Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 07:48 am GMT

PDB ID	:	7A5I
EMDB ID	:	EMD-11644
Title	:	Structure of the human mitoribosome with A- P-and E-site mt-tRNAs
Authors	:	Desai, N.; Yang, H.; Chandrasekaran, V.; Kazi, R.; Minczuk, M.; Ramakrishnan, V.
Deposited on	:	2020-08-21
Resolution	:	3.70 Å(reported)

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

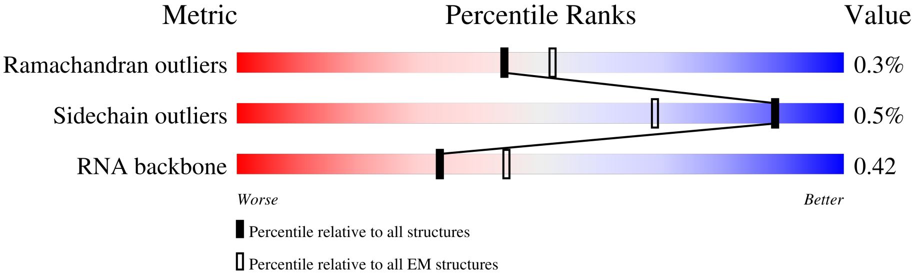
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

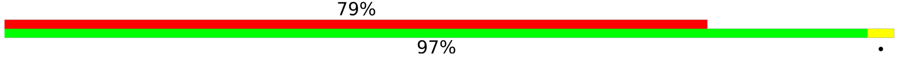
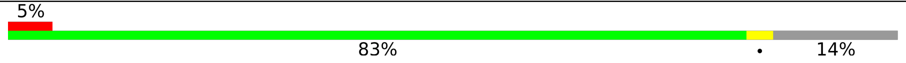
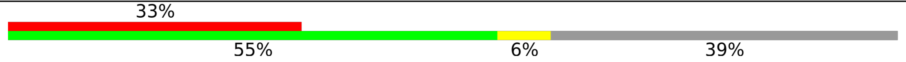
The reported resolution of this entry is 3.70 Å.

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.



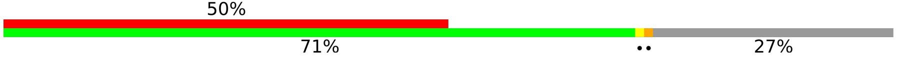
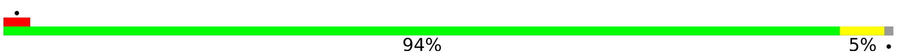
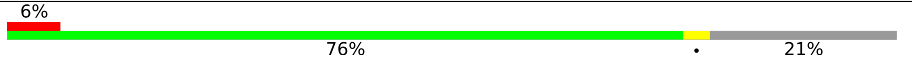
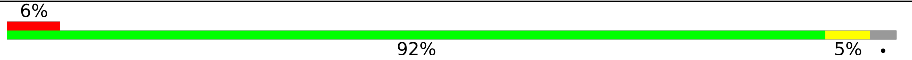
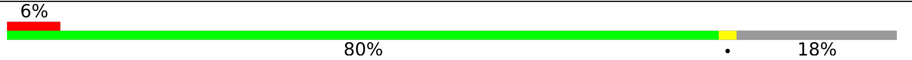
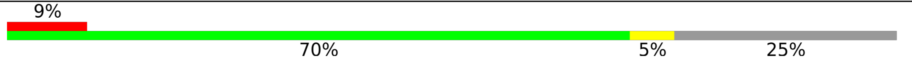
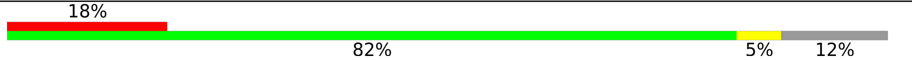
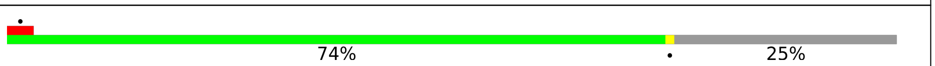
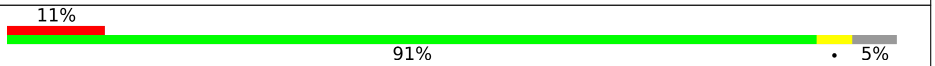
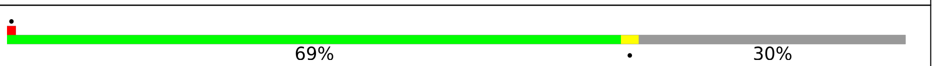
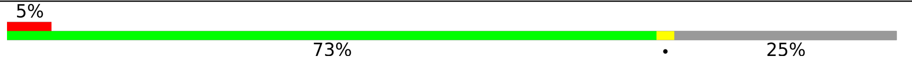
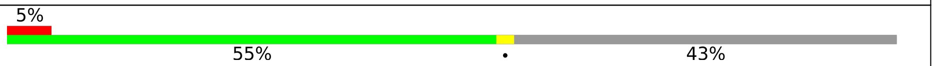
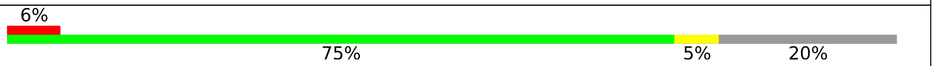
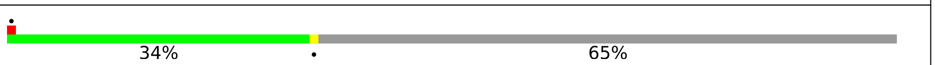
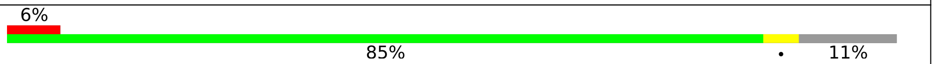
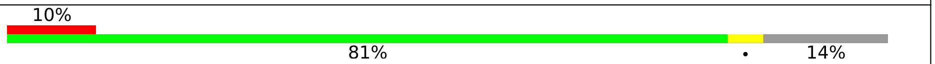
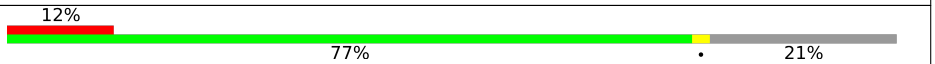
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Y2	29	
2	A3	1559	
3	B3	73	
4	D3	305	
5	E3	348	
6	F3	311	
7	H3	267	
8	I3	261	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	J3	192	 50% 71% •• 27%
10	K3	178	 • 94% 5% •
11	L3	145	 6% 76% • 21%
12	M3	296	 6% 92% 5% •
13	N3	251	 6% 80% • 18%
14	O3	175	 • 82% 5% 13%
15	P3	179	 • 74% • 26%
16	Q3	292	 9% 70% 5% 25%
17	R3	149	 6% 90% • 6%
18	S3	205	 • 74% • 24%
19	T3	212	 • 75% • 22%
20	U3	153	 • 71% • 27%
21	V3	216	 18% 82% 5% 12%
22	W3	148	 • 74% • 25%
23	X3	256	 11% 91% • 5%
24	Y3	250	 • 69% • 30%
25	Z3	161	 5% 73% • 25%
26	03	188	 5% 55% • 43%
27	13	65	 6% 75% 5% 20%
28	23	92	 49% • 50%
29	33	188	 • 49% • 49%
30	43	103	 • 34% • 65%
31	53	423	 6% 85% • 11%
32	63	380	 10% 81% • 14%
33	73	338	 12% 77% • 21%

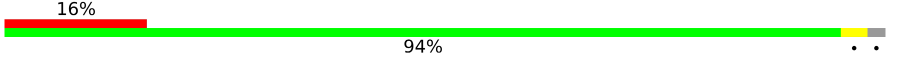
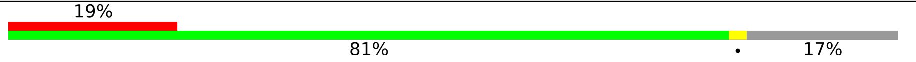
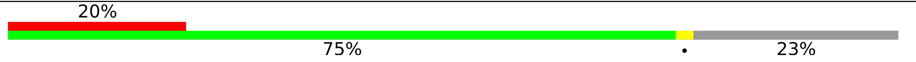
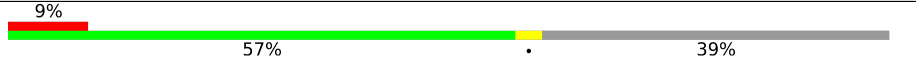
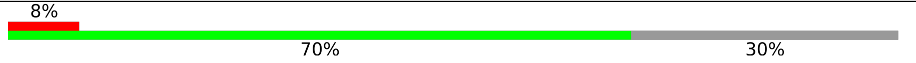
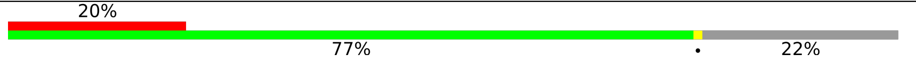
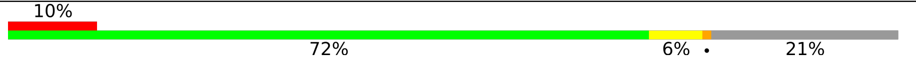
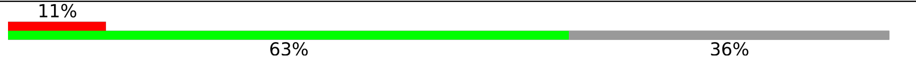
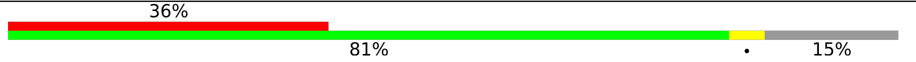
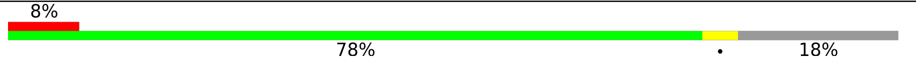
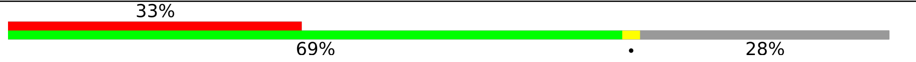
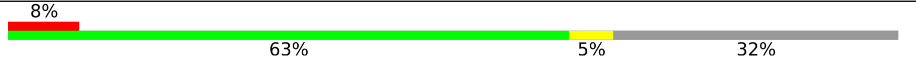
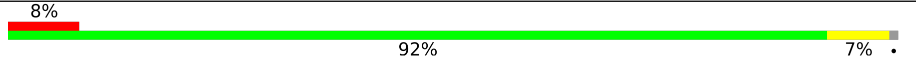
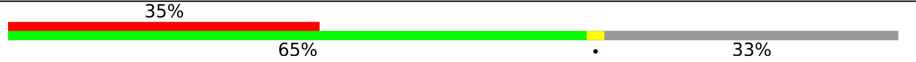
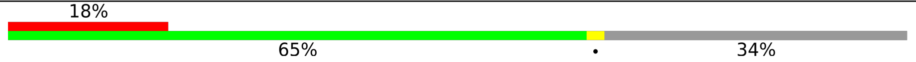
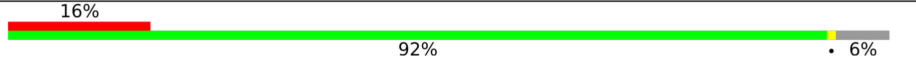
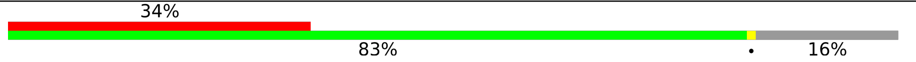
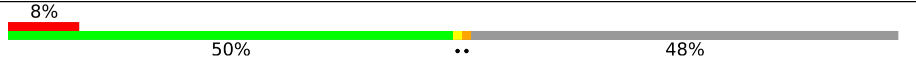
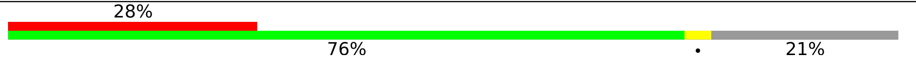
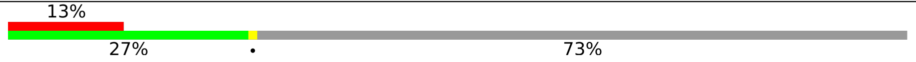
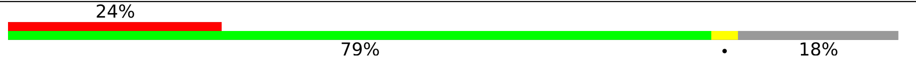
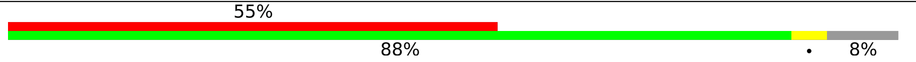
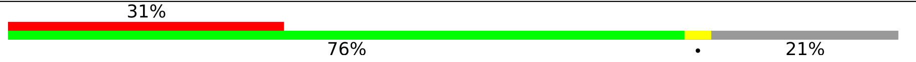
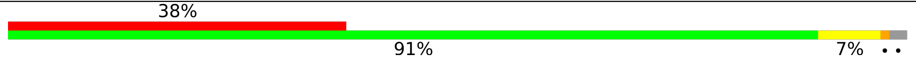
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	83	206	25% 46% • 52%
35	93	137	8% 77% • 20%
36	a3	142	5% 56% • 42%
37	b3	155	5% 92% • 5%
38	c3	332	8% 80% • 17%
39	d3	306	9% 51% • 47%
40	e3	279	53% 76% • 22%
41	f3	194	21% 66% • 32%
42	g3	166	• 77% • 22%
43	h3	158	14% 59% • • 37%
44	i3	128	• 72% • 24%
45	j3	123	6% 66% • 31%
46	k3	112	35% 72% • 25%
47	l3	138	• 16% • 83%
48	m3	128	7% 32% • 65%
49	o3	102	• 88% • 8%
50	p3	206	9% 60% • 38%
51	q3	222	11% 55% • 42%
52	r3	196	6% 73% • 26%
53	s3	439	7% 81% • 16%
54	A5	28	100% 100%
54	t3	28	86% 100%
55	B6	296	6% 70% • 27%
56	C6	167	10% 78% • 21%
57	D6	430	18% 72% • 25%

