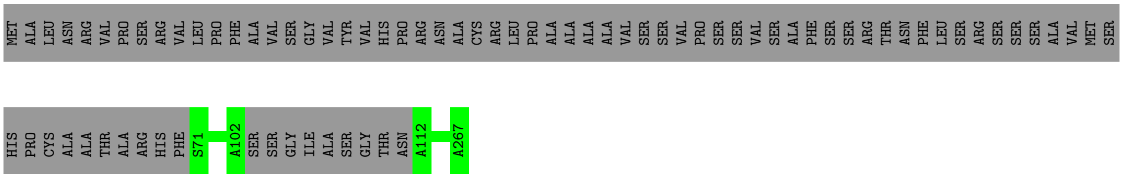
Chain N9:





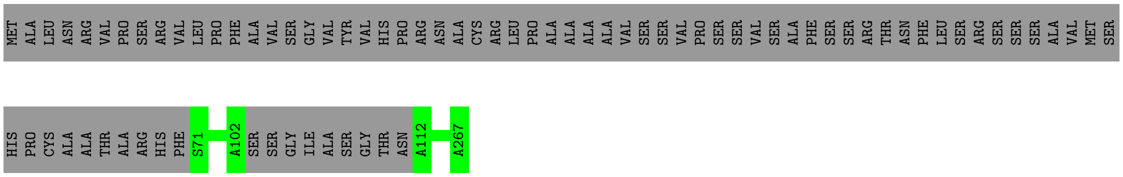
- Molecule 22: ATPTG4

Chain f7:



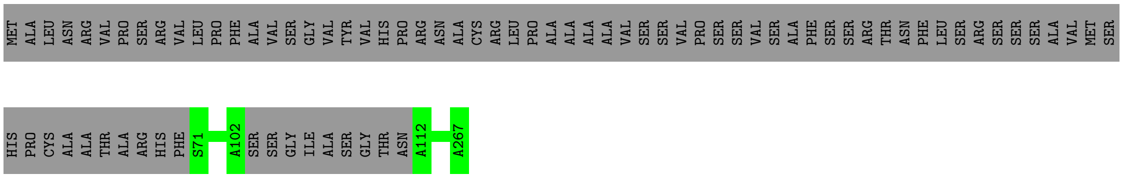
- Molecule 22: ATPTG4

Chain F7:



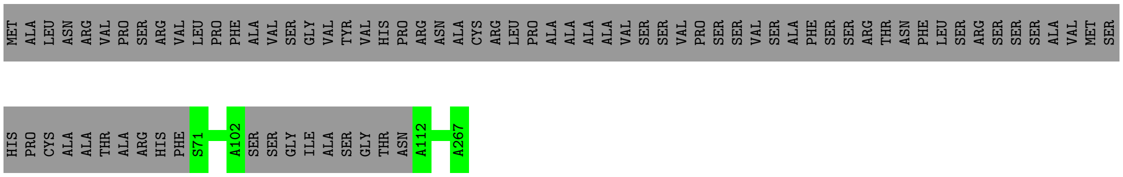
- Molecule 22: ATPTG4

Chain f8:



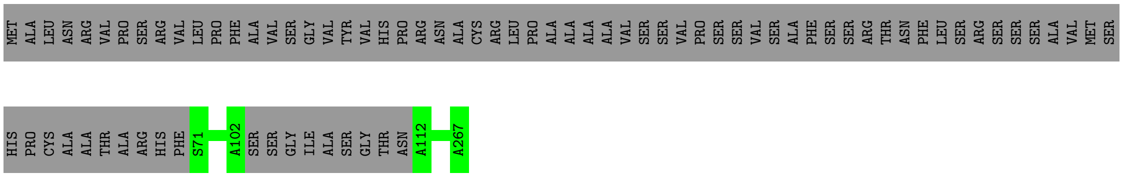
- Molecule 22: ATPTG4

Chain F8:



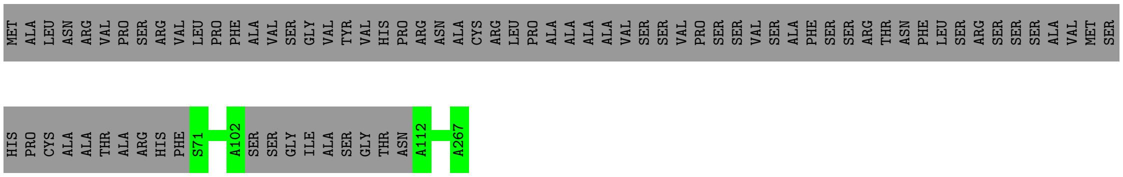
- Molecule 22: ATPTG4

Chain f9:



- Molecule 22: ATPTG4

Chain F9:



- Molecule 23: ATPTG16

Chain w7:

- Molecule 23: ATPTG16

Chain W7:

- Molecule 23: ATPTG16

Chain w8:

- Molecule 23: ATPTG16

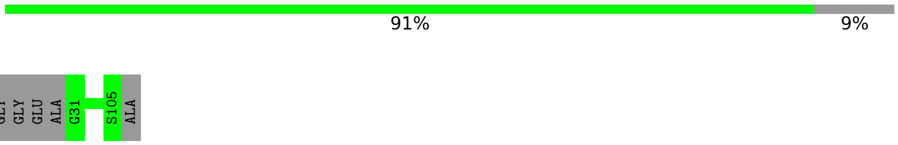
Chain W8:

- Molecule 23: ATPTG16

Chain w9:

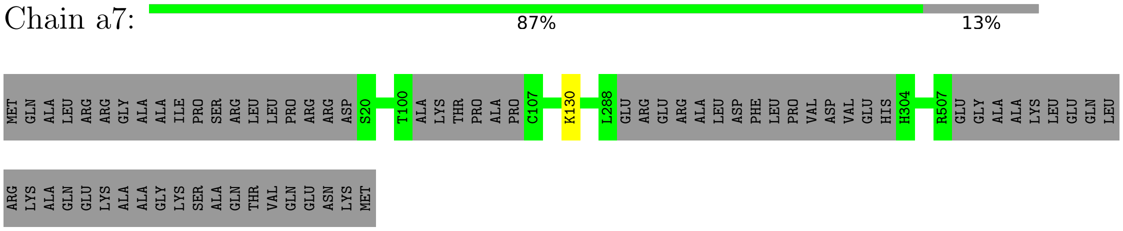
- Molecule 23: ATPTG16

Chain W9:



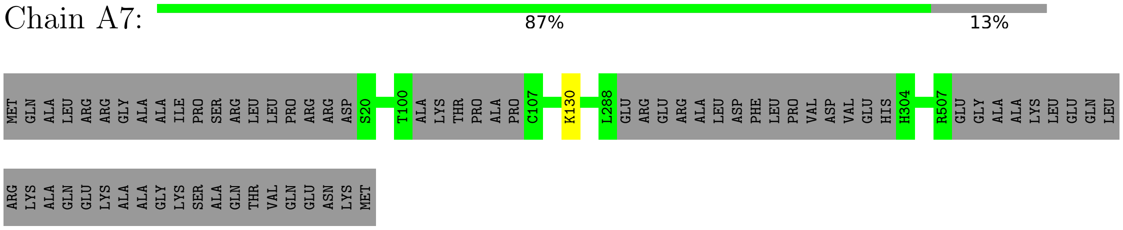
- Molecule 24: subunit d

Chain a7:



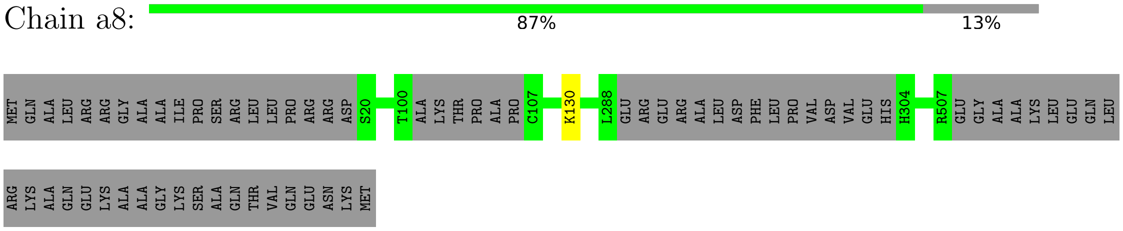
- Molecule 24: subunit d

Chain A7:



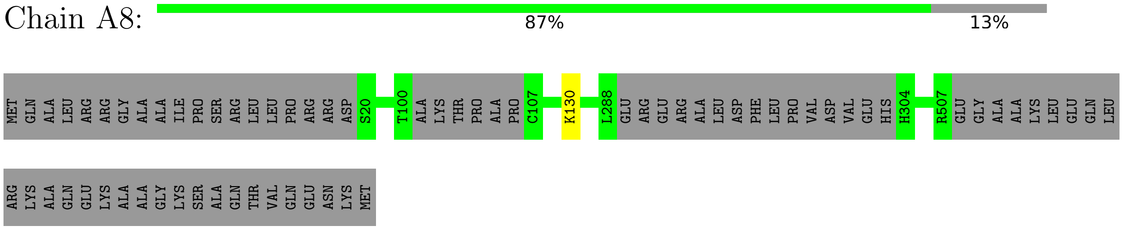
- Molecule 24: subunit d

Chain a8:



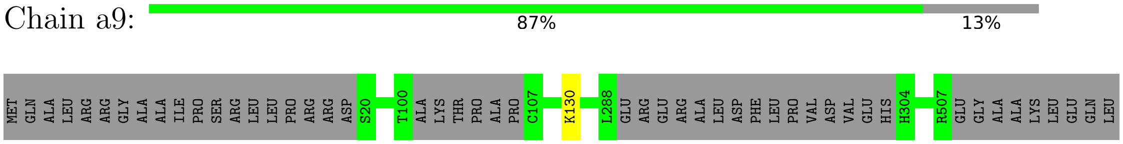
- Molecule 24: subunit d

Chain A8:



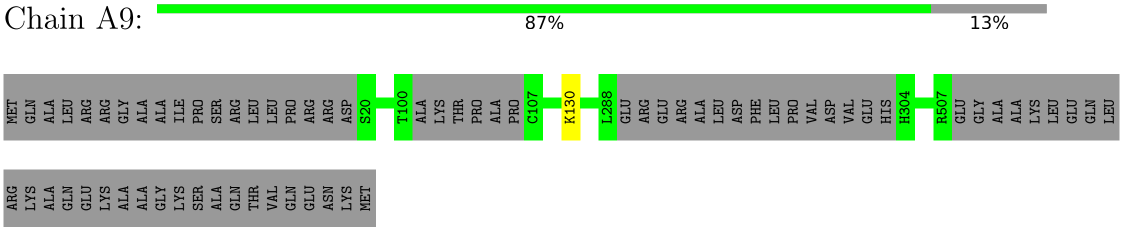
- Molecule 24: subunit d

Chain a9:



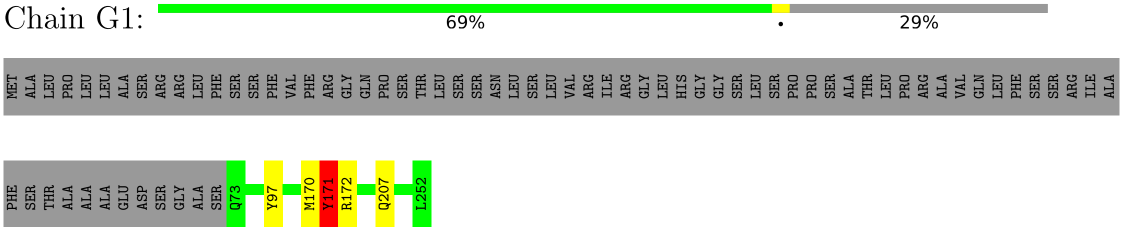
- Molecule 24: subunit d

Chain A9:



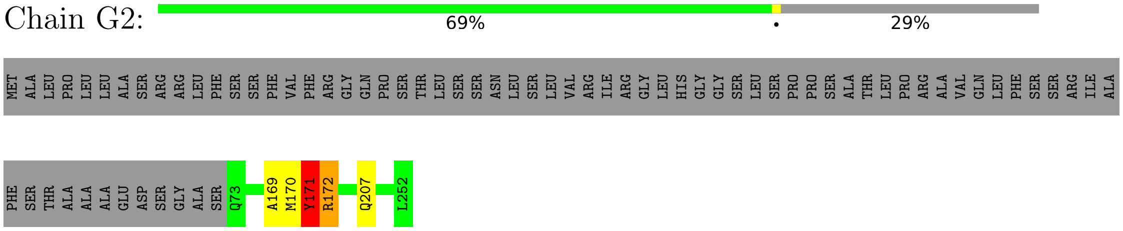
- Molecule 25: Oligomycin sensitivity conferring protein (OSCP)

Chain G1:



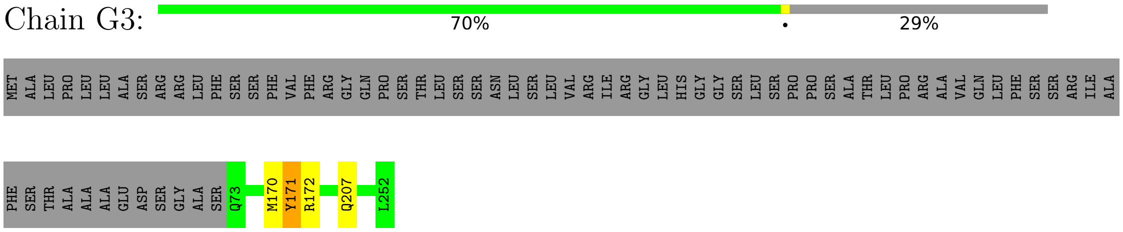
- Molecule 25: Oligomycin sensitivity conferring protein (OSCP)

Chain G2:



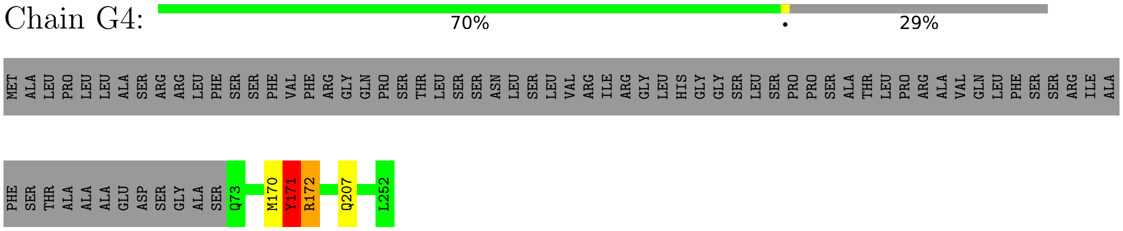
- Molecule 25: Oligomycin sensitivity conferring protein (OSCP)

Chain G3:



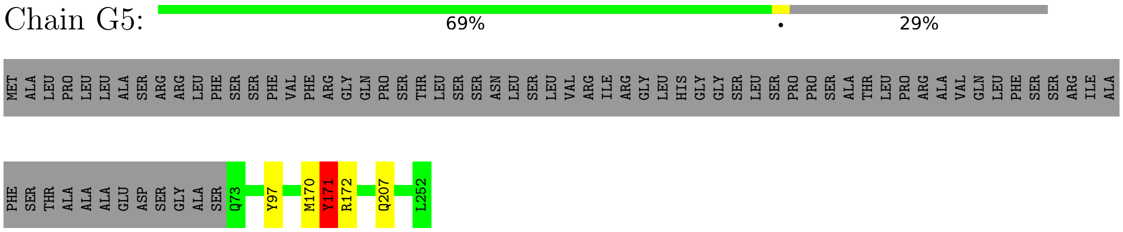
- Molecule 25: Oligomycin sensitivity conferring protein (OSCP)

Chain G4:



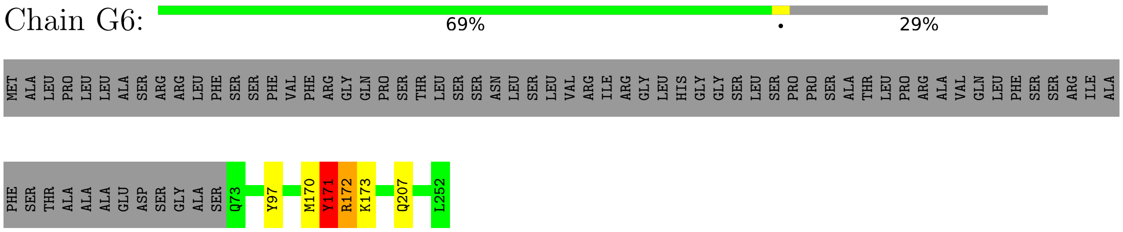
- Molecule 25: Oligomycin sensitivity conferring protein (OSCP)

Chain G5:



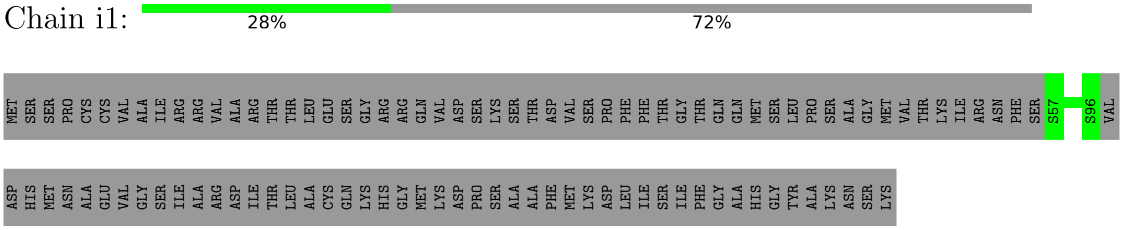
- Molecule 25: Oligomycin sensitivity conferring protein (OSCP)

Chain G6:



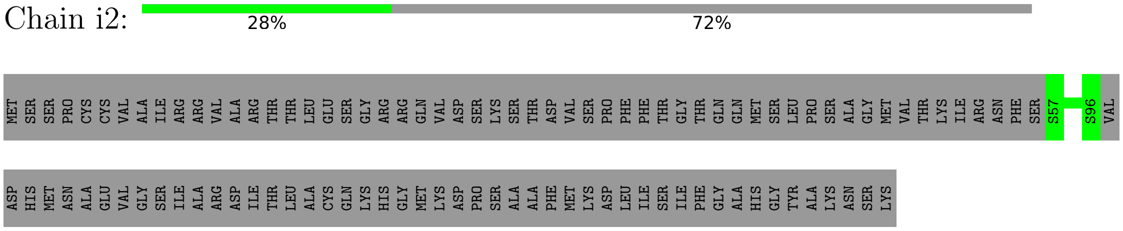
- Molecule 26: Inhibitor of F1

Chain i1:



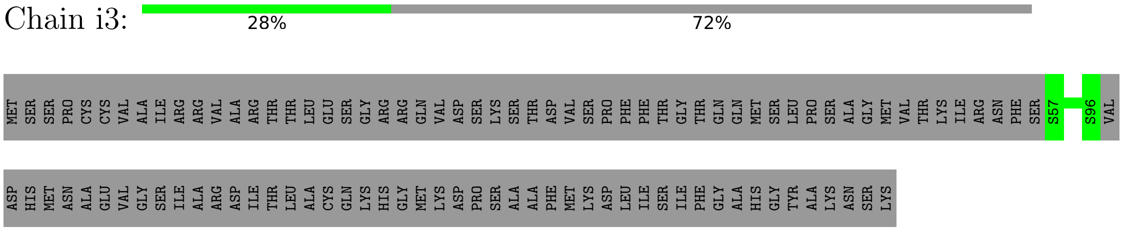
- Molecule 26: Inhibitor of F1

Chain i2:



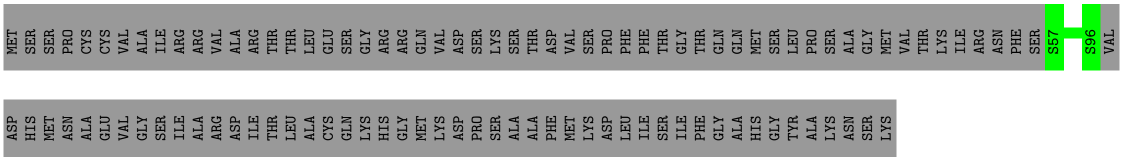
- Molecule 26: Inhibitor of F1

Chain i3:



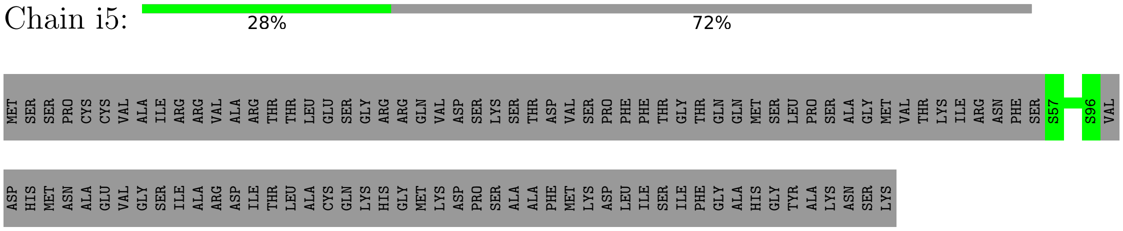
- Molecule 26: Inhibitor of F1

Chain i4:



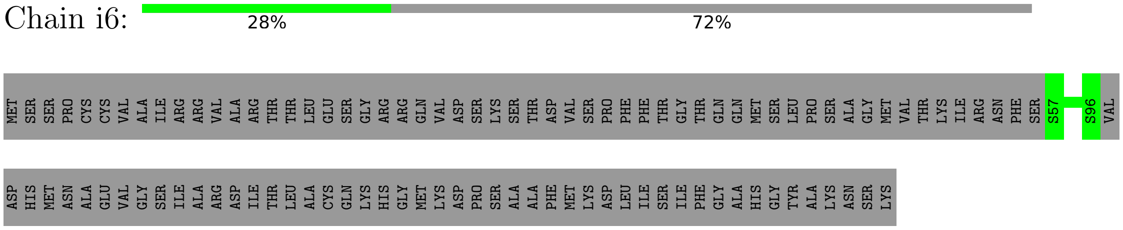
- Molecule 26: Inhibitor of F1

Chain i5:



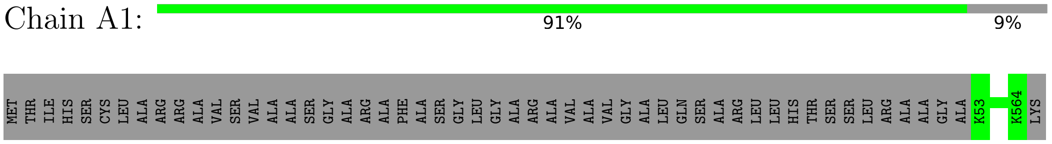
- Molecule 26: Inhibitor of F1

Chain i6:



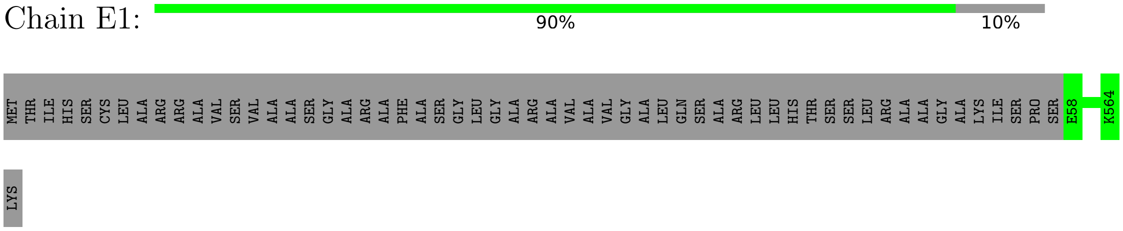
- Molecule 27: ATP synthase subunit alpha

Chain A1:



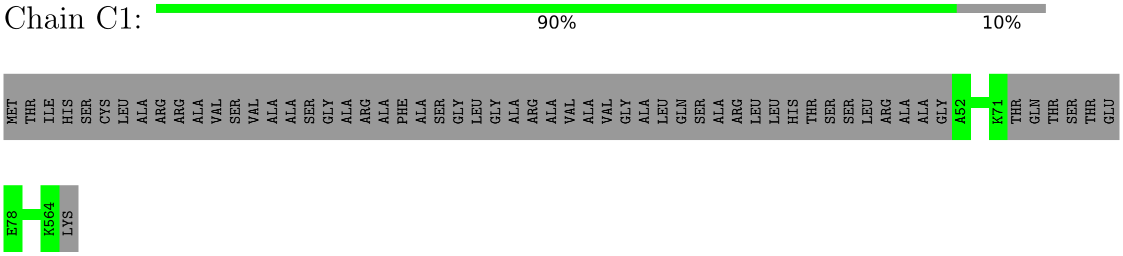
- Molecule 27: ATP synthase subunit alpha

Chain E1:



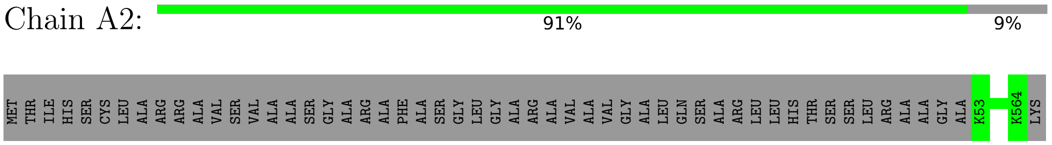
- Molecule 27: ATP synthase subunit alpha

Chain C1:



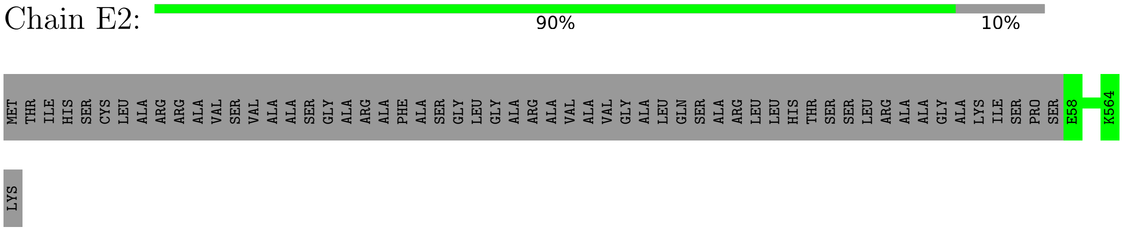
- Molecule 27: ATP synthase subunit alpha

Chain A2:



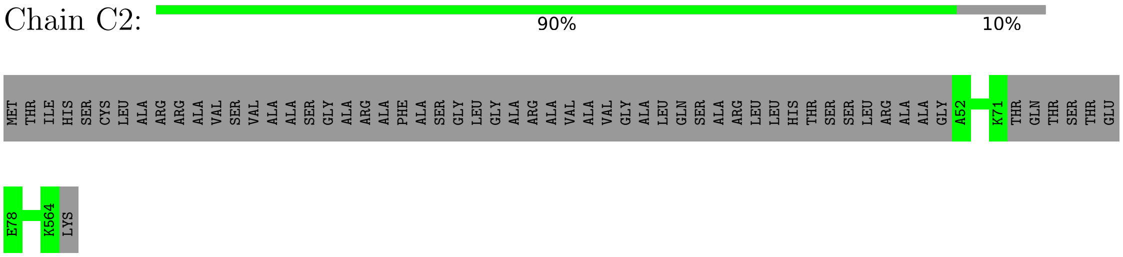
- Molecule 27: ATP synthase subunit alpha

Chain E2:



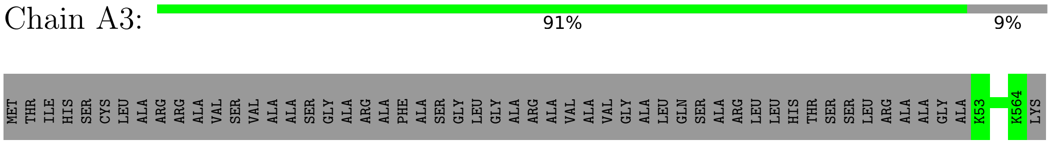
- Molecule 27: ATP synthase subunit alpha

Chain C2:



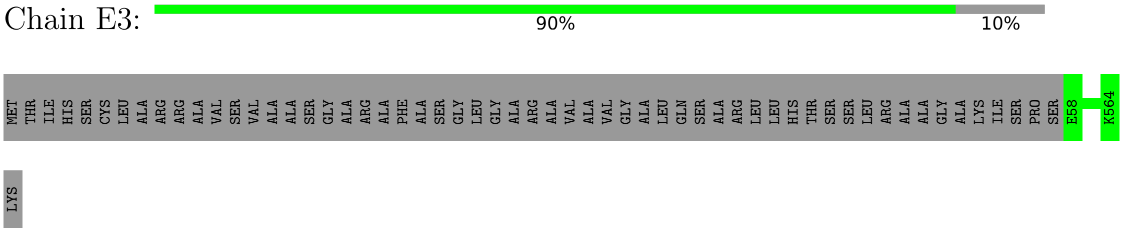
- Molecule 27: ATP synthase subunit alpha

Chain A3:



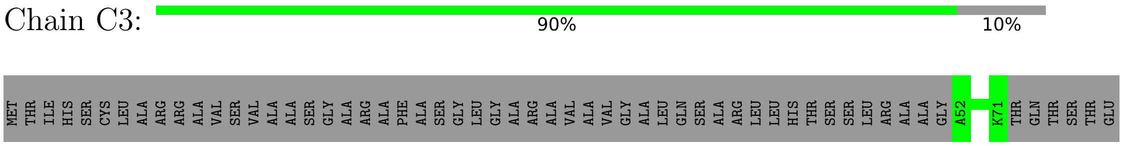
- Molecule 27: ATP synthase subunit alpha

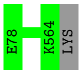
Chain E3:



- Molecule 27: ATP synthase subunit alpha

Chain C3:



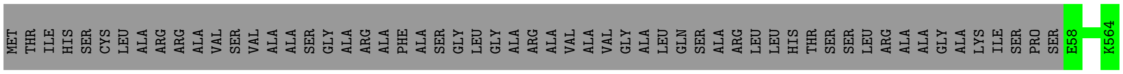


- Molecule 27: ATP synthase subunit alpha

Chain A4:

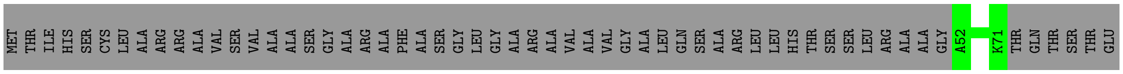
- Molecule 27: ATP synthase subunit alpha

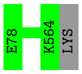
Chain E4:



- Molecule 27: ATP synthase subunit alpha

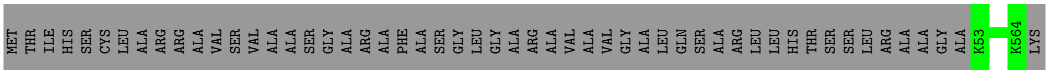
Chain C4:





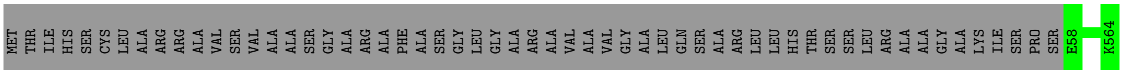
- Molecule 27: ATP synthase subunit alpha

Chain A5:



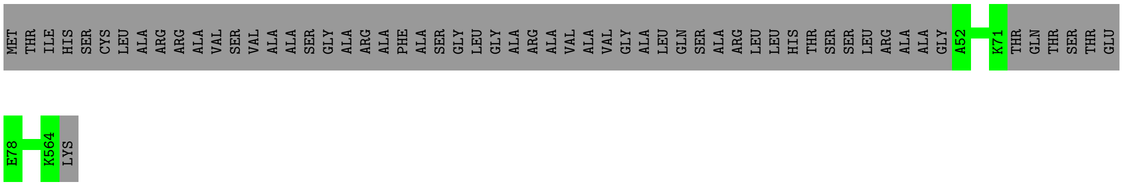
- Molecule 27: ATP synthase subunit alpha

Chain E5:



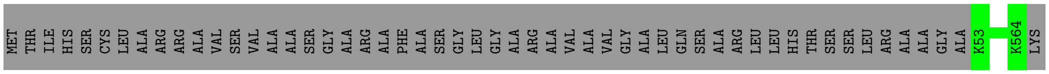
- Molecule 27: ATP synthase subunit alpha

Chain C5:



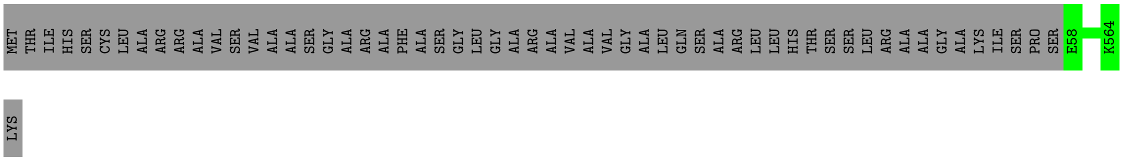
- Molecule 27: ATP synthase subunit alpha

Chain A6:



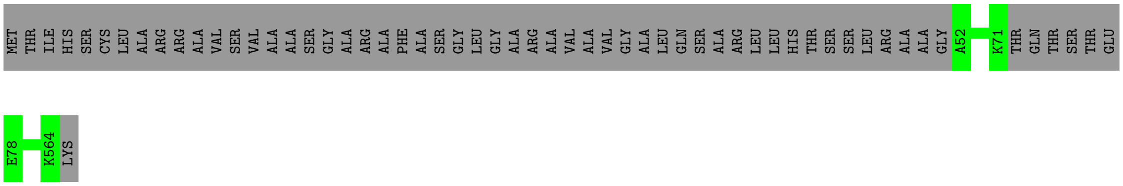
- Molecule 27: ATP synthase subunit alpha

Chain E6:



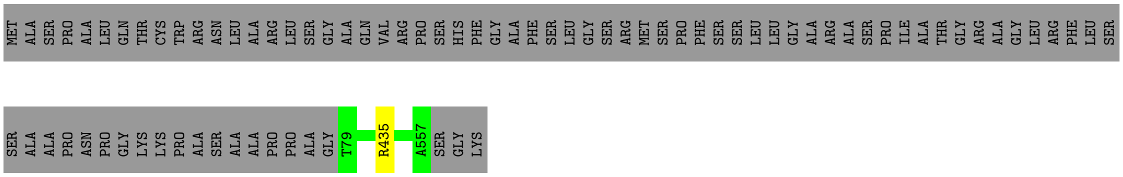
- Molecule 27: ATP synthase subunit alpha

Chain C6:



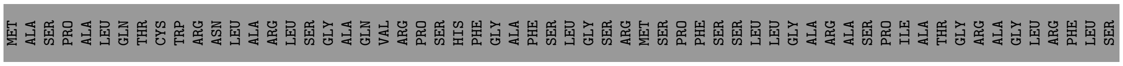
- Molecule 28: ATP synthase subunit beta

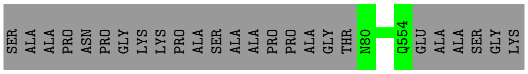
Chain B1:



- Molecule 28: ATP synthase subunit beta

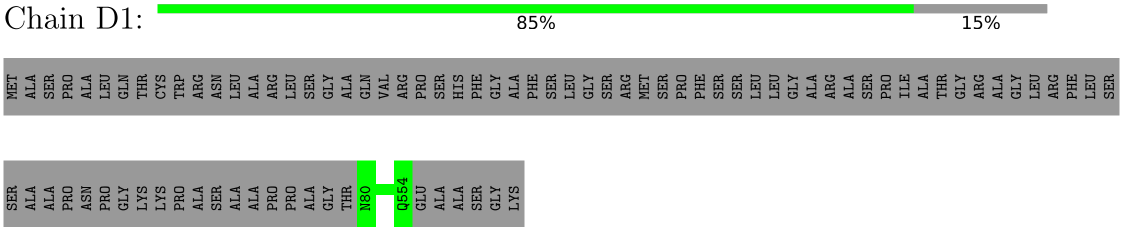
Chain F1:





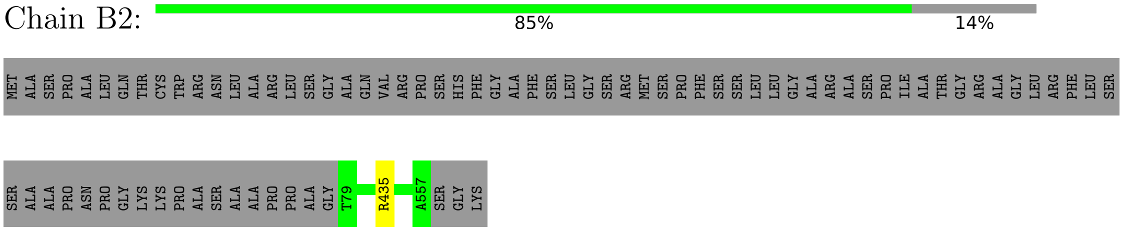
- Molecule 28: ATP synthase subunit beta

Chain D1:



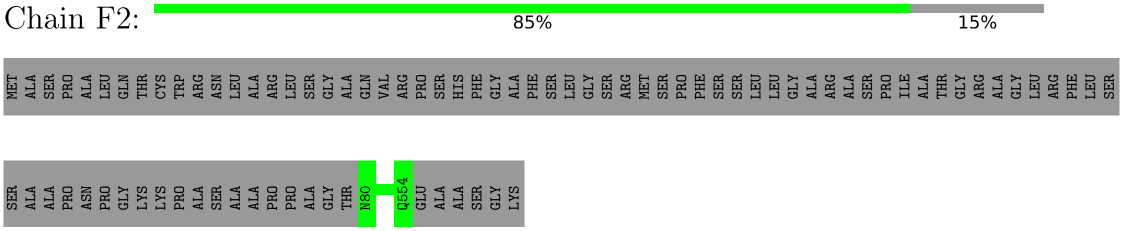
- Molecule 28: ATP synthase subunit beta

Chain B2:



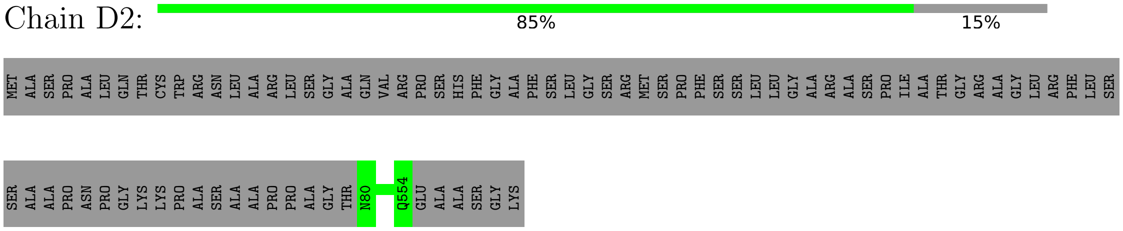
- Molecule 28: ATP synthase subunit beta

Chain F2:



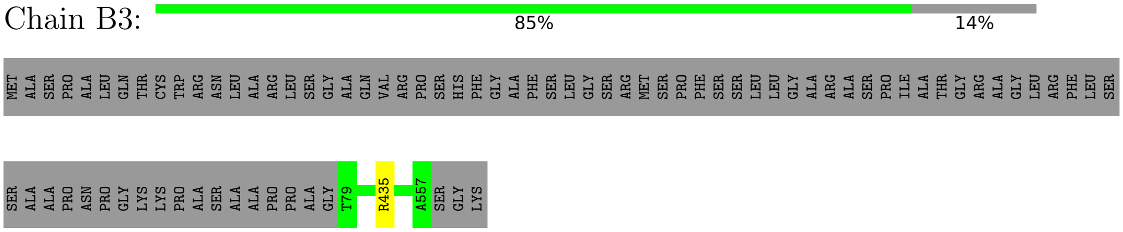
- Molecule 28: ATP synthase subunit beta

Chain D2:



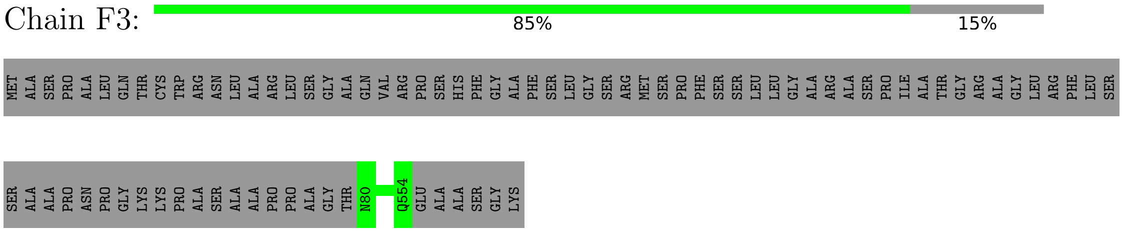
- Molecule 28: ATP synthase subunit beta

Chain B3:



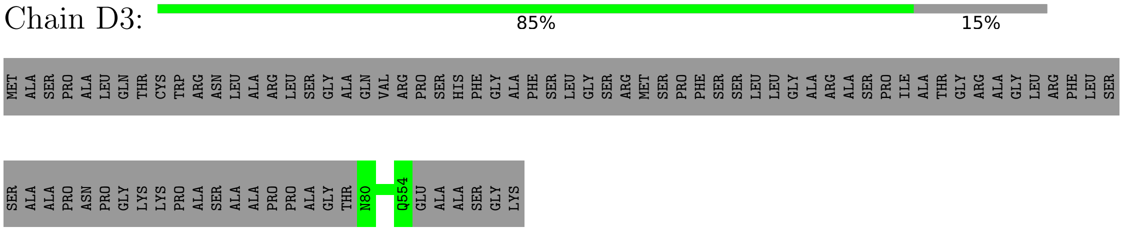
- Molecule 28: ATP synthase subunit beta

Chain F3:



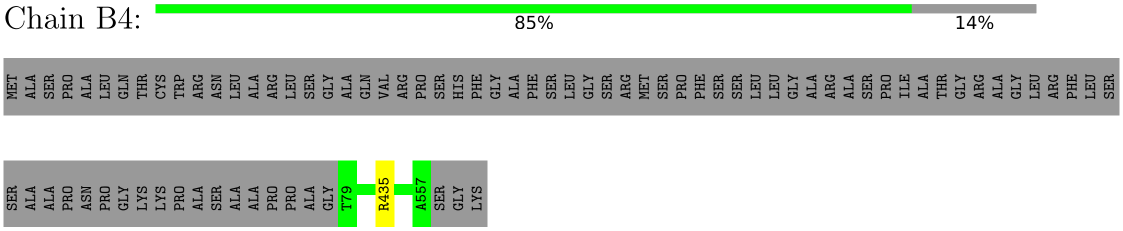
- Molecule 28: ATP synthase subunit beta

Chain D3:



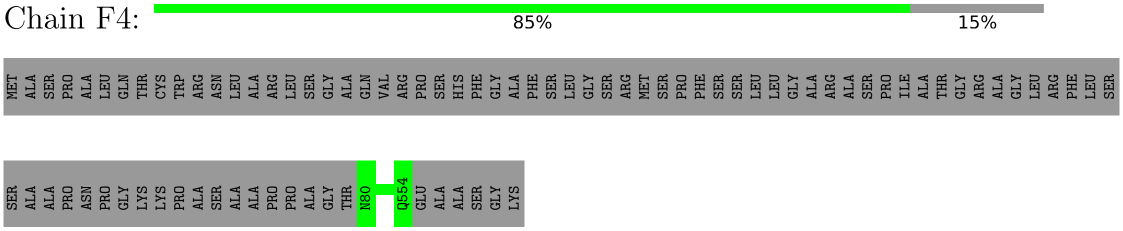
- Molecule 28: ATP synthase subunit beta

Chain B4:



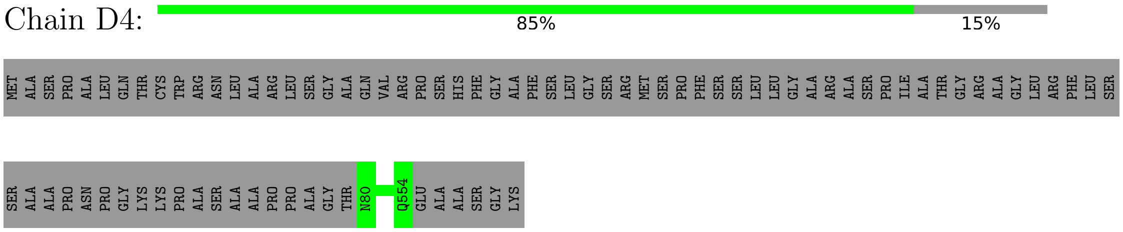
- Molecule 28: ATP synthase subunit beta

Chain F4:



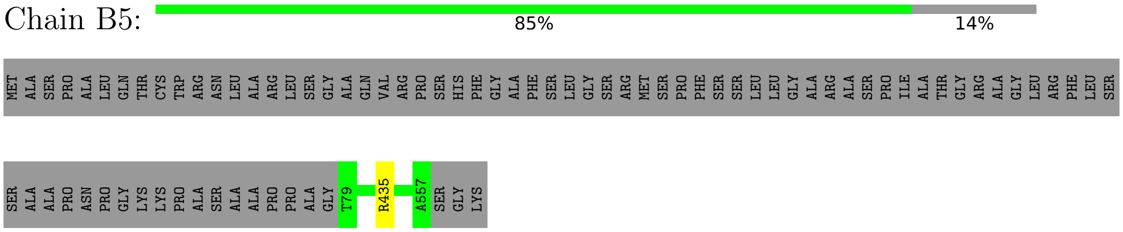
- Molecule 28: ATP synthase subunit beta

Chain D4:



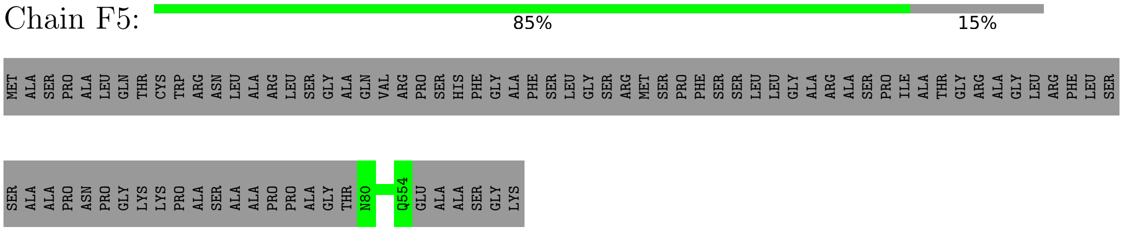
- Molecule 28: ATP synthase subunit beta

Chain B5:



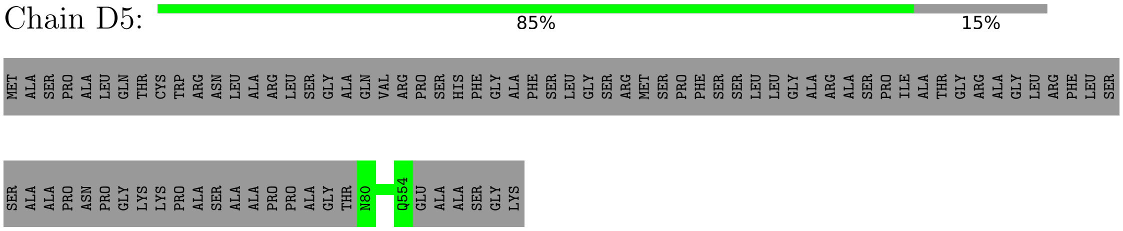
- Molecule 28: ATP synthase subunit beta

Chain F5:



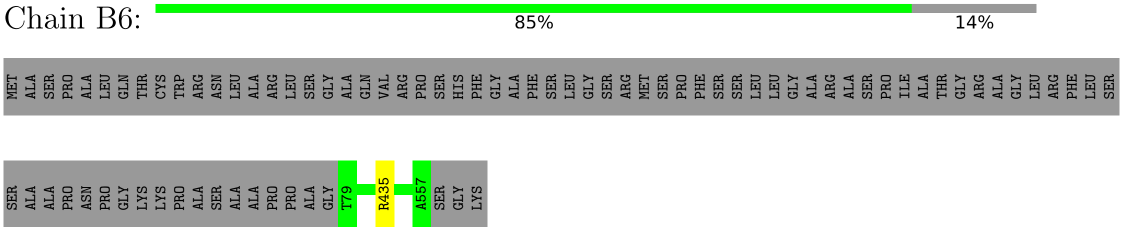
- Molecule 28: ATP synthase subunit beta

Chain D5:



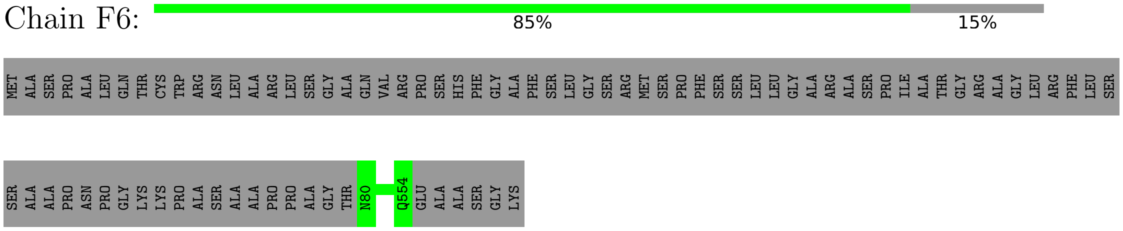
- Molecule 28: ATP synthase subunit beta

Chain B6:



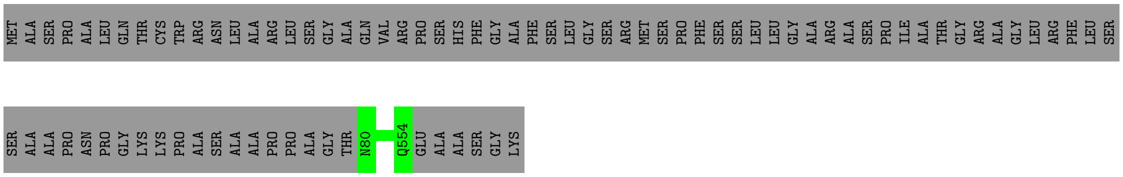
- Molecule 28: ATP synthase subunit beta

Chain F6:



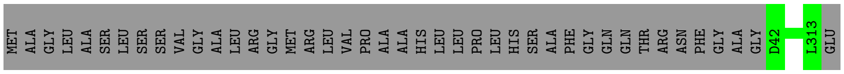
- Molecule 28: ATP synthase subunit beta

Chain D6:



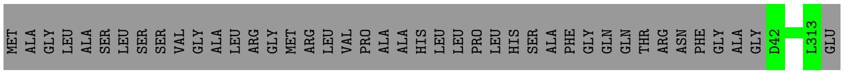
- Molecule 29: ATP synthase subunit gamma

Chain g1:



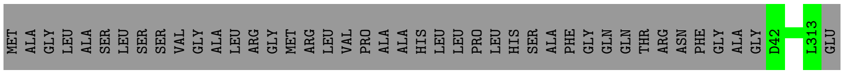
- Molecule 29: ATP synthase subunit gamma

Chain g2:



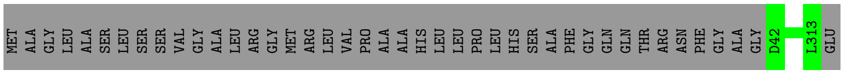
- Molecule 29: ATP synthase subunit gamma

Chain g3:



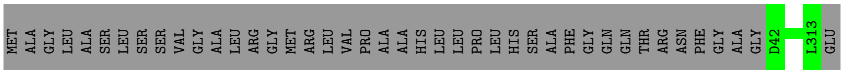
- Molecule 29: ATP synthase subunit gamma

Chain g4:



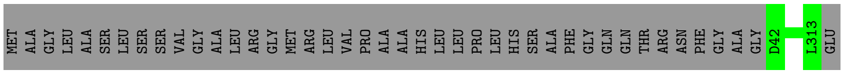
- Molecule 29: ATP synthase subunit gamma

Chain g5:



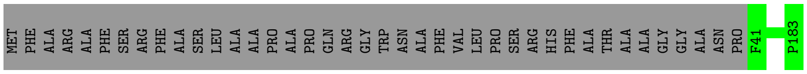
- Molecule 29: ATP synthase subunit gamma

Chain g6:



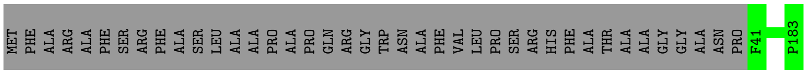
- Molecule 30: ATP synthase subunit delta

Chain d1:



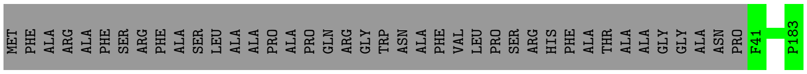
- Molecule 30: ATP synthase subunit delta

Chain d2:



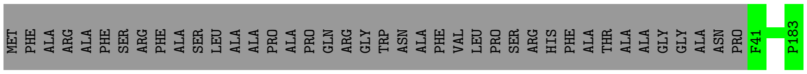
- Molecule 30: ATP synthase subunit delta

Chain d3:



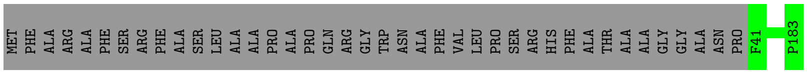
- Molecule 30: ATP synthase subunit delta

Chain d4:



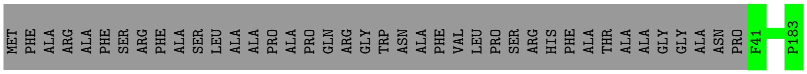
- Molecule 30: ATP synthase subunit delta

Chain d5:



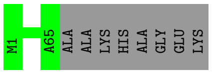
- Molecule 30: ATP synthase subunit delta

Chain d6:



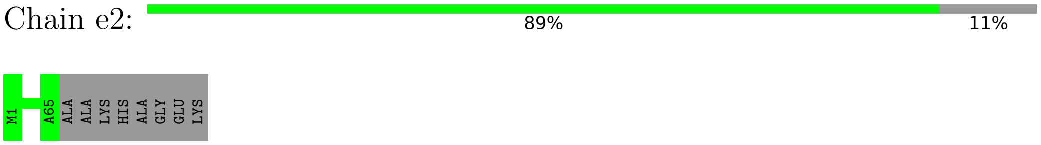
- Molecule 31: ATP synthase subunit epsilon

Chain e1:



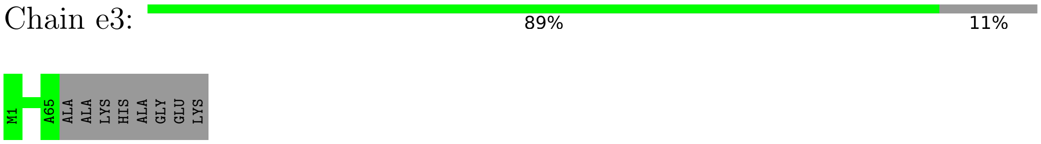
- Molecule 31: ATP synthase subunit epsilon

Chain e2:



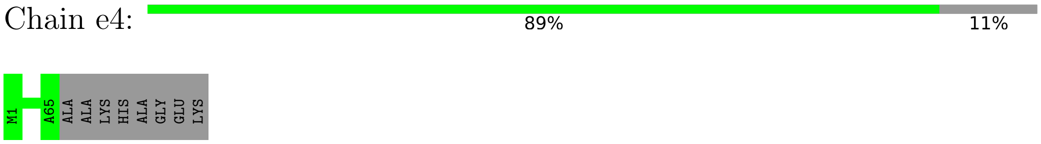
- Molecule 31: ATP synthase subunit epsilon

Chain e3:



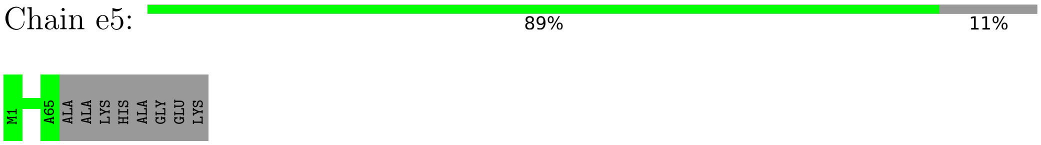
- Molecule 31: ATP synthase subunit epsilon

Chain e4:



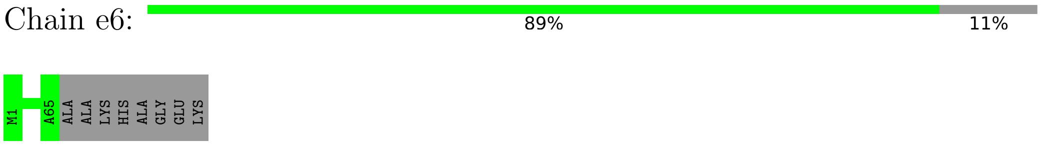
- Molecule 31: ATP synthase subunit epsilon

Chain e5:



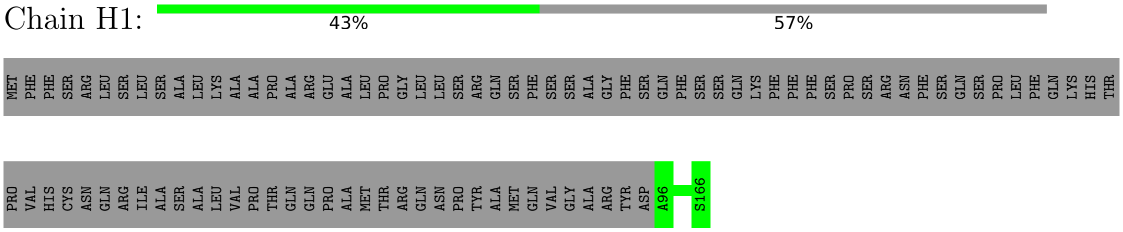
- Molecule 31: ATP synthase subunit epsilon

Chain e6:



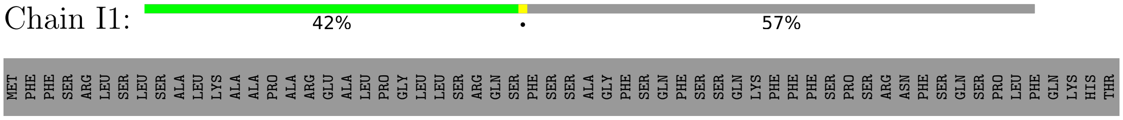
- Molecule 32: subunit c

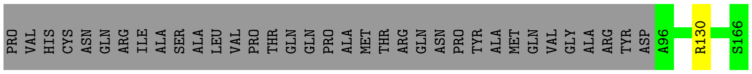
Chain H1:



- Molecule 32: subunit c

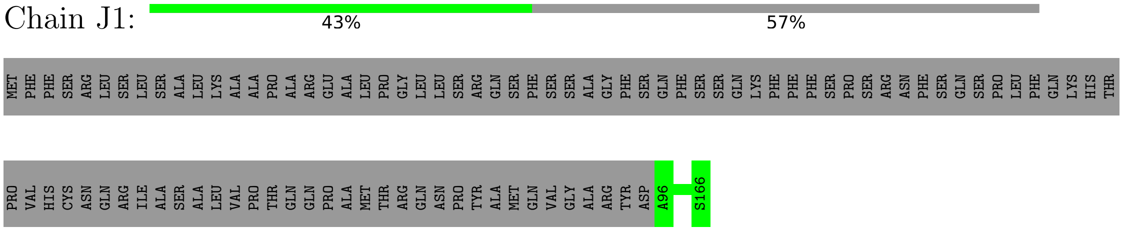
Chain I1:





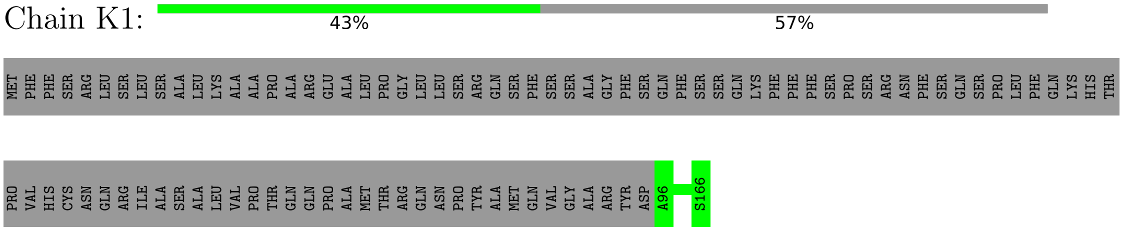
- Molecule 32: subunit c

Chain J1:



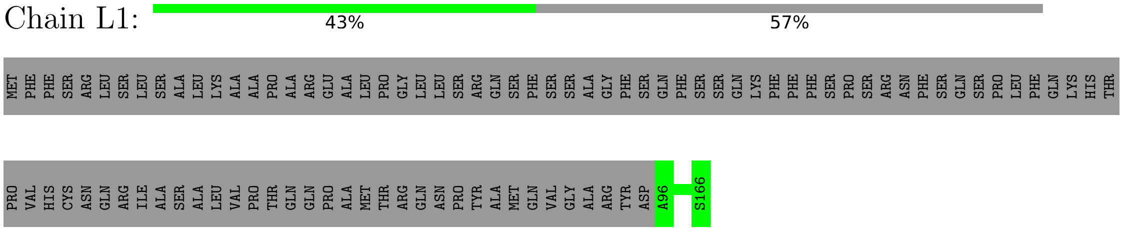
- Molecule 32: subunit c

Chain K1:



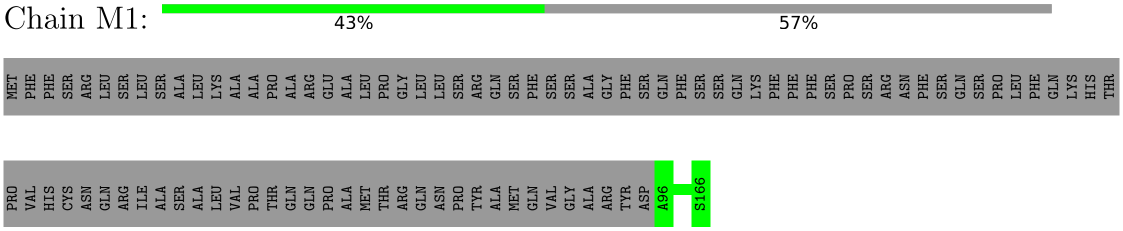
- Molecule 32: subunit c

Chain L1:



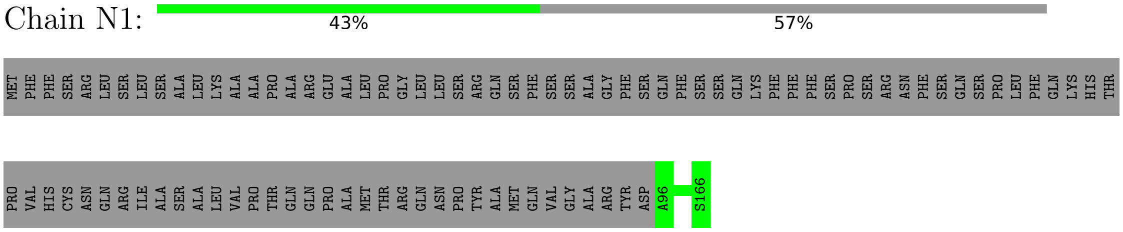
- Molecule 32: subunit c

Chain M1:



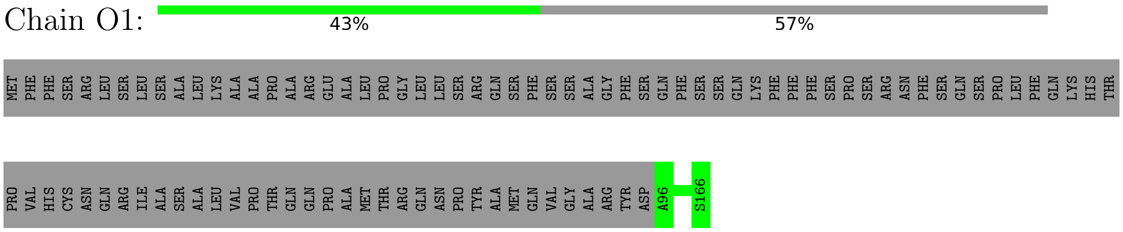
- Molecule 32: subunit c

Chain N1:



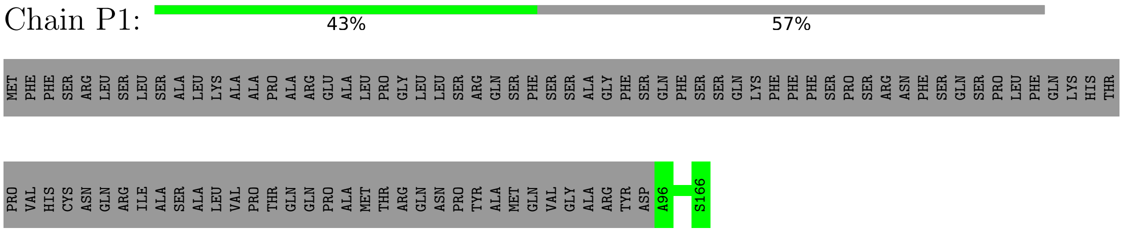
- Molecule 32: subunit c

Chain O1:



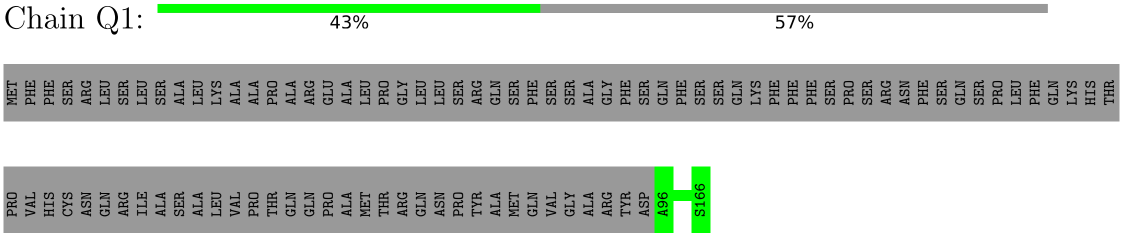
- Molecule 32: subunit c

Chain P1:



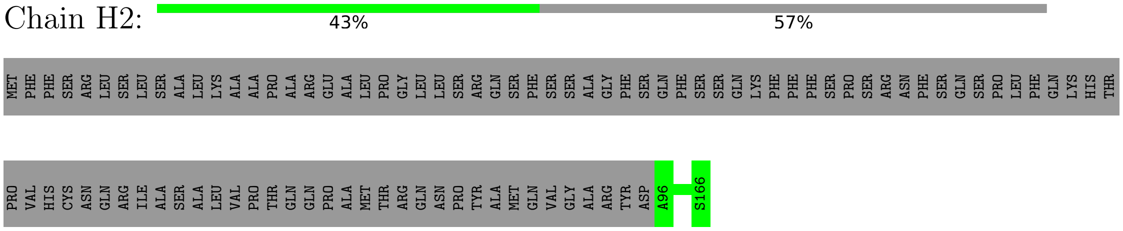
- Molecule 32: subunit c

Chain Q1:



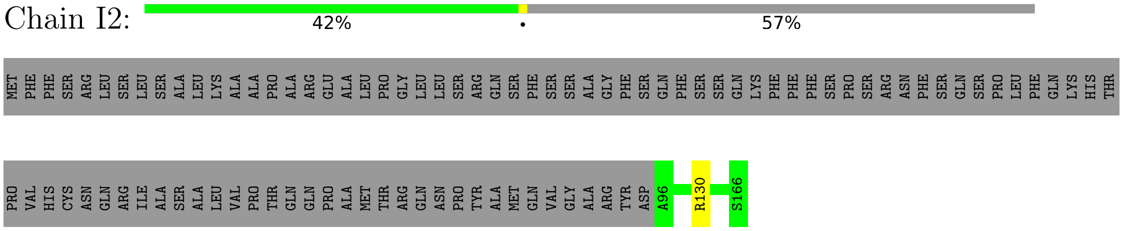
- Molecule 32: subunit c

Chain H2:



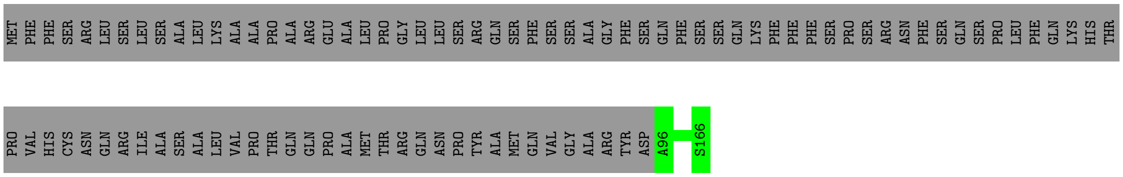
- Molecule 32: subunit c

Chain I2:



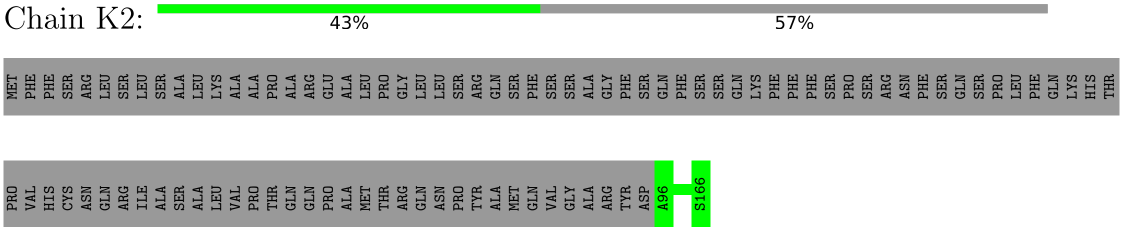
- Molecule 32: subunit c

Chain J2:



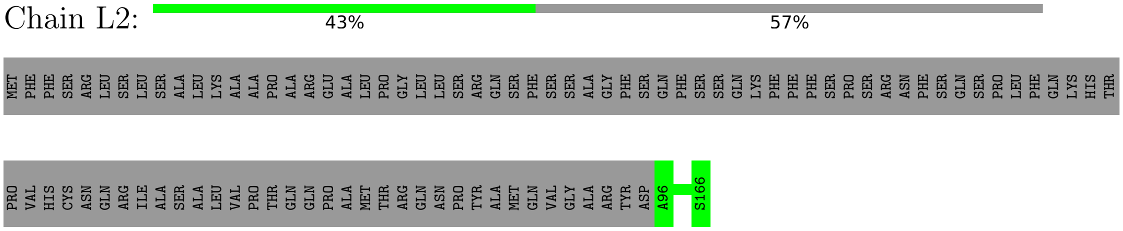
- Molecule 32: subunit c

Chain K2:



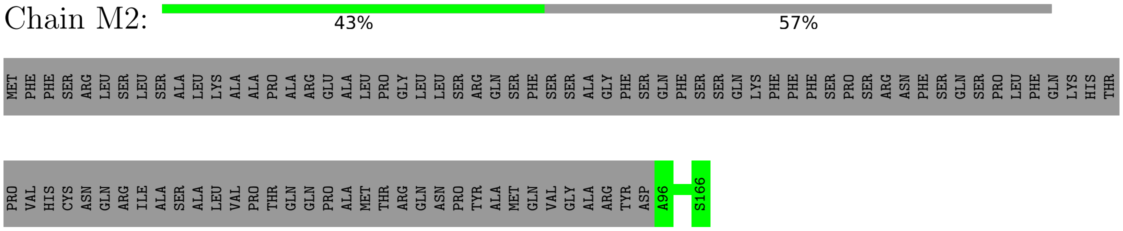
- Molecule 32: subunit c

Chain L2:



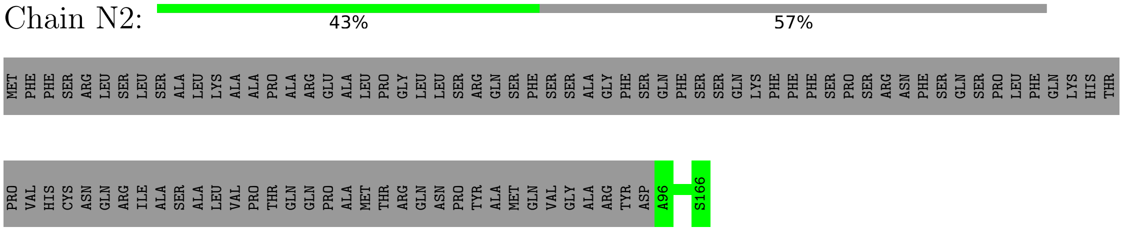
- Molecule 32: subunit c

Chain M2:



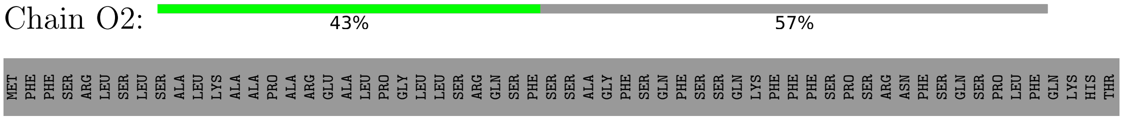
- Molecule 32: subunit c

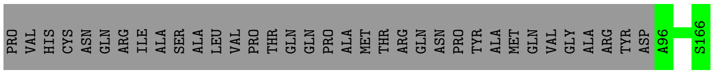
Chain N2:



- Molecule 32: subunit c

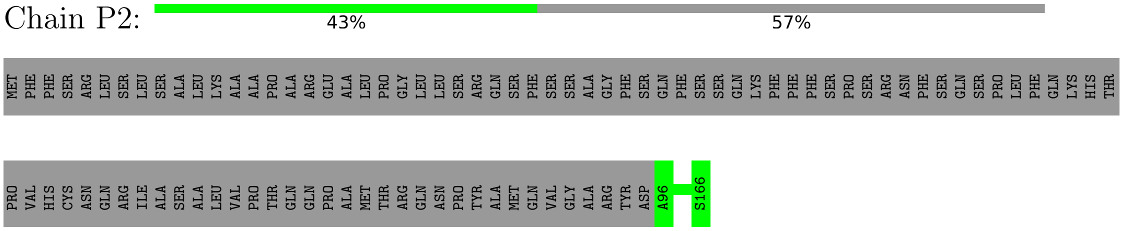
Chain O2:





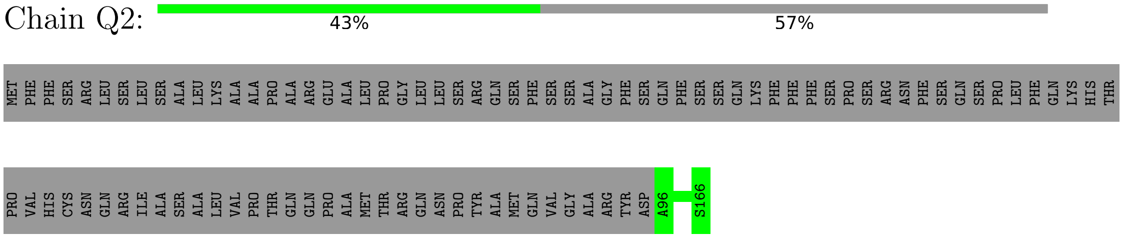
- Molecule 32: subunit c

Chain P2:



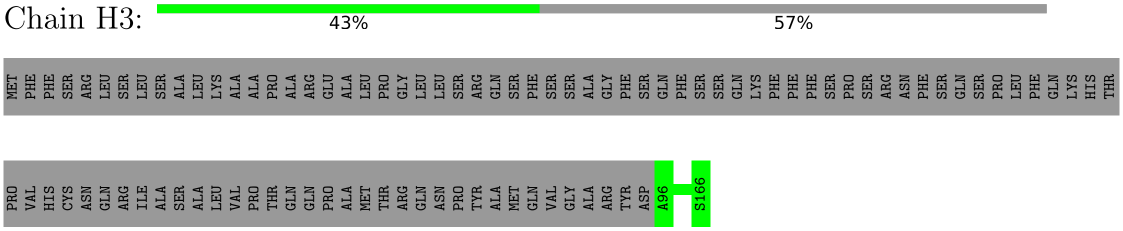
- Molecule 32: subunit c

Chain Q2:



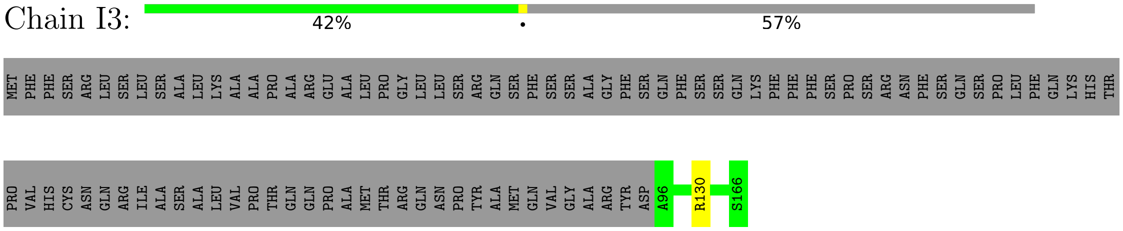
- Molecule 32: subunit c

Chain H3:



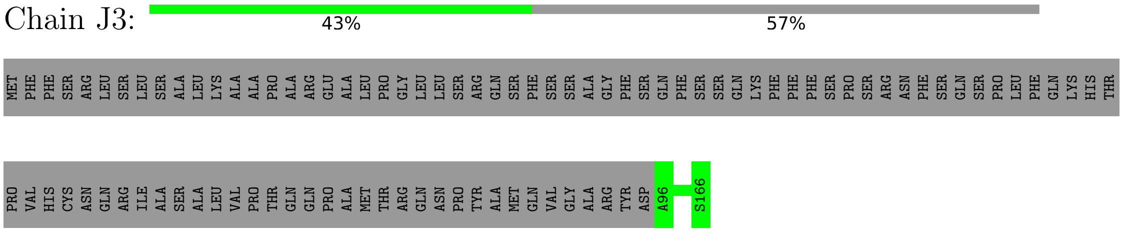
- Molecule 32: subunit c

Chain I3:



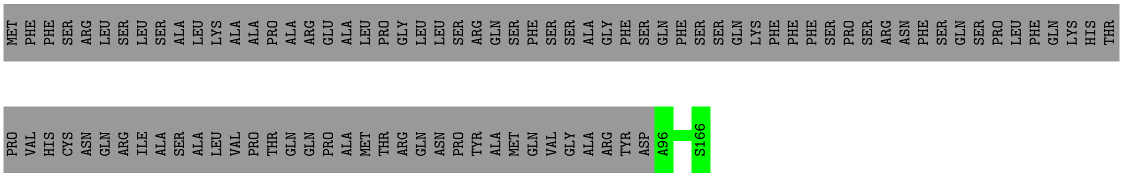
- Molecule 32: subunit c

Chain J3:



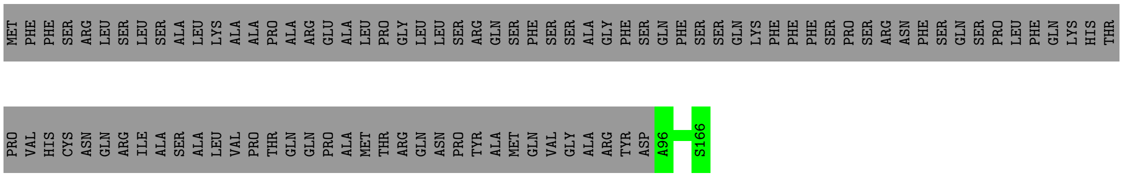
- Molecule 32: subunit c

Chain K3:



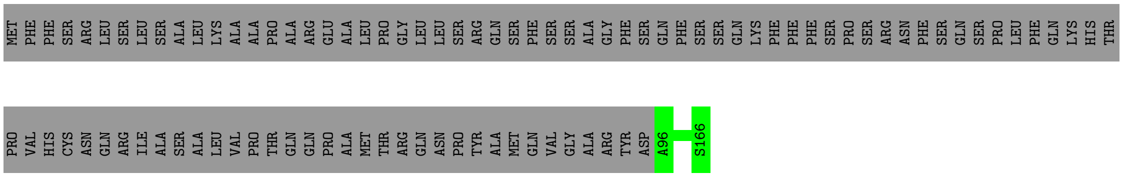
- Molecule 32: subunit c

Chain L3:



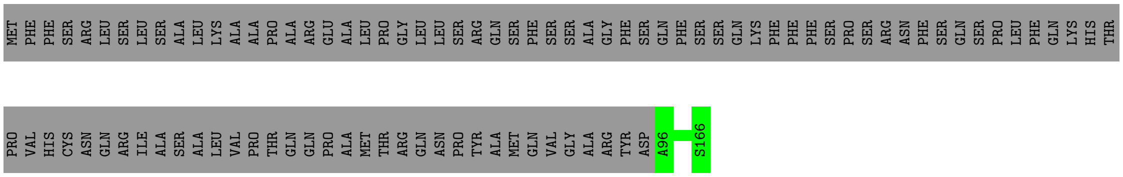
- Molecule 32: subunit c

Chain M3:



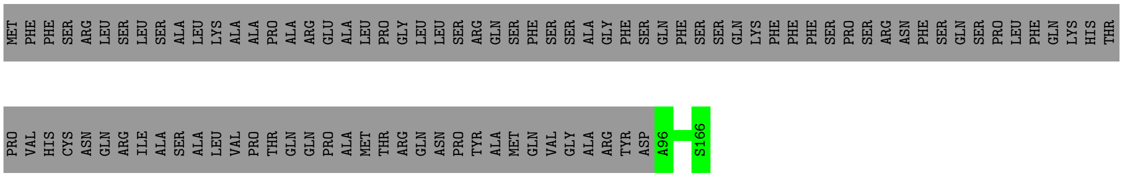
- Molecule 32: subunit c

Chain N3:



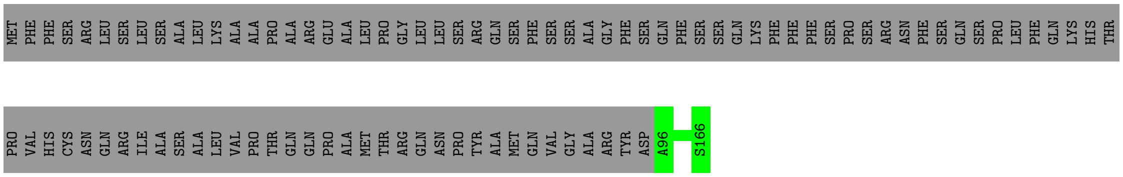
- Molecule 32: subunit c

Chain O3:



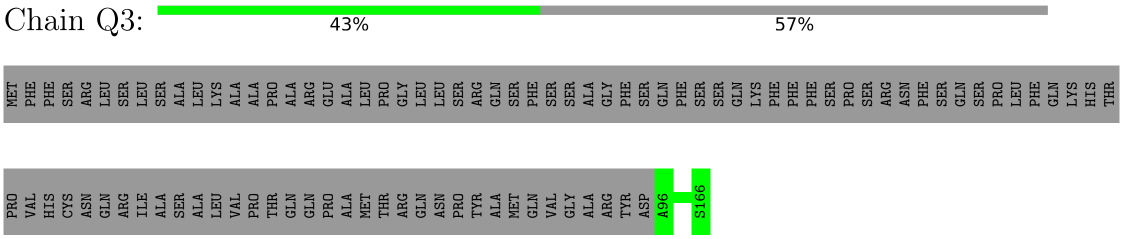
- Molecule 32: subunit c

Chain P3:



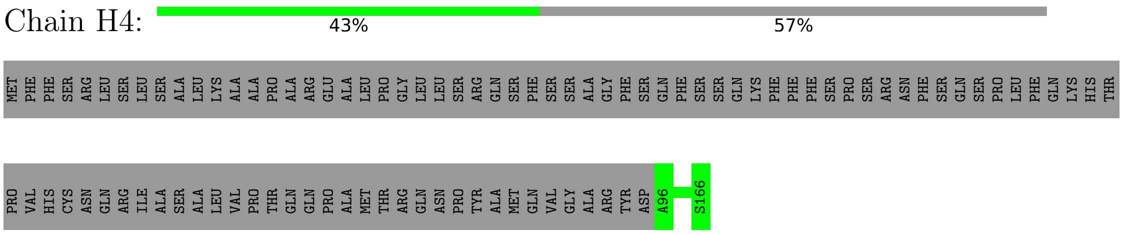
- Molecule 32: subunit c

Chain Q3:



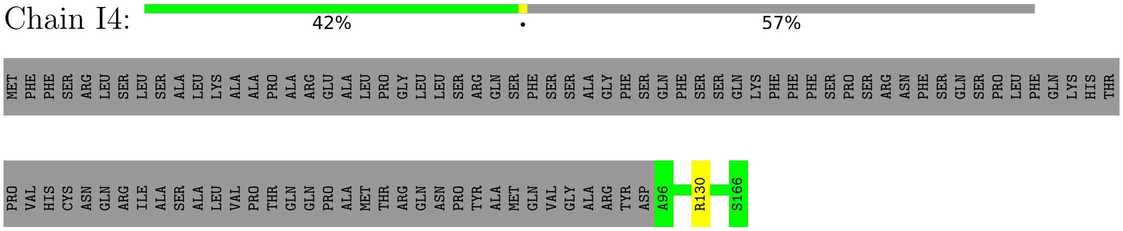
- Molecule 32: subunit c

Chain H4:



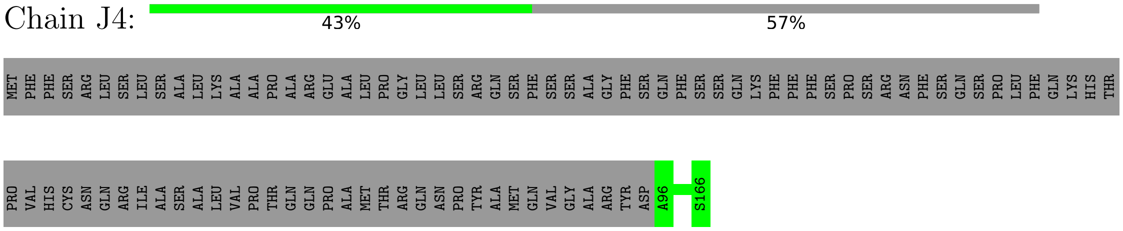
- Molecule 32: subunit c

Chain I4:



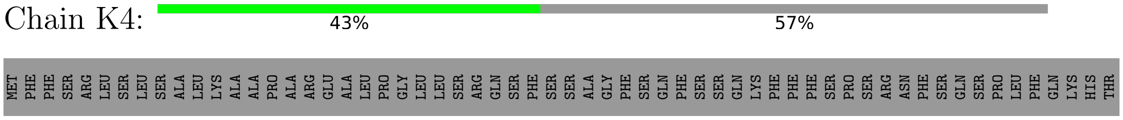
- Molecule 32: subunit c

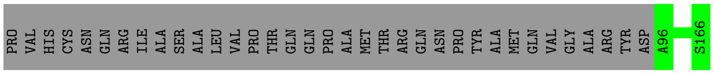
Chain J4:



- Molecule 32: subunit c

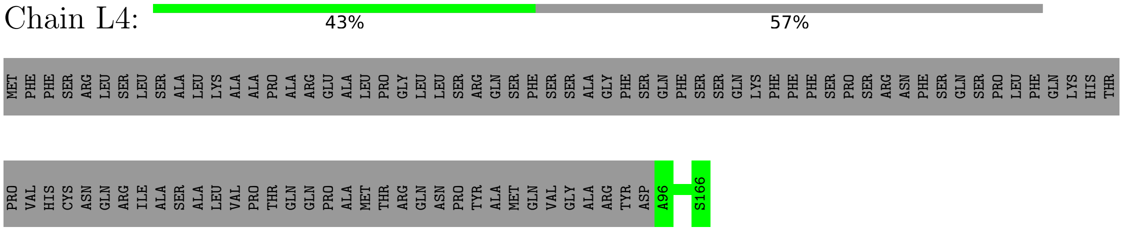
Chain K4:





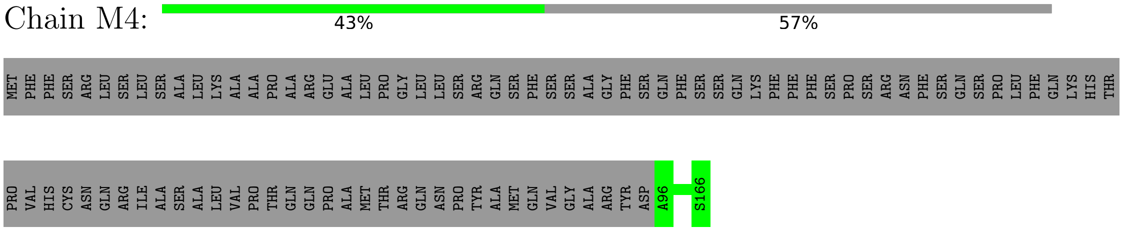
- Molecule 32: subunit c

Chain L4:



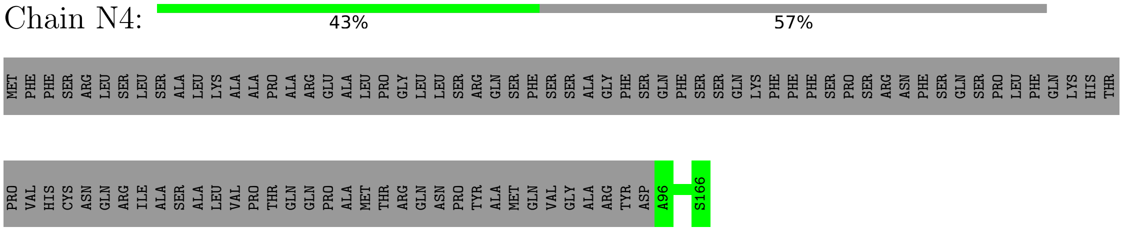
- Molecule 32: subunit c

Chain M4:



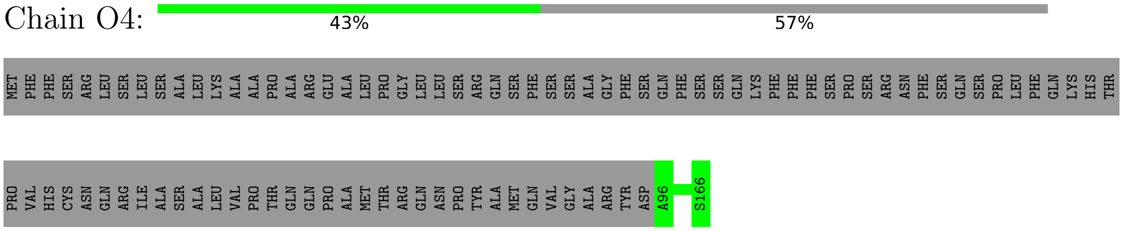
- Molecule 32: subunit c

Chain N4:



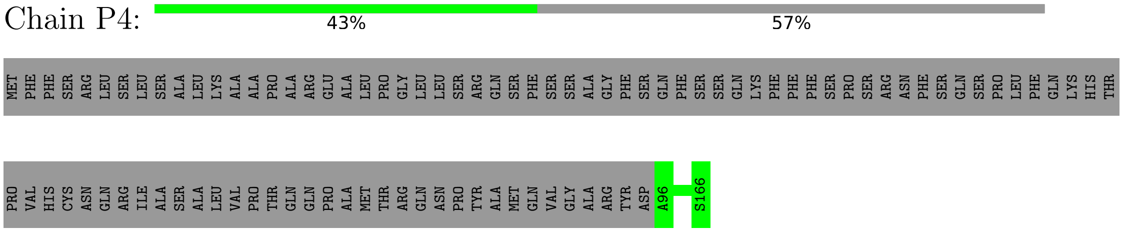
- Molecule 32: subunit c

Chain O4:



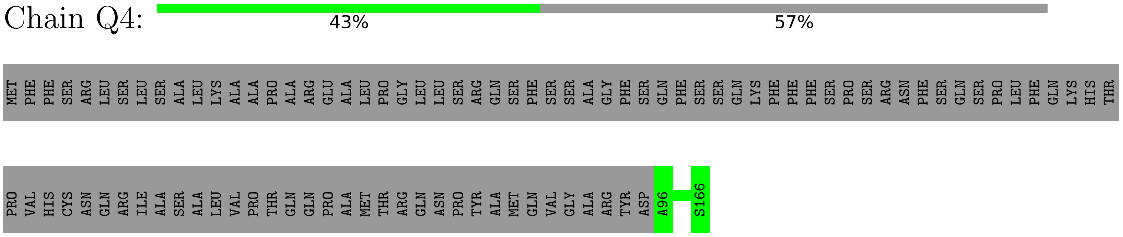
- Molecule 32: subunit c

Chain P4:



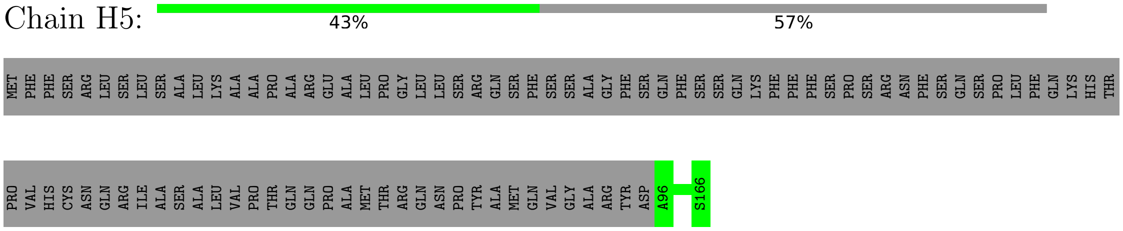
- Molecule 32: subunit c

Chain Q4:



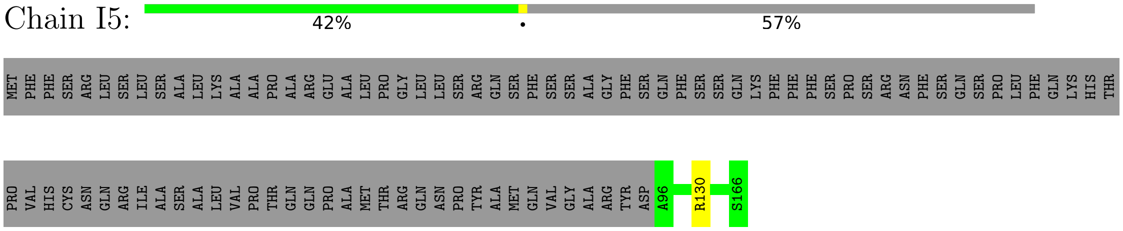
- Molecule 32: subunit c

Chain H5:



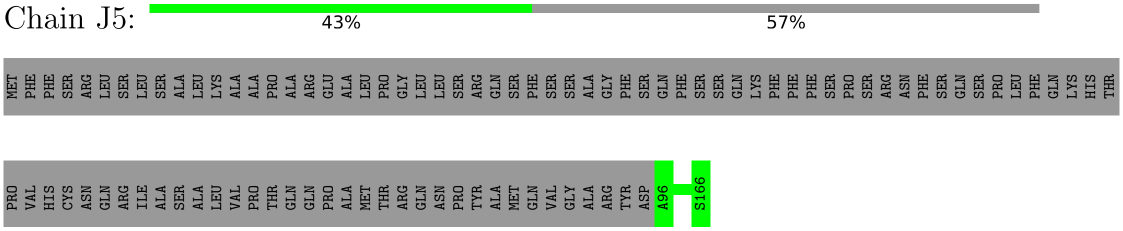
- Molecule 32: subunit c

Chain I5:



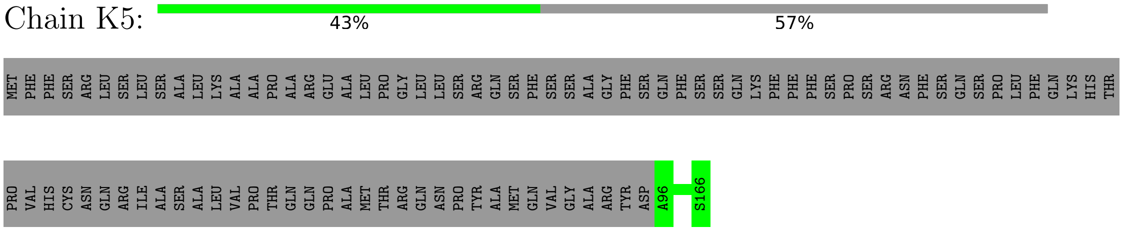
- Molecule 32: subunit c

Chain J5:



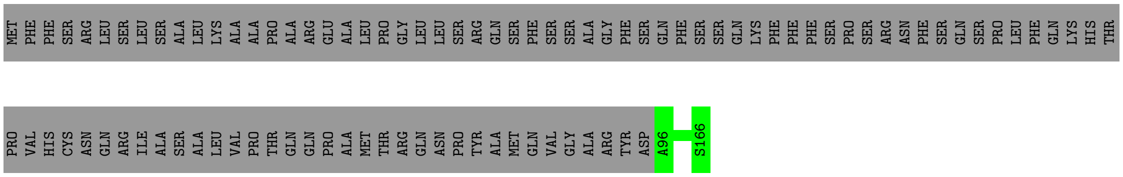
- Molecule 32: subunit c

Chain K5:



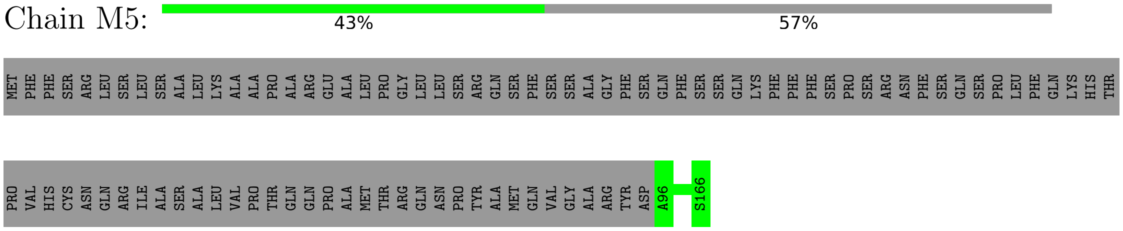
- Molecule 32: subunit c

Chain L5:



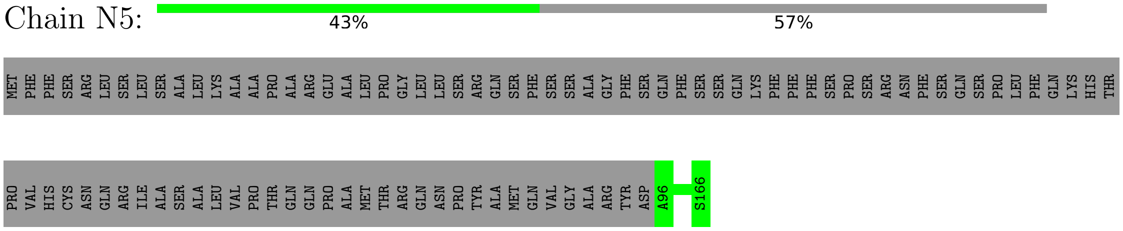
- Molecule 32: subunit c

Chain M5:



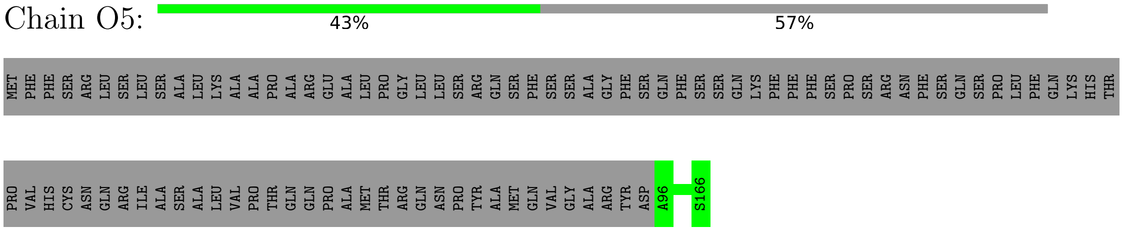
- Molecule 32: subunit c

Chain N5:



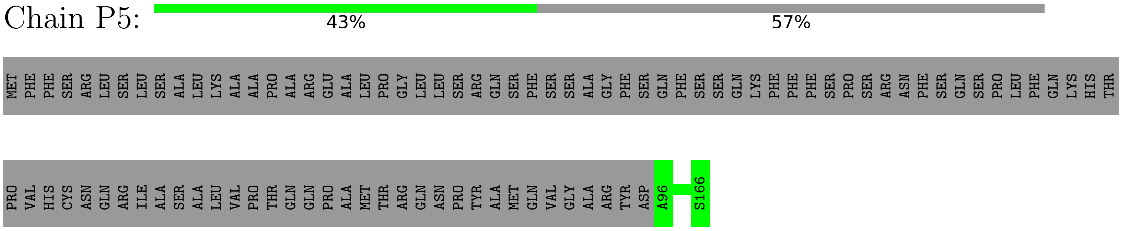
- Molecule 32: subunit c

Chain O5:



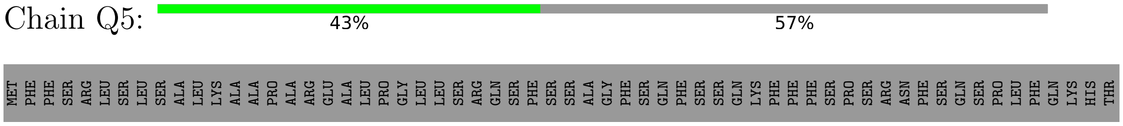
- Molecule 32: subunit c

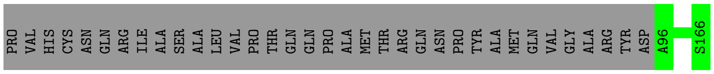
Chain P5:



- Molecule 32: subunit c

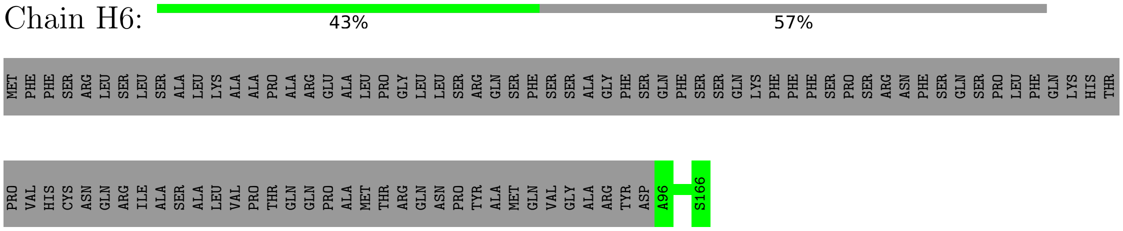
Chain Q5:





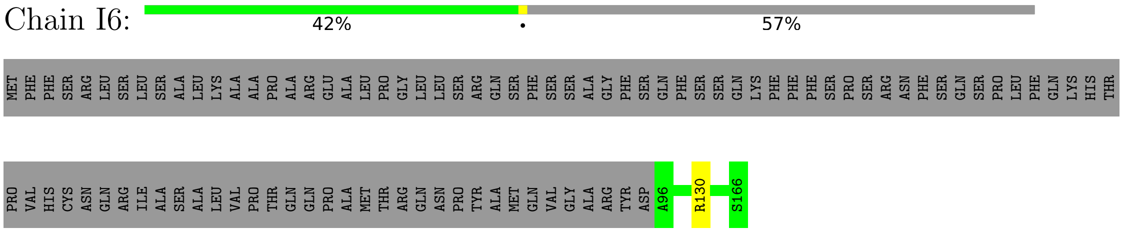
- Molecule 32: subunit c

Chain H6:



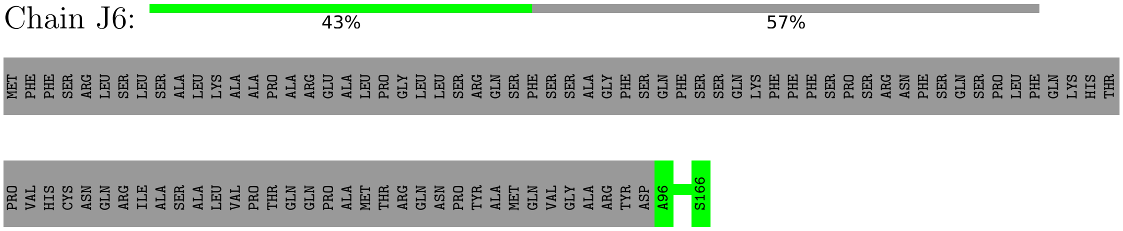
- Molecule 32: subunit c

Chain I6:



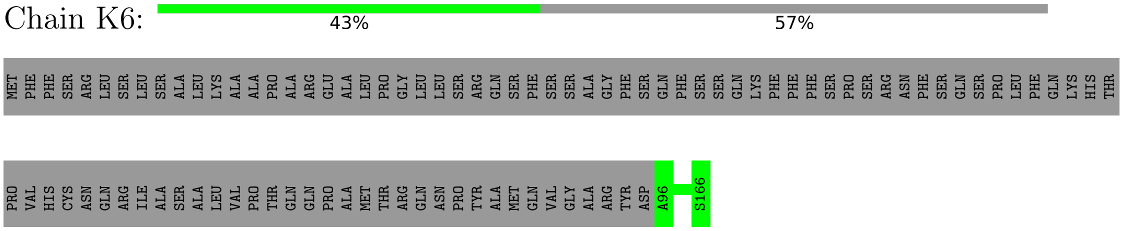
- Molecule 32: subunit c

Chain J6:



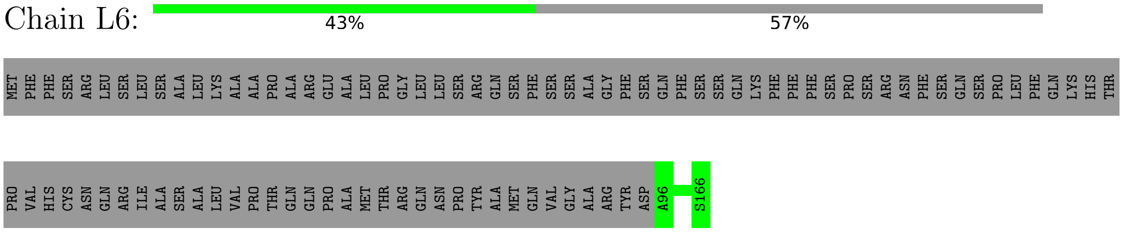
- Molecule 32: subunit c

Chain K6:



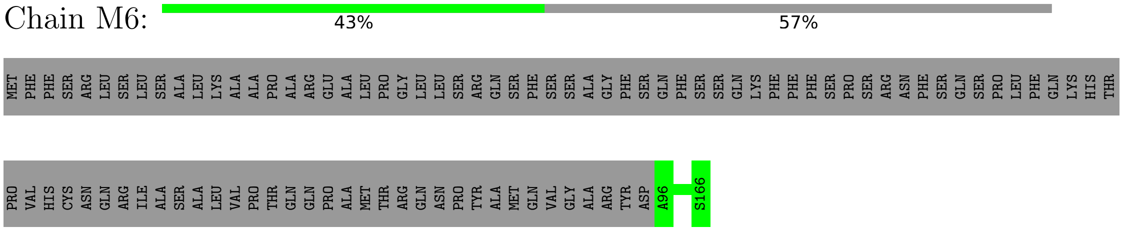
- Molecule 32: subunit c

Chain L6:



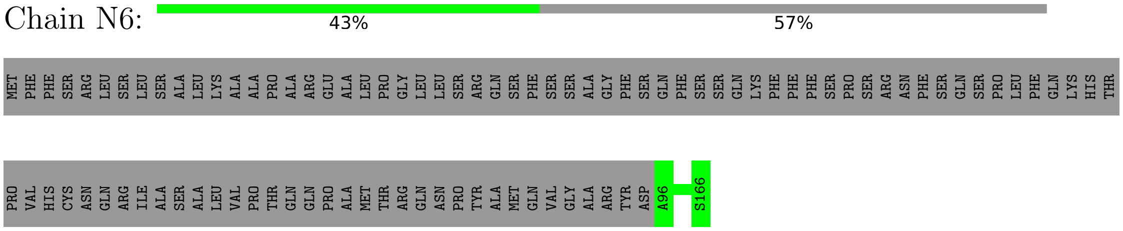
- Molecule 32: subunit c

Chain M6:



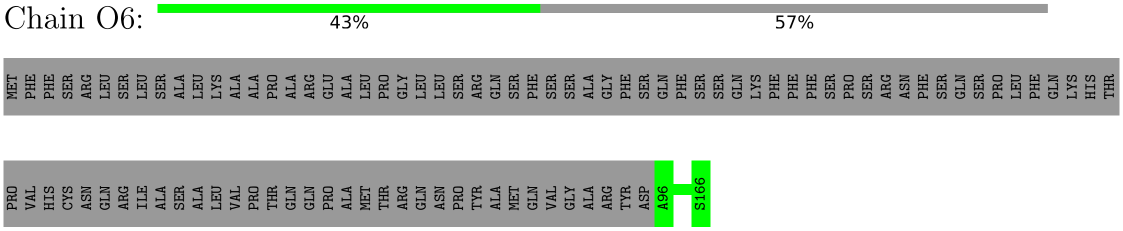
- Molecule 32: subunit c

Chain N6:



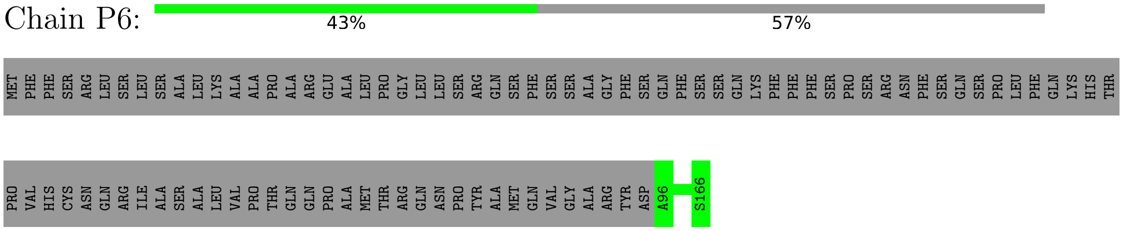
- Molecule 32: subunit c

Chain O6:



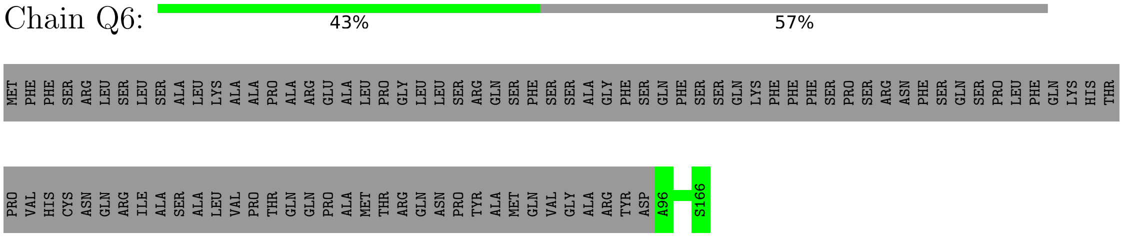
- Molecule 32: subunit c

Chain P6:



- Molecule 32: subunit c

Chain Q6:



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 ($e^-/\text{Å}^2$)	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.

The worst 5 of 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

There are no chirality outliers.

5 of 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
7	J7	89	PHE	Peptide
7	j7	89	PHE	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

5 of 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

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	I3	130	ARG
10	H9	117	ARG
28	B4	435	ARG
13	b9	509	ARG
21	N9	82	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
25	G4	201	GLN
28	D4	361	GLN
27	E6	527	ASN
28	B3	80	ASN
28	D3	361	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.