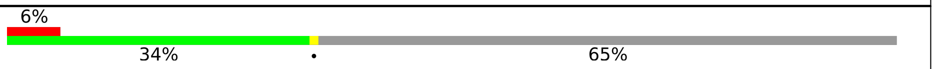
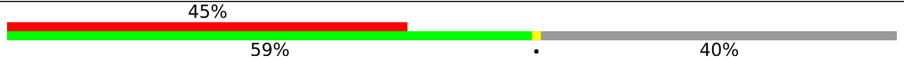
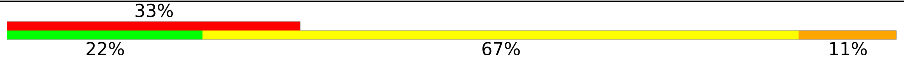
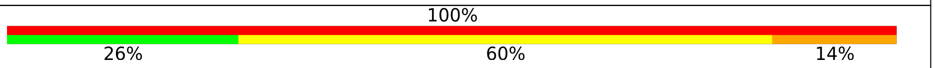
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
58	E6	125	
59	F6	242	
60	G6	396	
61	H6	201	
62	I6	194	
63	J6	138	
64	K6	128	
65	L6	257	
66	M6	137	
67	N6	130	
68	O6	258	
69	P6	142	
70	Q6	87	
71	R6	360	
72	S6	190	
73	T6	173	
74	U6	205	
75	V6	414	
76	W6	187	
77	X6	398	
78	Y6	395	
79	Z6	106	
80	a6	218	
81	b6	323	
82	c6	118	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
83	d6	199	
84	e6	689	
85	A6	954	
86	i4	9	
87	94	73	
87	99	73	
87	X	73	

2 Entry composition (i)

There are 91 unique types of molecules in this entry. The entry contains 163843 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	Y2	29	145	87	29	29	0	0

- Molecule 2 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	A3	1485	31529	14146	5687	10211	1485	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	3107	U	UNK	conflict	GB 1025814679

- Molecule 3 is a RNA chain called mt-tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	B3	56	1191	534	214	387	56	0	0

- Molecule 4 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D3	236	1842	1145	373	315	9	0	0

- Molecule 5 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E3	300	2365	1523	410	422	10	0	0

- Molecule 6 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F3	250	2013	1294	365	348	6	0	0

- Molecule 7 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	H3	95	784	498	152	134	0	0

- Molecule 8 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I3	158	1283	828	235	210	10	0	0

- Molecule 9 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J3	140	1061	680	192	187	2	0	0

- Molecule 10 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K3	177	1451	934	259	251	7	0	0

- Molecule 11 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L3	115	889	559	171	154	5	0	0

- Molecule 12 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M3	287	2305	1472	425	402	6	0	0

- Molecule 13 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N3	205	1654	1056	308	280	10	0	0

- Molecule 14 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O3	152	1245	784	239	215	7	0	0

- Molecule 15 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P3	133	1080	677	209	189	5	0	0

- Molecule 16 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q3	219	1822	1168	322	323	9	0	0

- Molecule 17 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R3	140	1153	732	231	186	4	0	0

- Molecule 18 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	S3	156	1251	806	222	219	4	0	0

- Molecule 19 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T3	166	1368	875	254	232	7	0	0

- Molecule 20 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U3	111	Total	C	N	O	S	0	0
			922	591	176	153	2		

- Molecule 21 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V3	189	Total	C	N	O	S	0	0
			1551	987	278	278	8		

- Molecule 22 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W3	111	Total	C	N	O	S	0	0
			871	558	164	146	3		

- Molecule 23 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X3	243	Total	C	N	O	S	0	0
			2027	1310	350	362	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X3	148	ALA	THR	conflict	UNP Q13084
X3	149	SER	PRO	conflict	UNP Q13084
X3	150	GLY	LYS	conflict	UNP Q13084

- Molecule 24 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y3	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 25 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z3	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 26 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	03	108	880	545	172	157	6	0	0

- Molecule 27 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	13	52	433	278	83	70	2	0	0

- Molecule 28 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	23	46	376	233	83	59	1	0	0

- Molecule 29 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	33	95	831	539	162	127	3	0	0

- Molecule 30 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	43	36	322	203	70	46	3	0	0

- Molecule 31 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	53	376	3064	1987	529	538	10	0	0

- Molecule 32 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	63	325	2636	1692	465	470	9	0	0

- Molecule 33 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	73	266	2158	1383	371	388	16	0	0

- Molecule 34 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	83	99	836	535	144	155	2	0	0

- Molecule 35 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	93	109	873	565	152	154	2	0	0

- Molecule 36 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	a3	82	686	434	124	123	5	0	0

- Molecule 37 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	b3	148	1178	733	229	213	3	0	0

- Molecule 38 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	c3	275	2217	1415	383	410	9	0	0

- Molecule 39 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	d3	162	1347	870	234	235	8	0	0

- Molecule 40 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	e3	217	Total 1762	C 1124	N 310	O 323	S 5	0	0

- Molecule 41 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	f3	131	Total 1039	C 663	N 169	O 203	S 4	0	0

- Molecule 42 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	g3	129	Total 1067	C 690	N 185	O 190	S 2	0	0

- Molecule 43 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h3	100	Total 827	C 524	N 146	O 155	S 2	0	0

- Molecule 44 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	i3	97	Total 827	C 532	N 165	O 126	S 4	0	0

- Molecule 45 is a protein called cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	j3	85	Total 684	C 423	N 133	O 126	S 2	0	0

- Molecule 46 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	k3	84	Total 655	C 407	N 122	O 121	S 5	0	0

- Molecule 47 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	l3	23	Total 221	C 137	N 52	O 32	0	0

- Molecule 48 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	m3	45	Total 372	C 232	N 76	O 62	S 2	0	0

- Molecule 49 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	o3	94	Total 797	C 501	N 165	O 128	S 3	0	0

- Molecule 50 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	p3	127	Total 1058	C 661	N 201	O 192	S 4	0	0

- Molecule 51 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	q3	128	Total 1076	C 671	N 208	O 192	S 5	0	0

- Molecule 52 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	r3	146	Total 1203	C 764	N 232	O 199	S 8	0	0

- Molecule 53 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s3	370	Total 3036	C 1946	N 542	O 534	S 14	0	0

- Molecule 54 is a protein called Unknown protein/protein extension.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	t3	28	Total	C	N	O	0	0
			140	84	28	28		
54	A5	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 55 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B6	217	Total	C	N	O	S	0	0
			1768	1131	321	306	10		

- Molecule 56 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	C6	132	Total	C	N	O	S	0	0
			1082	699	195	184	4		

- Molecule 57 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	D6	322	Total	C	N	O	S	0	0
			2557	1611	476	457	13		

- Molecule 58 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	E6	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 59 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	F6	201	Total	C	N	O	S	0	0
			1668	1069	305	283	11		

- Molecule 60 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	G6	305	Total	C	N	O	S	0	0
			2516	1599	448	455	14		

- Molecule 61 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	H6	122	Total 999	C 643	N 168	O 185	S 3	0	0

- Molecule 62 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	I6	136	Total 1011	C 637	N 192	O 178	S 4	0	0

- Molecule 63 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	J6	108	Total 838	C 521	N 169	O 142	S 6	0	0

- Molecule 64 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	K6	101	Total 861	C 537	N 179	O 140	S 5	0	0

- Molecule 65 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	L6	164	Total 1382	C 883	N 257	O 235	S 7	0	0

- Molecule 66 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	M6	116	Total 920	C 582	N 182	O 150	S 6	0	0

- Molecule 67 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	N6	107	Total 846	C 549	N 153	O 141	S 3	0	0

- Molecule 68 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	O6	185	Total 1528	C 970	N 285	O 267	S 6	0	0

- Molecule 69 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	P6	96	Total 774	C 498	N 133	O 135	S 8	0	0

- Molecule 70 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Q6	86	Total 740	C 458	N 150	O 124	S 8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q6	50	ARG	CYS	conflict	UNP P82921

- Molecule 71 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	R6	242	Total 2008	C 1285	N 343	O 372	S 8	0	0

- Molecule 72 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	S6	126	Total 1042	C 673	N 183	O 185	S 1	0	0

- Molecule 73 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	T6	162	Total 1330	C 850	N 231	O 238	S 11	0	0

- Molecule 74 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	U6	173	Total 1461	C 900	N 294	O 263	S 4	0	0

- Molecule 75 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	V6	328	Total 2702	C 1737	N 452	O 502	S 11	0	0

- Molecule 76 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	W6	97	Total 766	C 486	N 137	O 139	S 4	0	0

- Molecule 77 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	X6	316	Total 2531	C 1625	N 440	O 455	S 11	0	0

- Molecule 78 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Y6	108	Total 914	C 593	N 150	O 169	S 2	0	0

- Molecule 79 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Z6	87	Total 740	C 473	N 133	O 130	S 4	0	0

- Molecule 80 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	a6	201	Total 1684	C 1065	N 322	O 292	S 5	0	0

- Molecule 81 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	b6	256	Total 2076	C 1321	N 350	O 395	S 10	0	0

- Molecule 82 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	c6	116	Total 925	C 574	N 181	O 162	S 8	0	0

- Molecule 83 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	d6	69	Total 610	C 393	N 130	O 86	S 1	0	0

- Molecule 84 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	e6	414	Total 2838	C 1805	N 490	O 529	S 14	0	0

- Molecule 85 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	A6	928	Total 19716	C 8840	N 3560	O 6388	P 928	0	0

- Molecule 86 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	i4	9	Total 196	C 88	N 39	O 60	P 9	0	0

- Molecule 87 is a RNA chain called mt-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	99	73	Total 1547	C 696	N 280	O 499	P 72	0	0
87	94	73	Total 1547	C 696	N 280	O 499	P 72	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
87	X	73	1547	696	280	499	72	0	0

- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
88	A3	96	96	96	0
88	D3	1	1	1	0
88	g3	1	1	1	0
88	o3	1	1	1	0
88	G6	1	1	1	0
88	A6	27	27	27	0

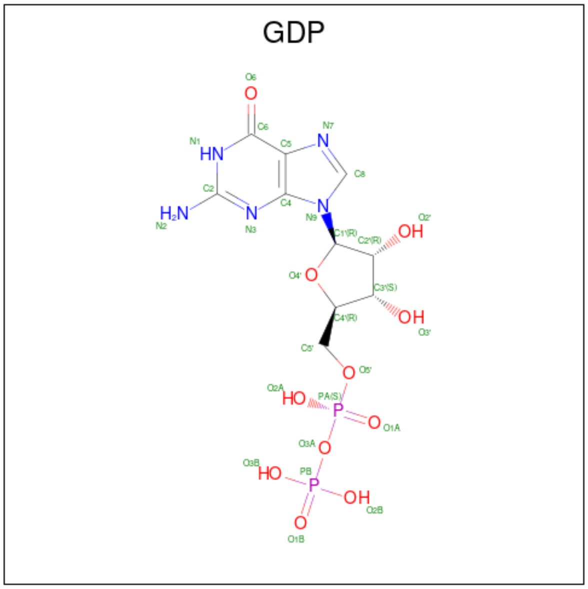
- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
89	03	1	1	1	0
89	43	1	1	1	0
89	r3	1	1	1	0
89	B6	1	1	1	0
89	O6	1	1	1	0
89	P6	1	1	1	0
89	T6	1	1	1	0

- Molecule 90 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
90	A5	1	1	1	0

- Molecule 91 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

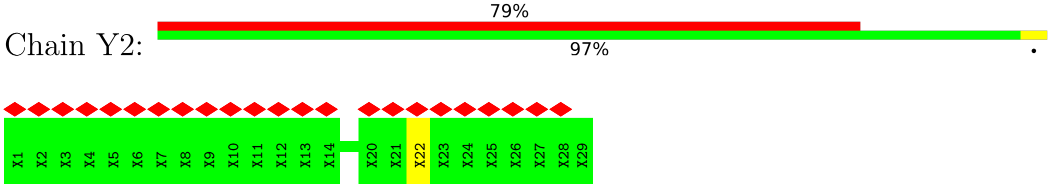


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
91	X6	1	28	10	5	11	2	0

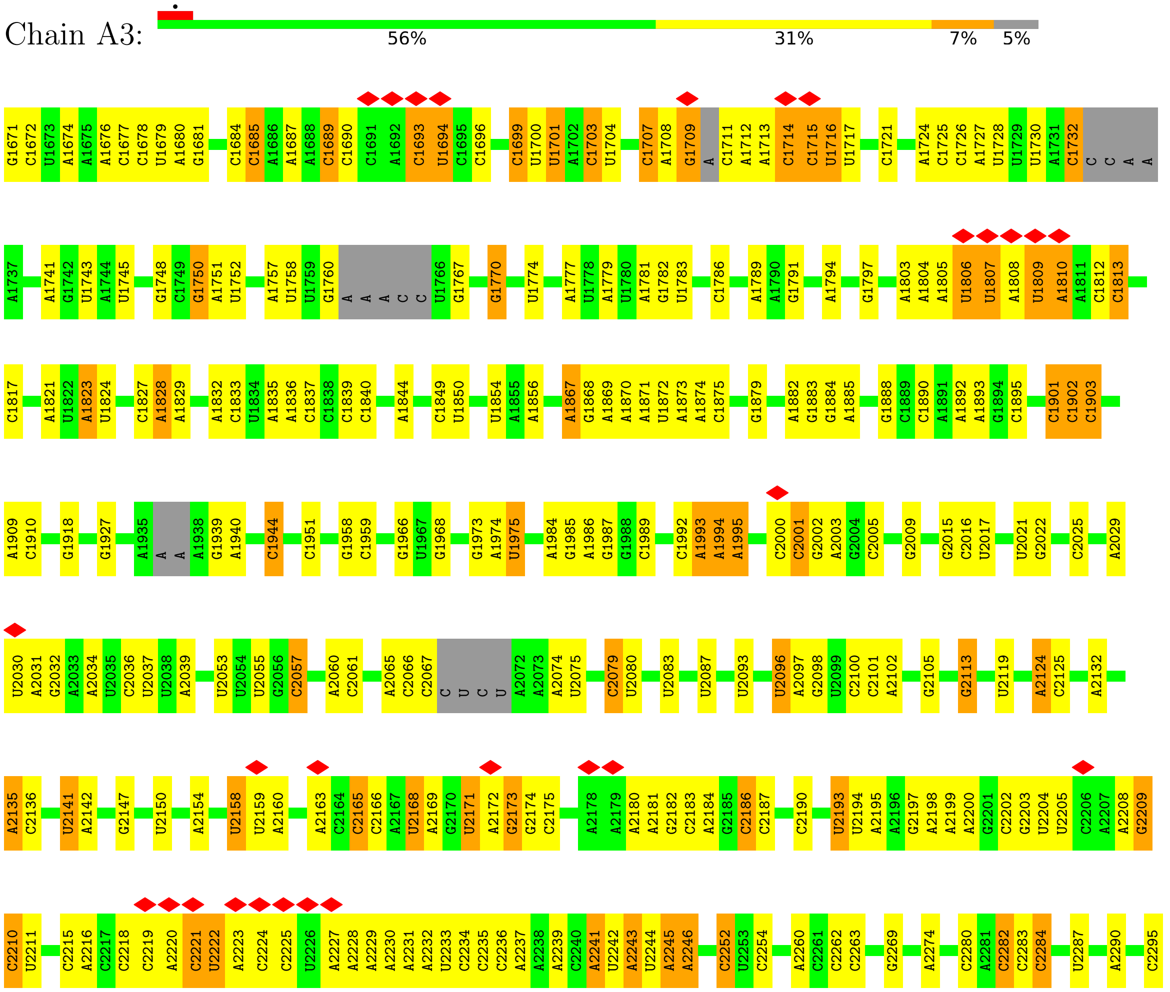
3 Residue-property plots

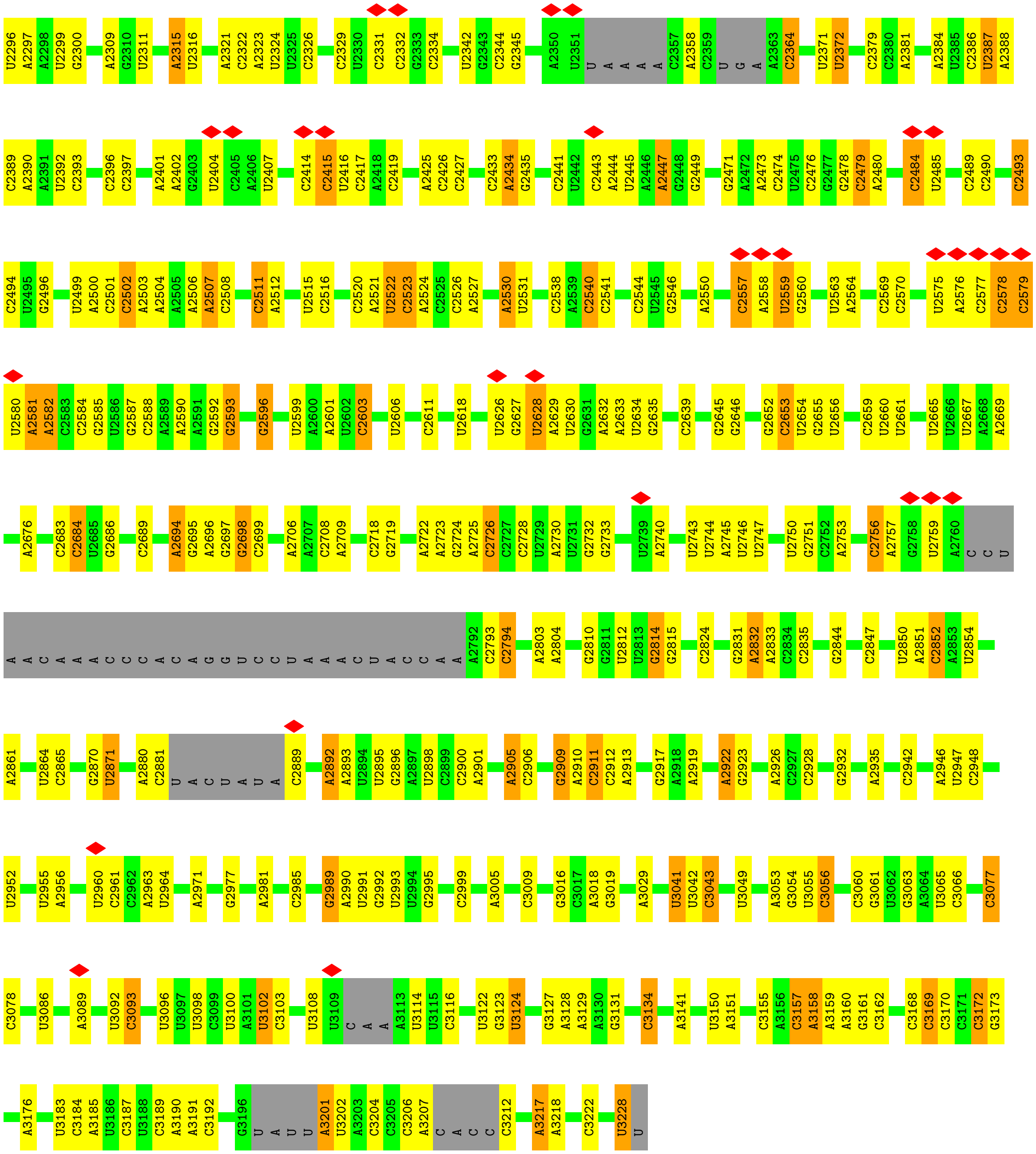
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: nascent chain



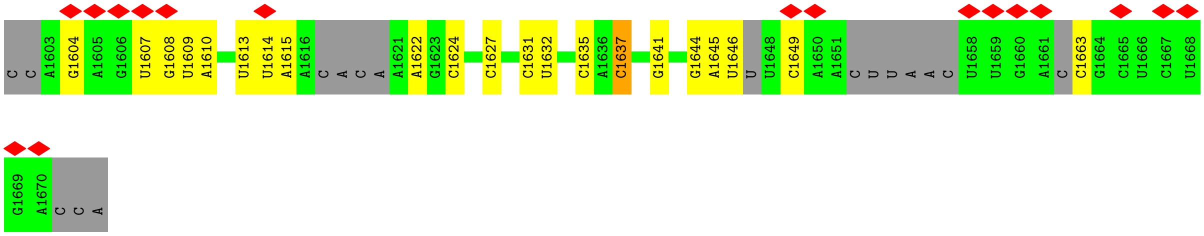
- Molecule 2: 16S rRNA



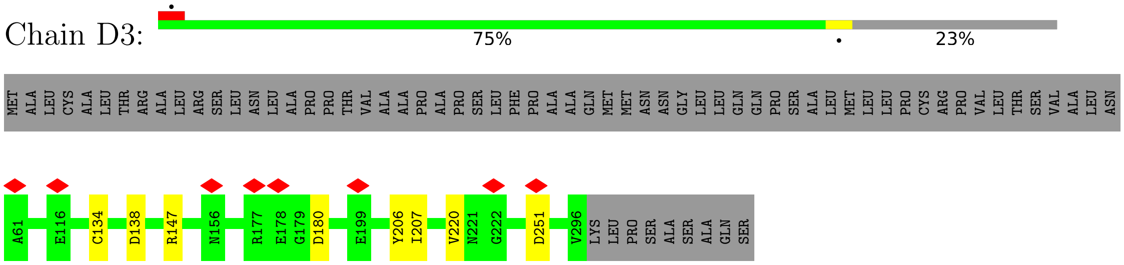


- Molecule 3: mt-tRNAVal

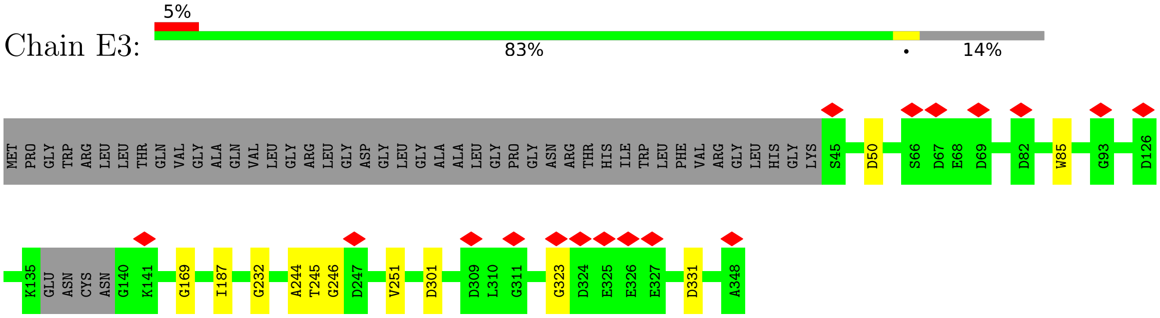
Chain B3:



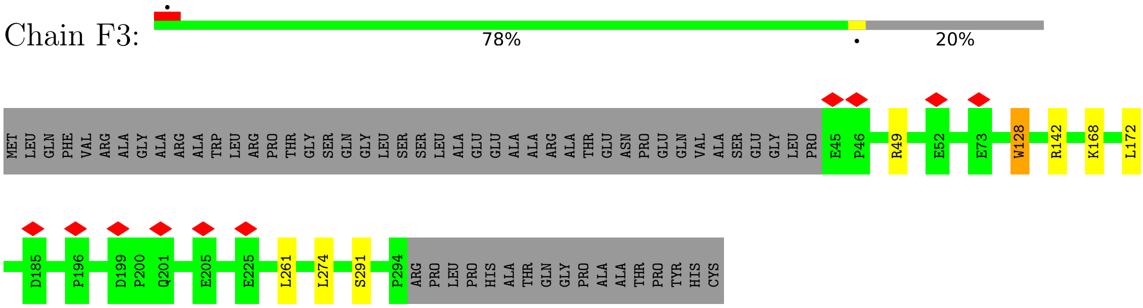
- Molecule 4: 39S ribosomal protein L2, mitochondrial



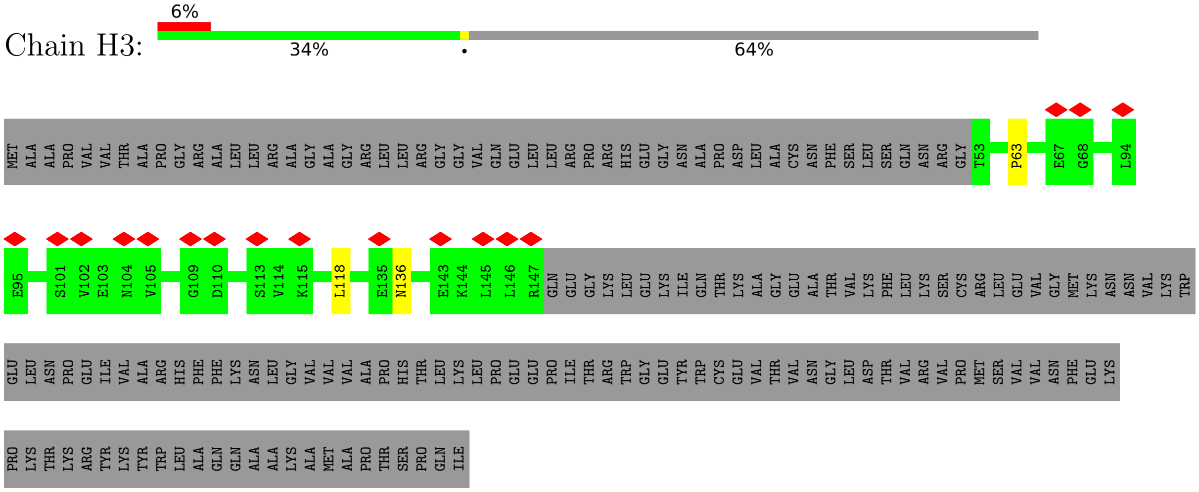
- Molecule 5: 39S ribosomal protein L3, mitochondrial



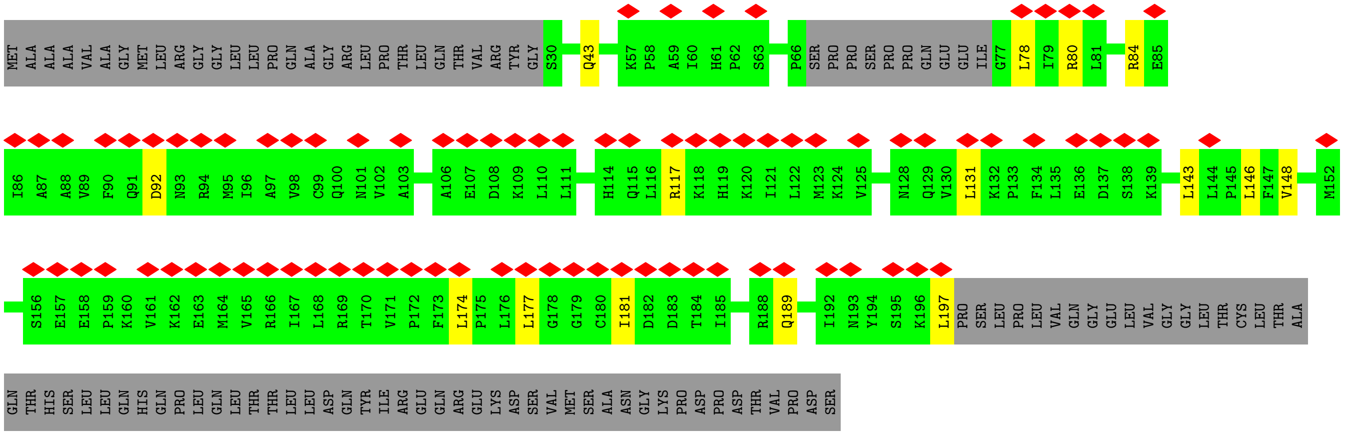
- Molecule 6: 39S ribosomal protein L4, mitochondrial



- Molecule 7: 39S ribosomal protein L9, mitochondrial

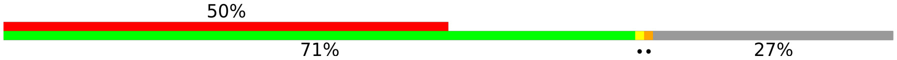


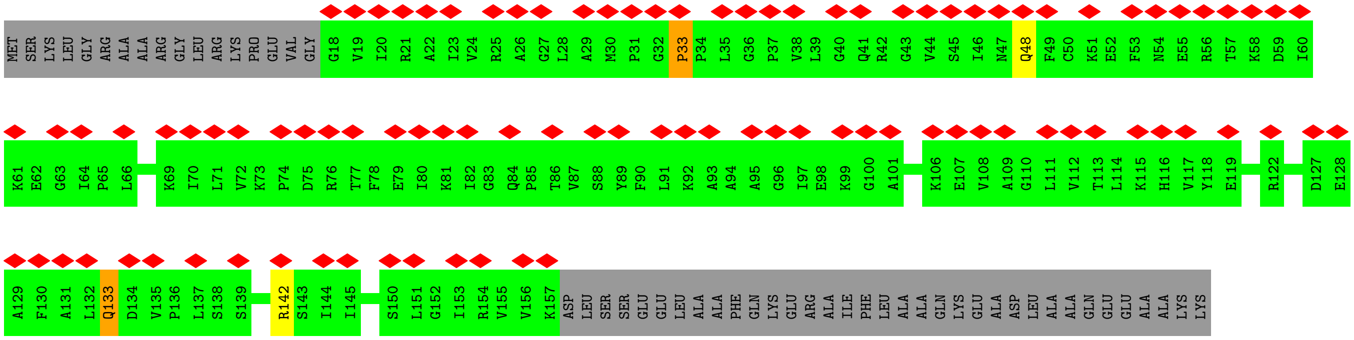
- Molecule 8: 39S ribosomal protein L10, mitochondrial



- Molecule 9: 39S ribosomal protein L11, mitochondrial

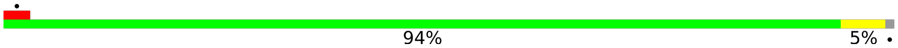
Chain J3:

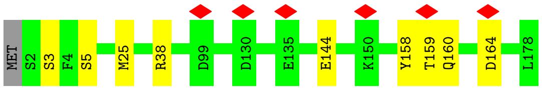




- Molecule 10: 39S ribosomal protein L13, mitochondrial

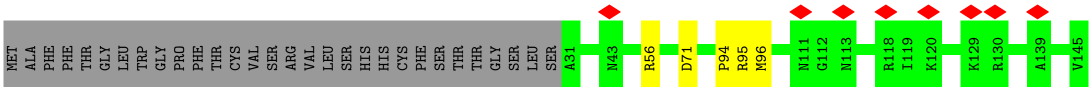
Chain K3:





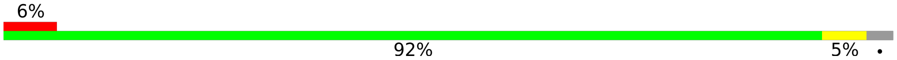
- Molecule 11: 39S ribosomal protein L14, mitochondrial

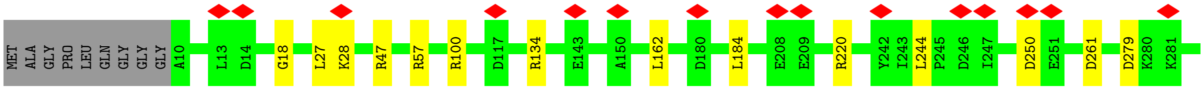
Chain L3:

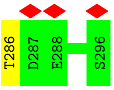


- Molecule 12: 39S ribosomal protein L15, mitochondrial

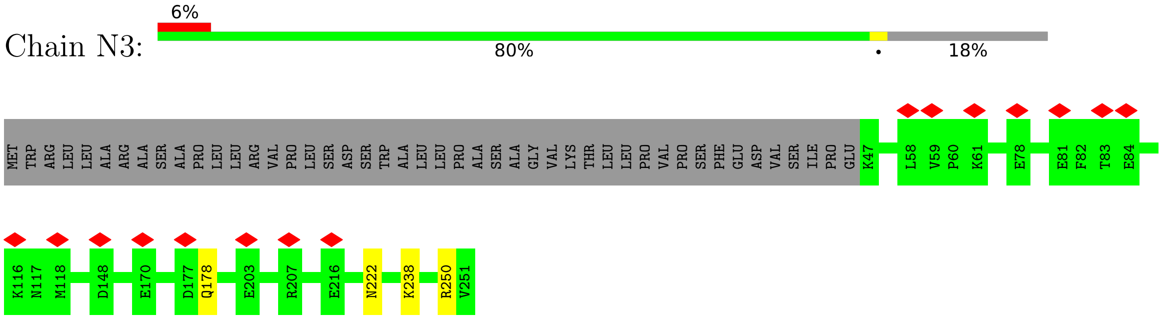
Chain M3:



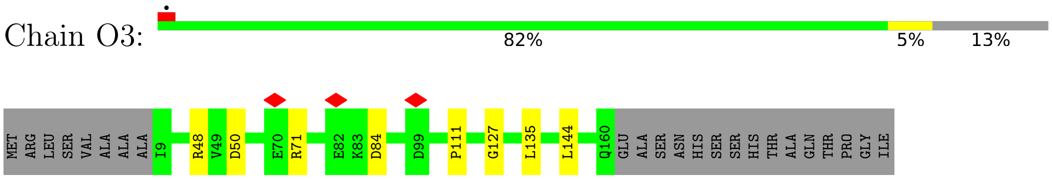




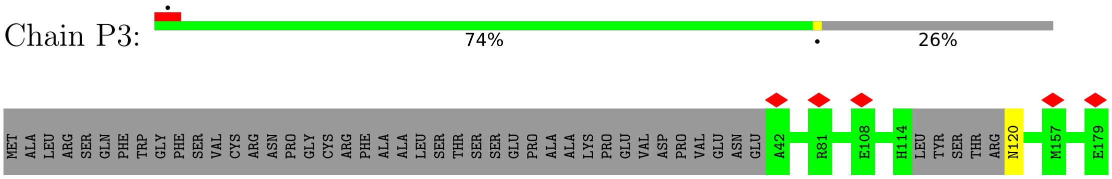
- Molecule 13: 39S ribosomal protein L16, mitochondrial



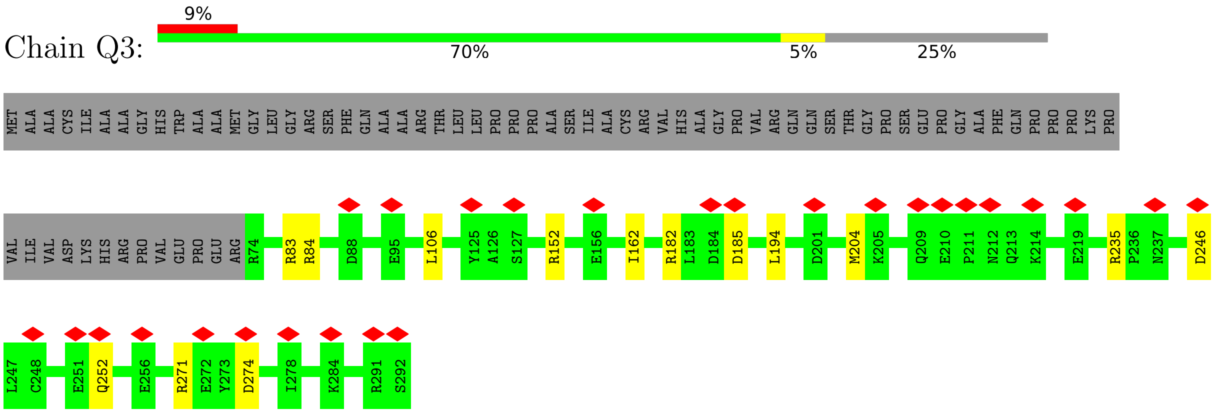
- Molecule 14: 39S ribosomal protein L17, mitochondrial



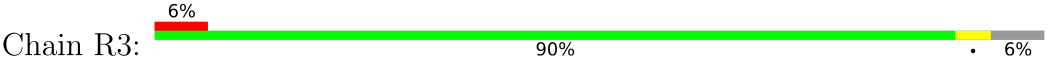
- Molecule 15: Mitochondrial ribosomal protein L18, isoform CRA_b

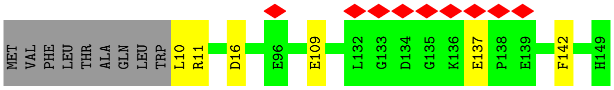


- Molecule 16: 39S ribosomal protein L19, mitochondrial



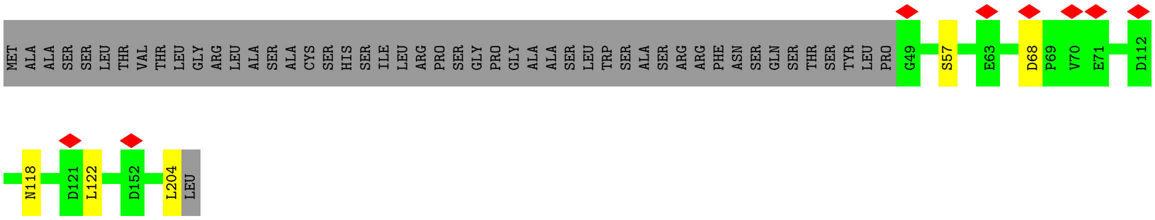
- Molecule 17: 39S ribosomal protein L20, mitochondrial





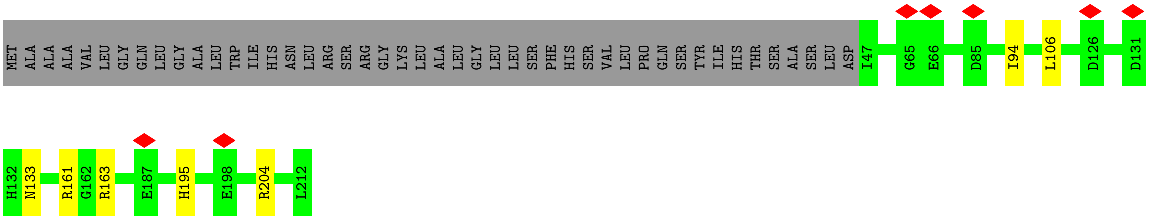
- Molecule 18: 39S ribosomal protein L21, mitochondrial

Chain S3:



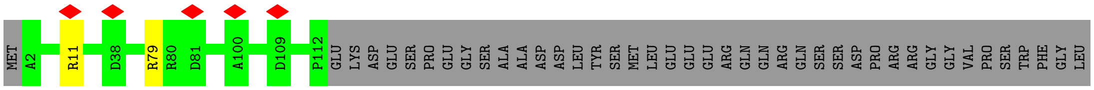
- Molecule 19: 39S ribosomal protein L22, mitochondrial

Chain T3:



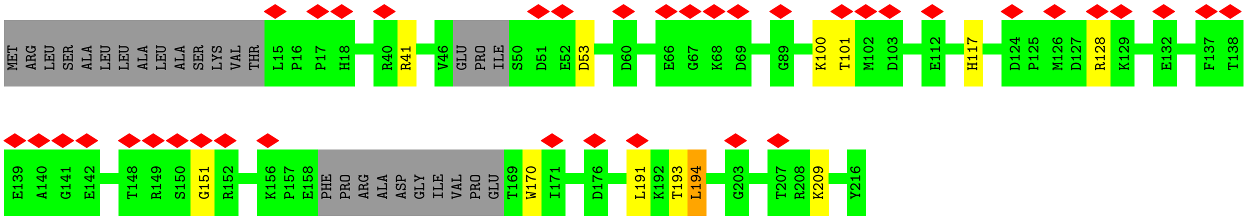
- Molecule 20: 39S ribosomal protein L23, mitochondrial

Chain U3:



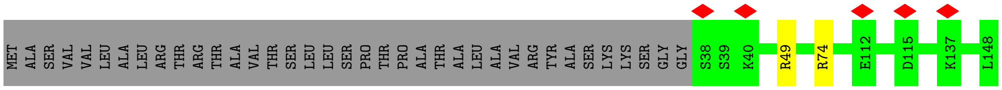
- Molecule 21: 39S ribosomal protein L24, mitochondrial

Chain V3:



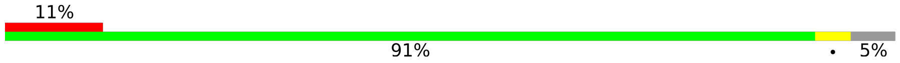
- Molecule 22: 39S ribosomal protein L27, mitochondrial

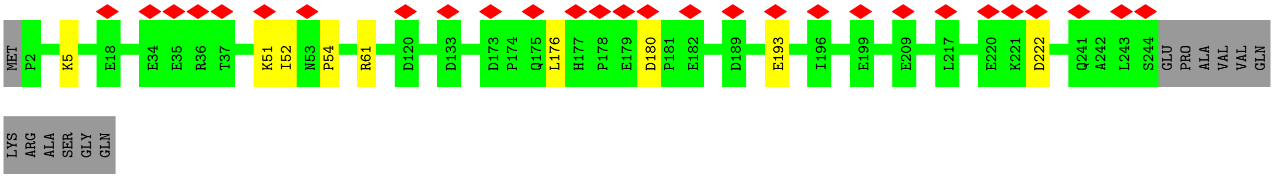
Chain W3:



- Molecule 23: 39S ribosomal protein L28, mitochondrial

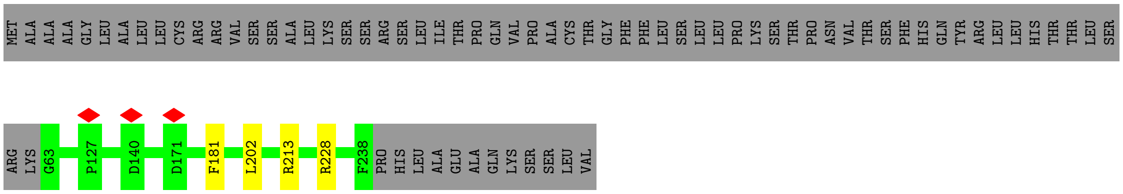
Chain X3:





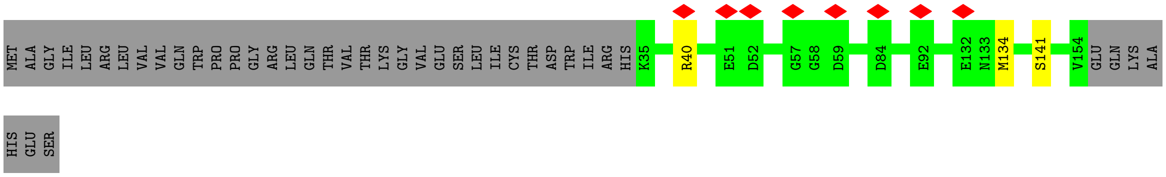
- Molecule 24: 39S ribosomal protein L47, mitochondrial

Chain Y3:



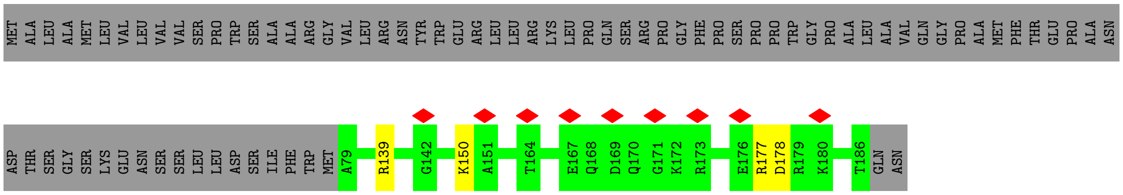
- Molecule 25: 39S ribosomal protein L30, mitochondrial

Chain Z3:



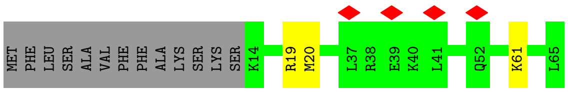
- Molecule 26: 39S ribosomal protein L32, mitochondrial

Chain 03:

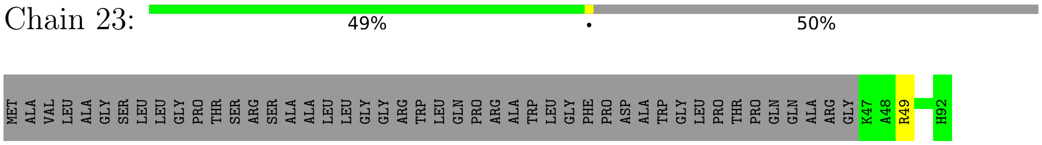


- Molecule 27: 39S ribosomal protein L33, mitochondrial

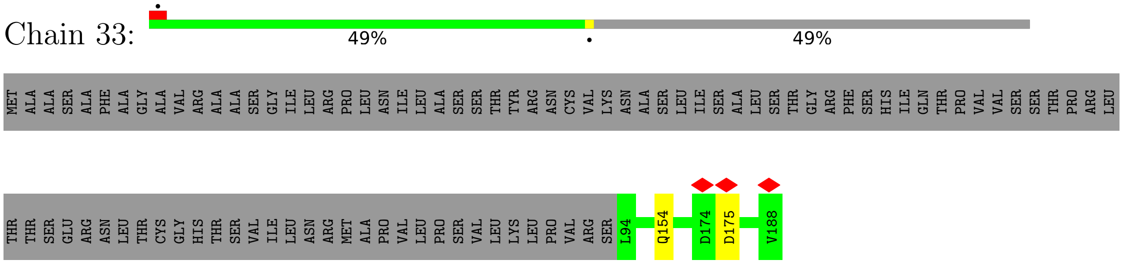
Chain 13:



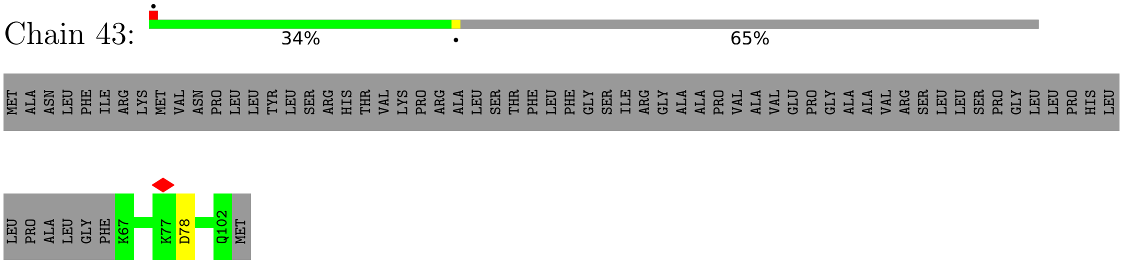
- Molecule 28: 39S ribosomal protein L34, mitochondrial



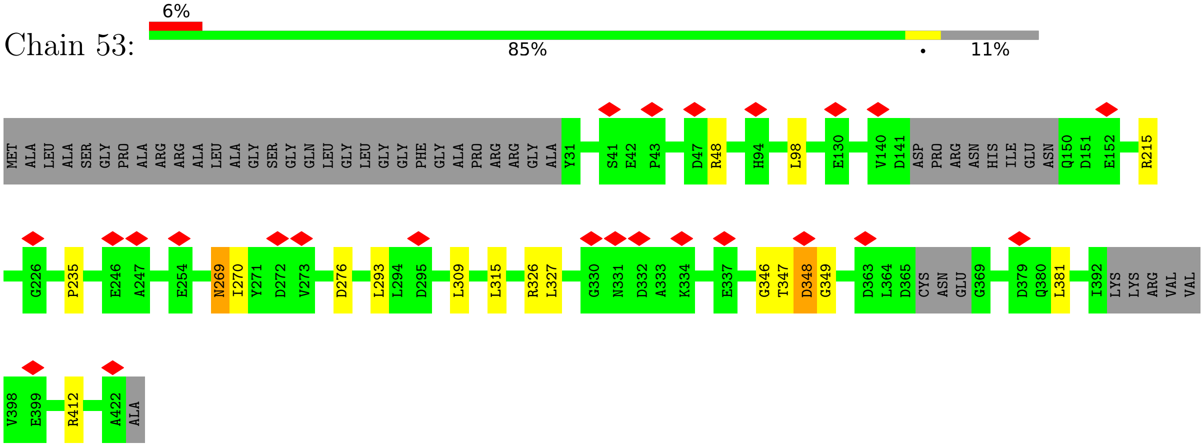
- Molecule 29: 39S ribosomal protein L35, mitochondrial



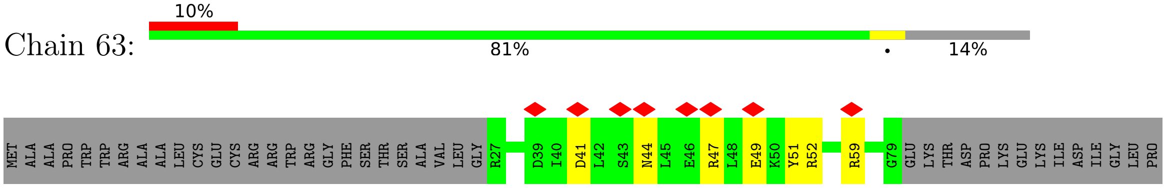
- Molecule 30: 39S ribosomal protein L36, mitochondrial

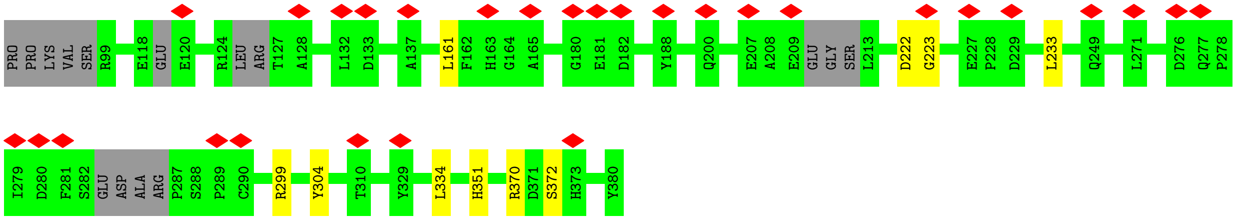


- Molecule 31: 39S ribosomal protein L37, mitochondrial



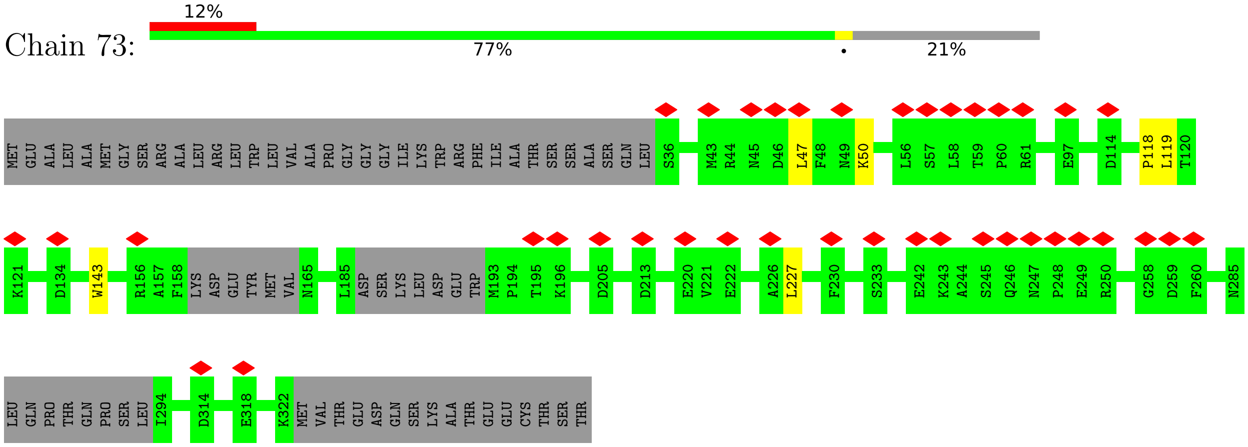
- Molecule 32: 39S ribosomal protein L38, mitochondrial





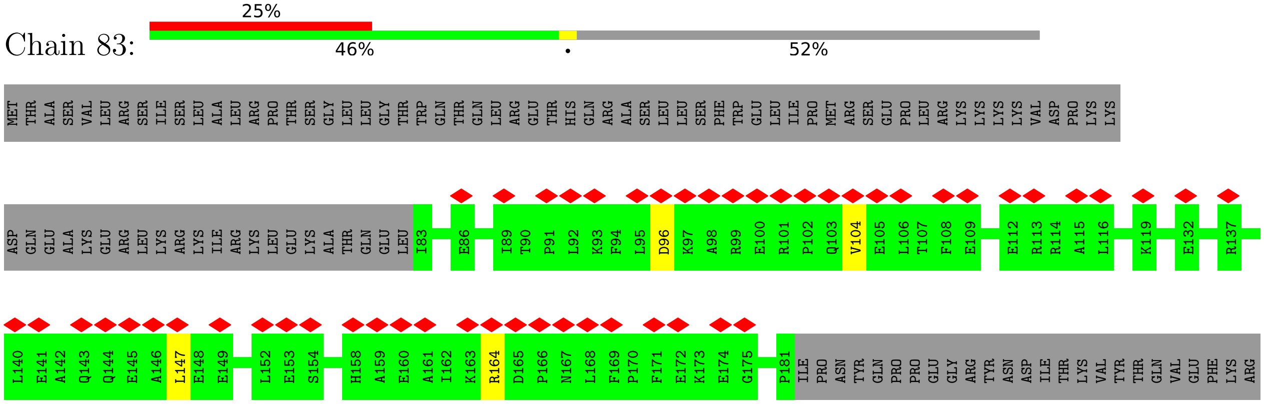
- Molecule 33: 39S ribosomal protein L39, mitochondrial

Chain 73:



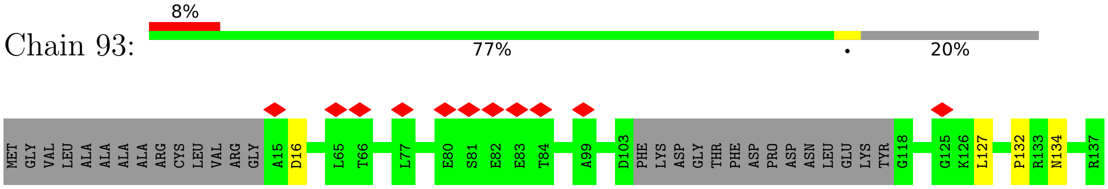
- Molecule 34: 39S ribosomal protein L40, mitochondrial

Chain 83:



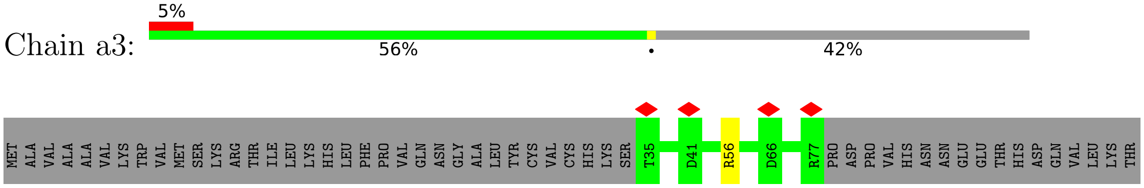
- Molecule 35: 39S ribosomal protein L41, mitochondrial

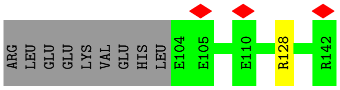
Chain 93:



- Molecule 36: 39S ribosomal protein L42, mitochondrial

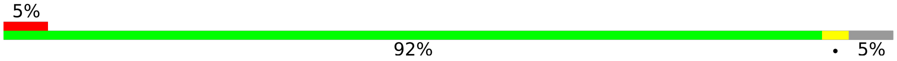
Chain a3:

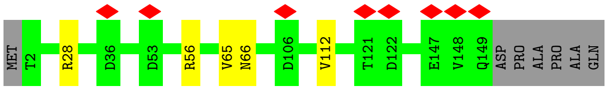




- Molecule 37: 39S ribosomal protein L43, mitochondrial

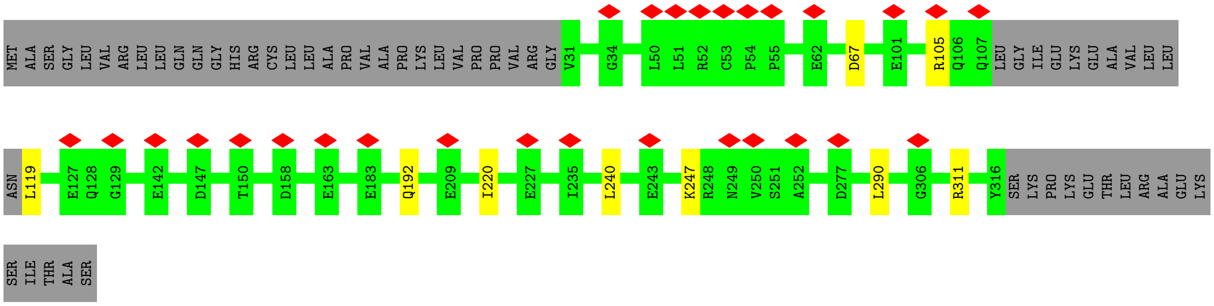
Chain b3:





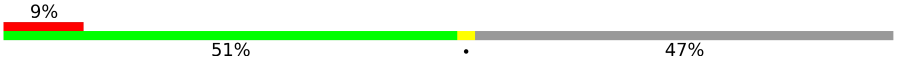
- Molecule 38: 39S ribosomal protein L44, mitochondrial

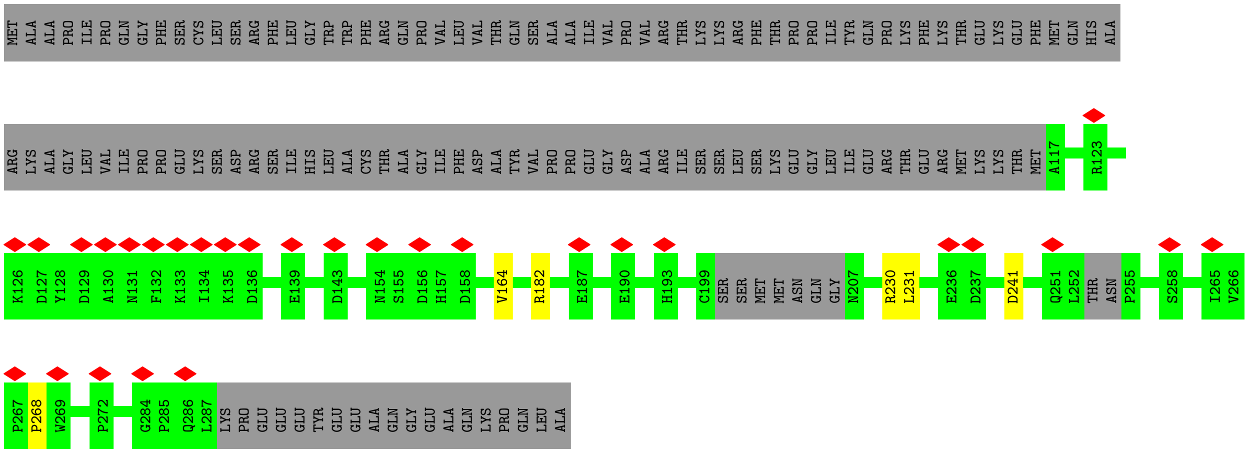
Chain c3:



- Molecule 39: 39S ribosomal protein L45, mitochondrial

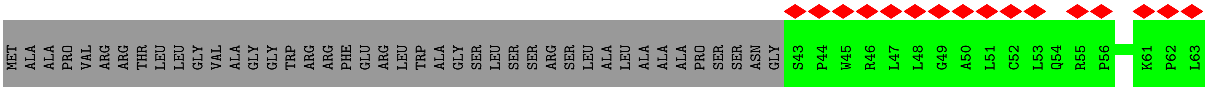
Chain d3:

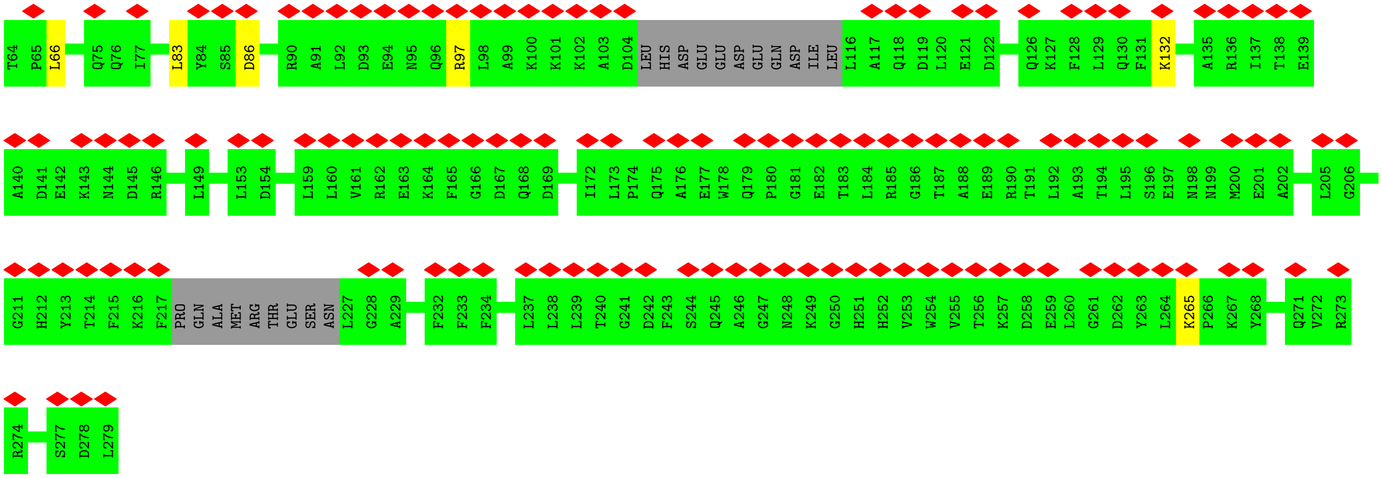




- Molecule 40: 39S ribosomal protein L46, mitochondrial

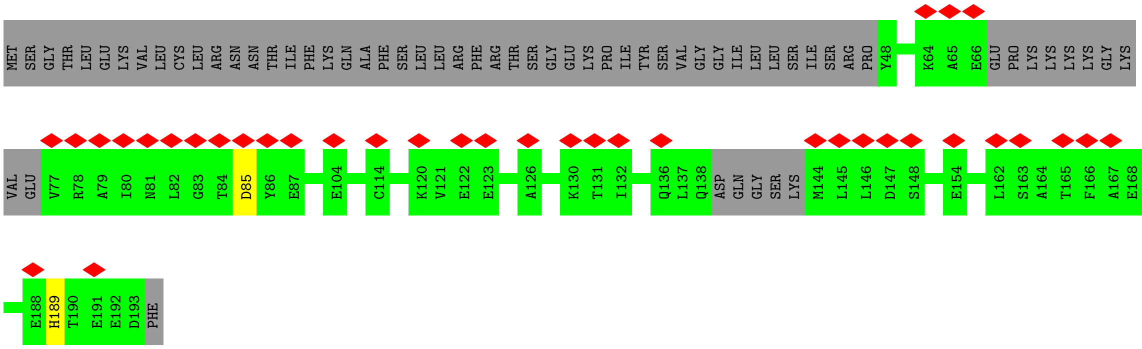
Chain e3:





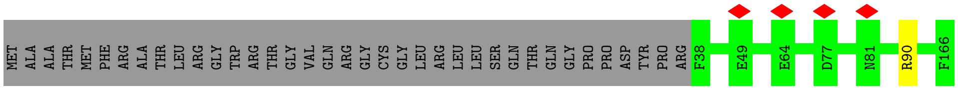
- Molecule 41: 39S ribosomal protein L48, mitochondrial

Chain f3:



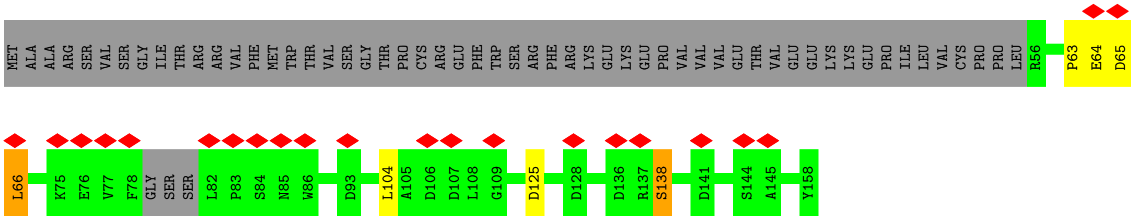
- Molecule 42: 39S ribosomal protein L49, mitochondrial

Chain g3:



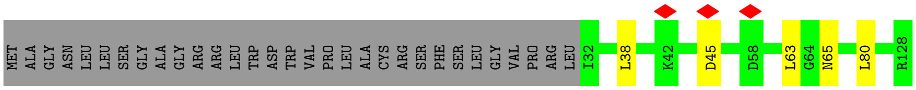
- Molecule 43: 39S ribosomal protein L50, mitochondrial

Chain h3:



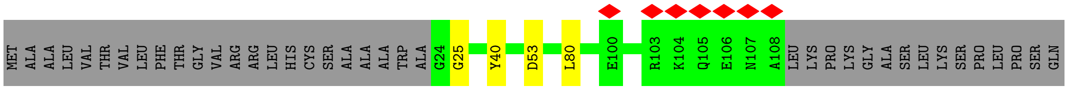
- Molecule 44: 39S ribosomal protein L51, mitochondrial

Chain i3:



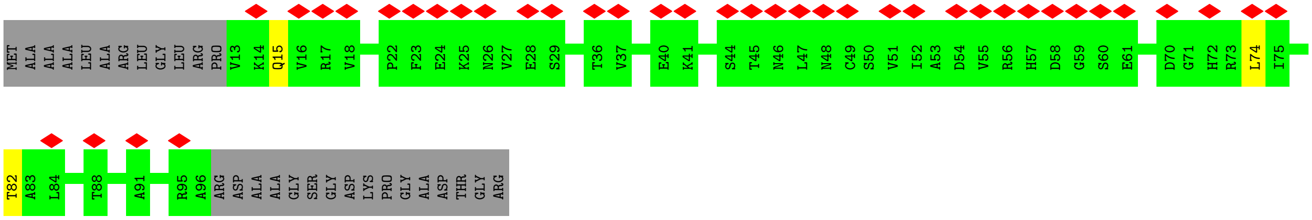
- Molecule 45: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA

Chain j3:



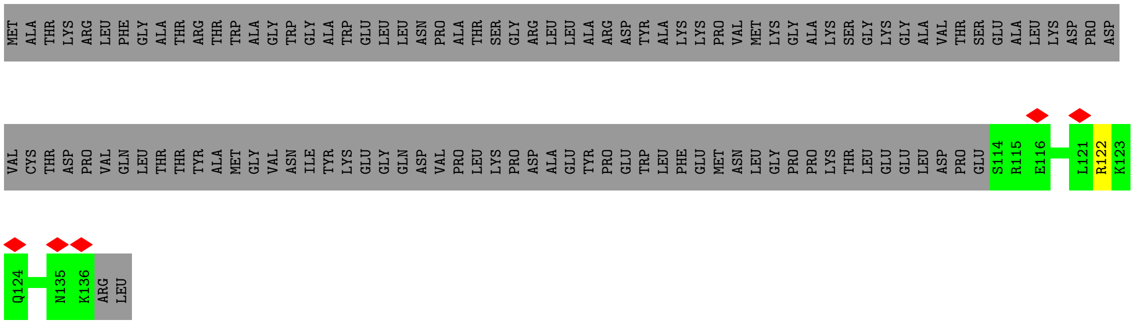
- Molecule 46: 39S ribosomal protein L53, mitochondrial

Chain k3:



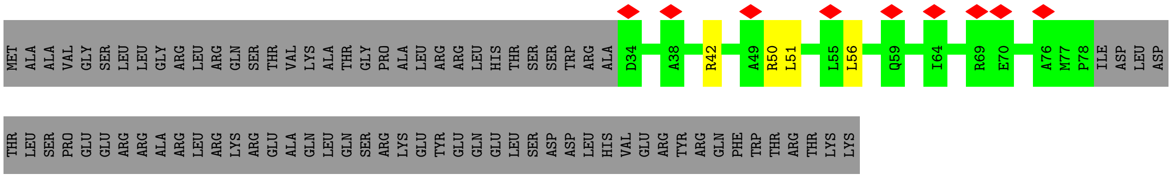
- Molecule 47: 39S ribosomal protein L54, mitochondrial

Chain l3:



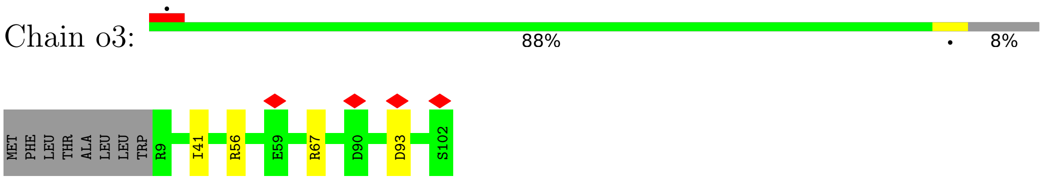
- Molecule 48: 39S ribosomal protein L55, mitochondrial

Chain m3:



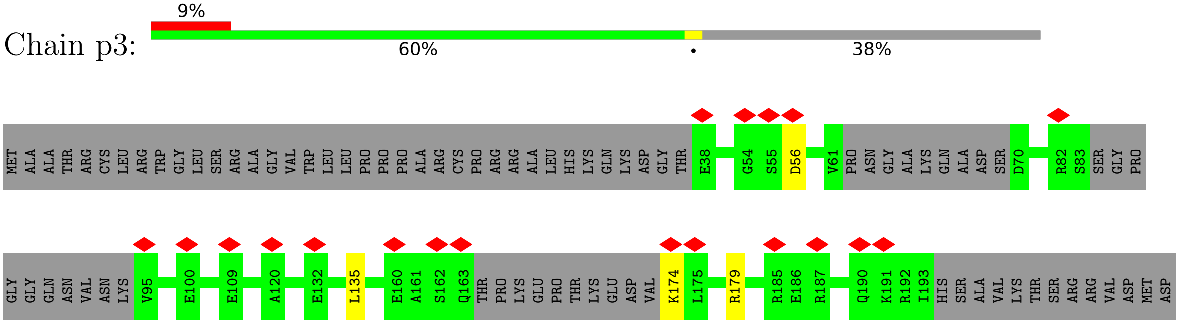
- Molecule 49: Ribosomal protein 63, mitochondrial

Chain o3:



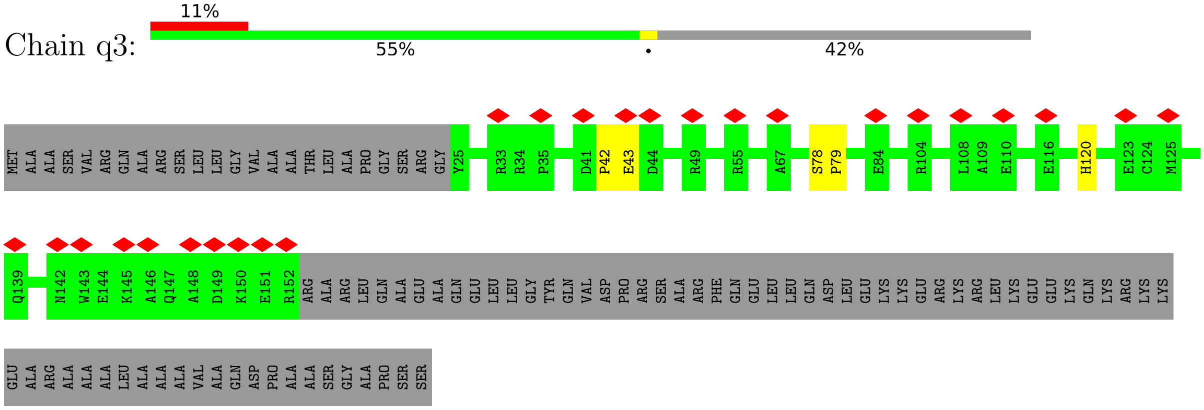
- Molecule 50: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p3:



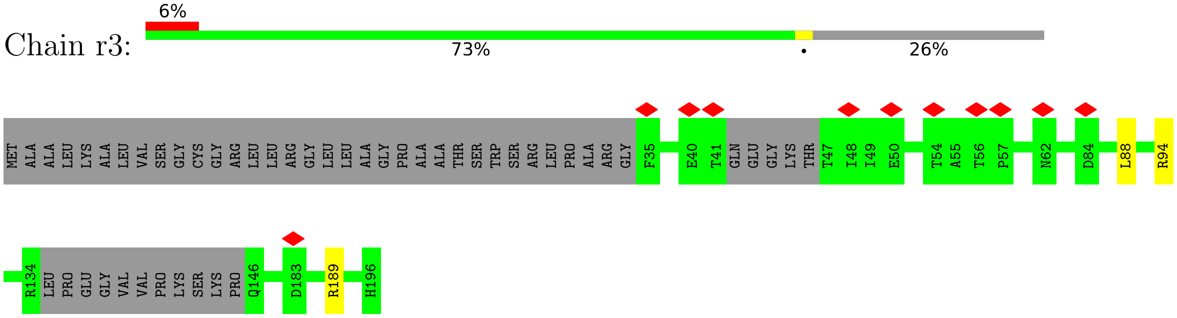
- Molecule 51: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q3:



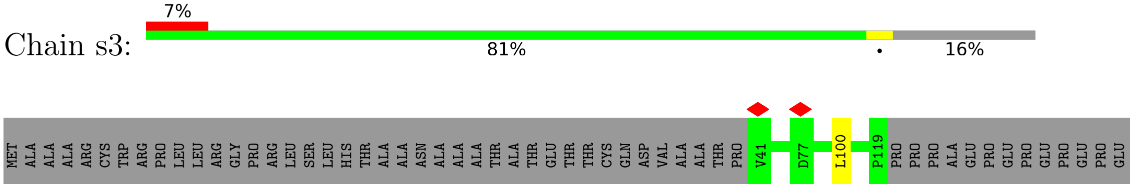
- Molecule 52: 39S ribosomal protein S18a, mitochondrial

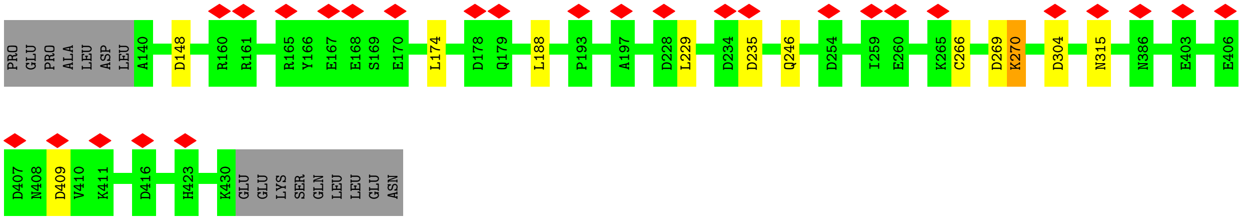
Chain r3:



- Molecule 53: 39S ribosomal protein S30, mitochondrial

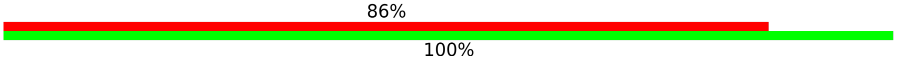
Chain s3:

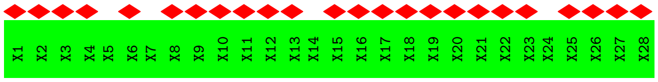




- Molecule 54: Unknown protein/protein extension

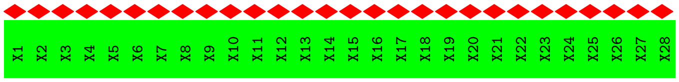
Chain t3:





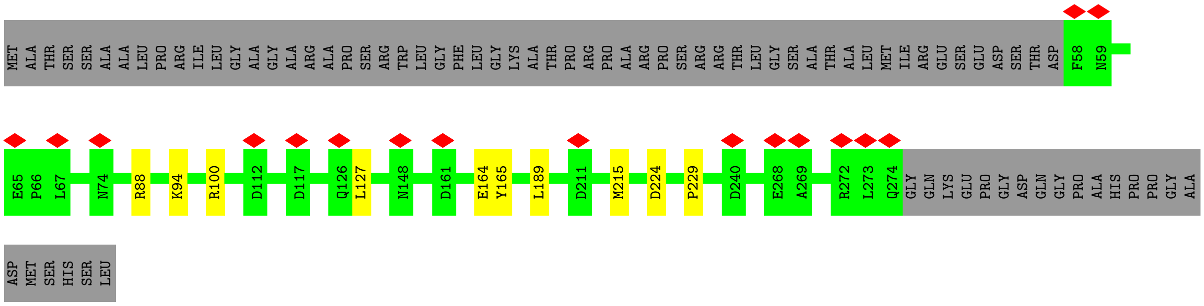
- Molecule 54: Unknown protein/protein extension

Chain A5:



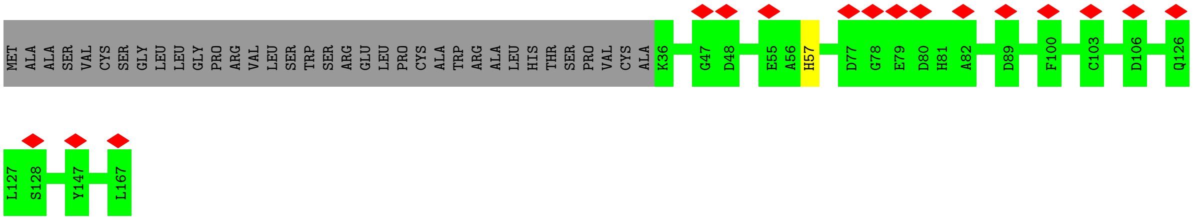
- Molecule 55: 28S ribosomal protein S2, mitochondrial

Chain B6:



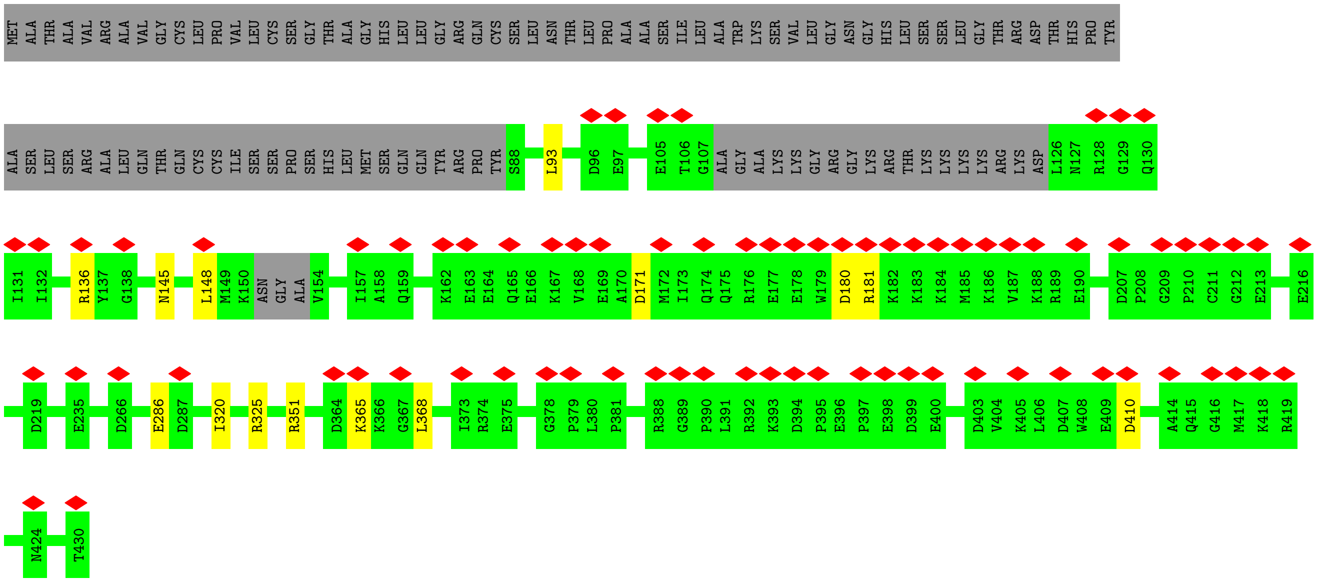
- Molecule 56: 28S ribosomal protein S24, mitochondrial

Chain C6:



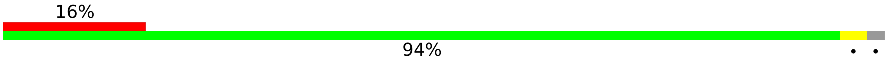
- Molecule 57: 28S ribosomal protein S5, mitochondrial

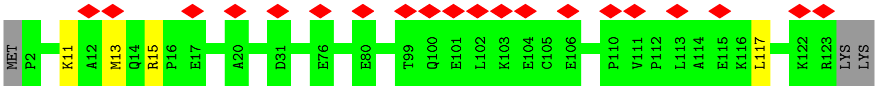
Chain D6:



- Molecule 58: 28S ribosomal protein S6, mitochondrial

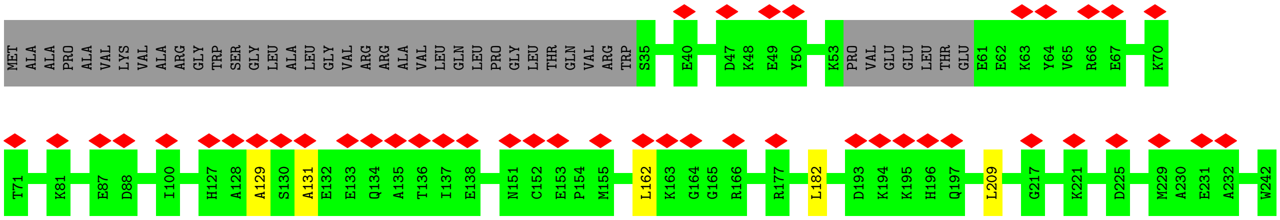
Chain E6:





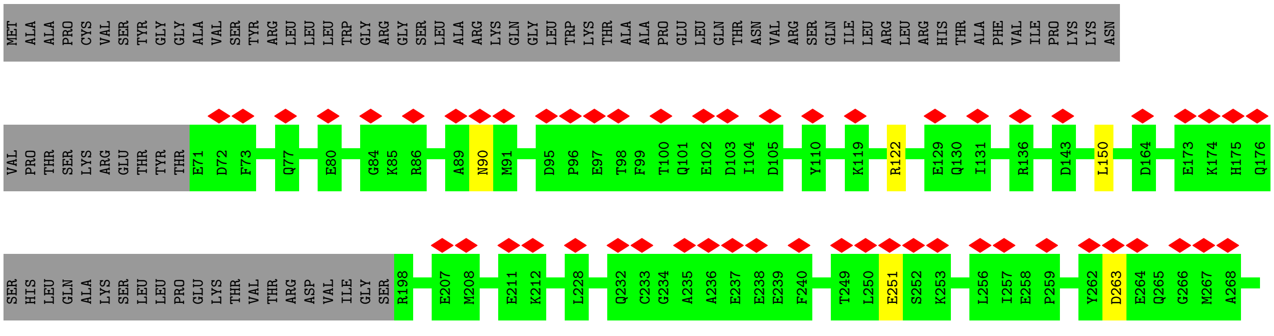
- Molecule 59: 28S ribosomal protein S7, mitochondrial

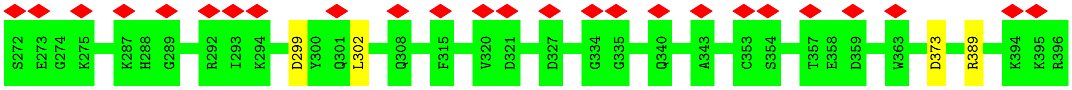
Chain F6:



- Molecule 60: 28S ribosomal protein S9, mitochondrial

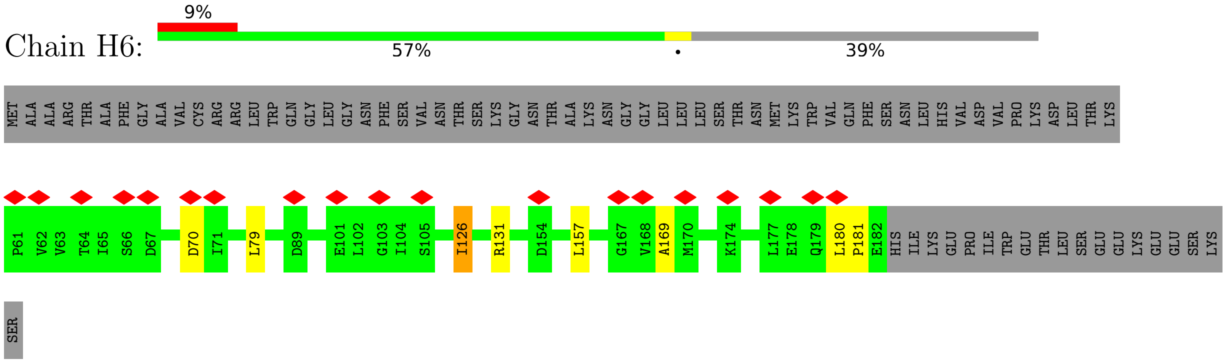
Chain G6:





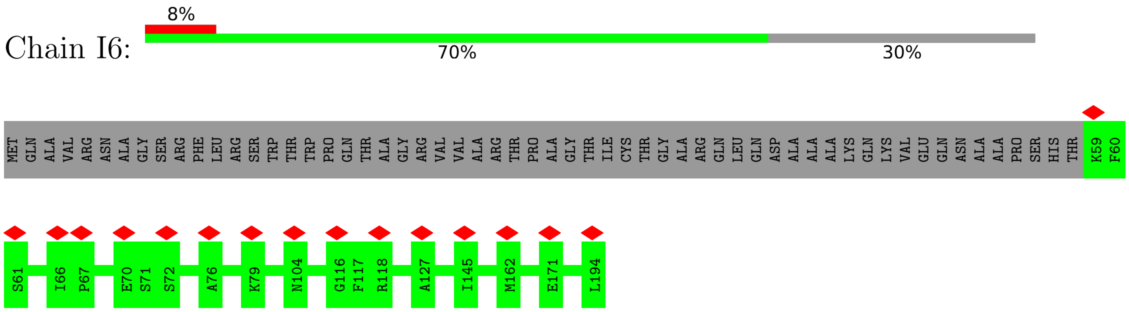
- Molecule 61: 28S ribosomal protein S10, mitochondrial

Chain H6:



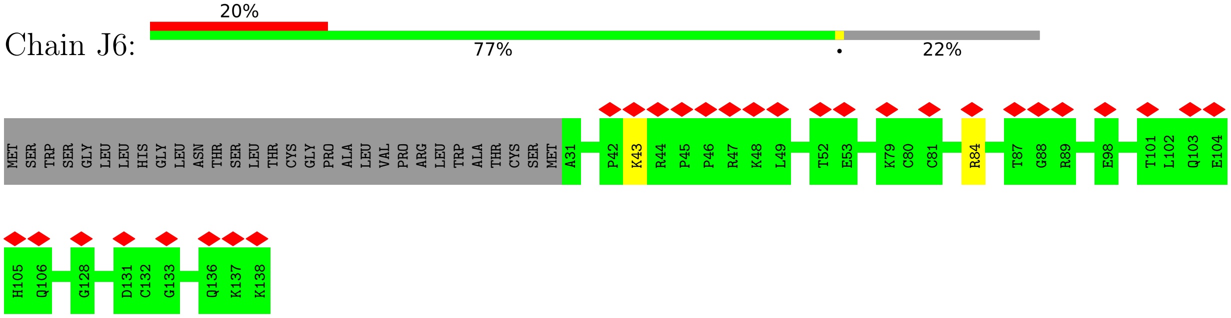
- Molecule 62: 28S ribosomal protein S11, mitochondrial

Chain I6:



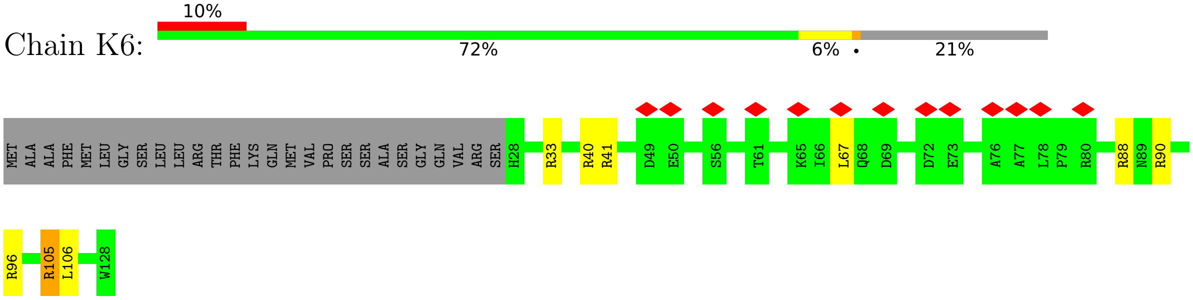
- Molecule 63: 28S ribosomal protein S12, mitochondrial

Chain J6:

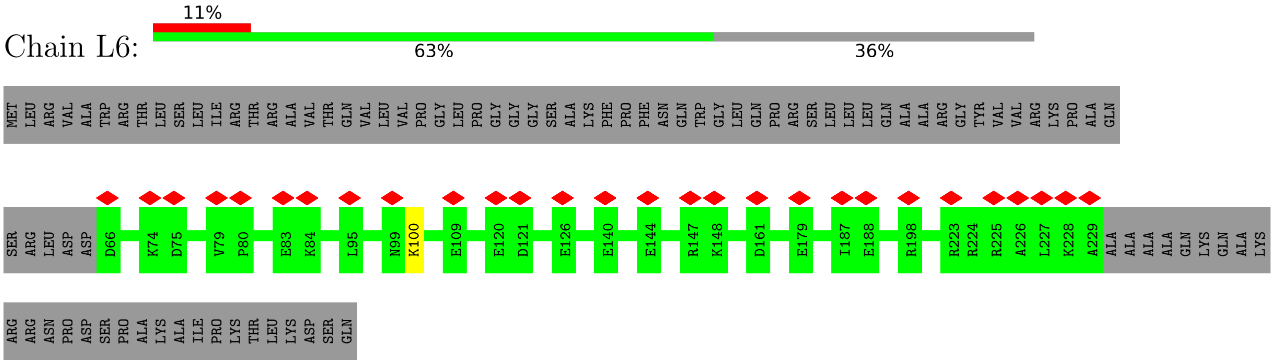


- Molecule 64: 28S ribosomal protein S14, mitochondrial

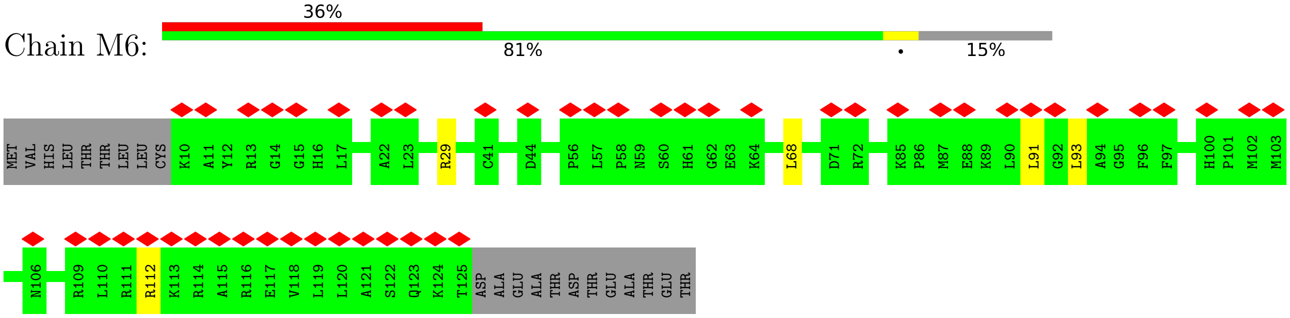
Chain K6:



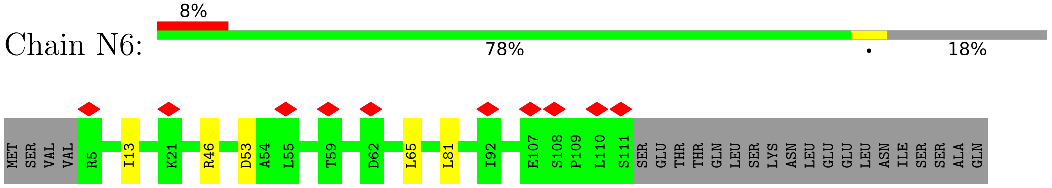
- Molecule 65: 28S ribosomal protein S15, mitochondrial



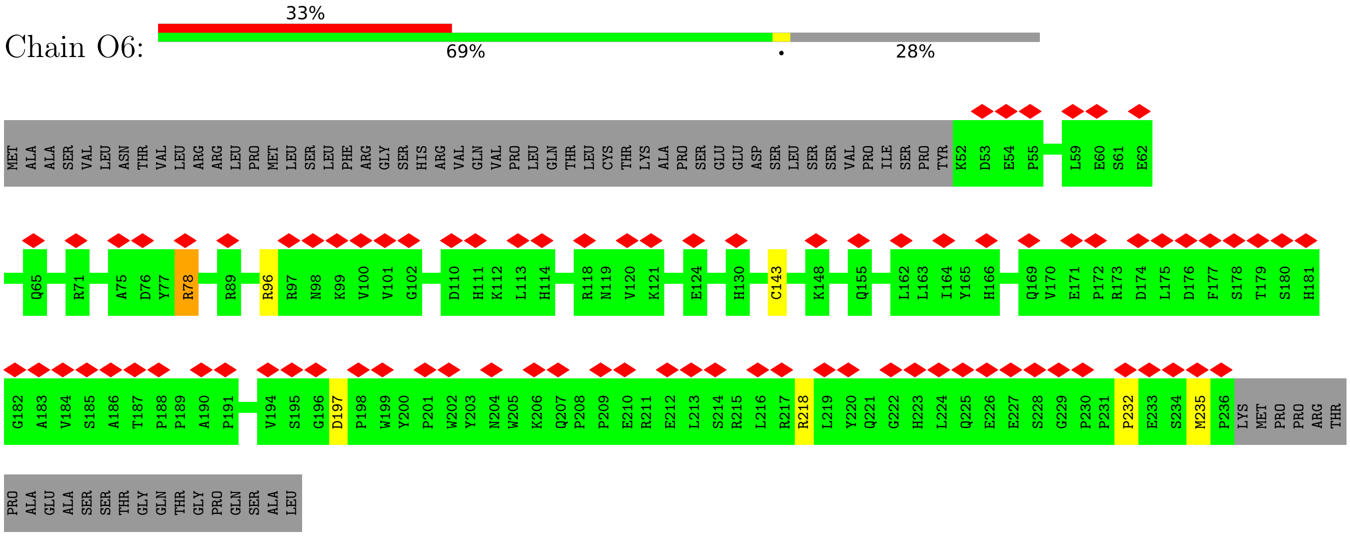
- Molecule 66: 28S ribosomal protein S16, mitochondrial



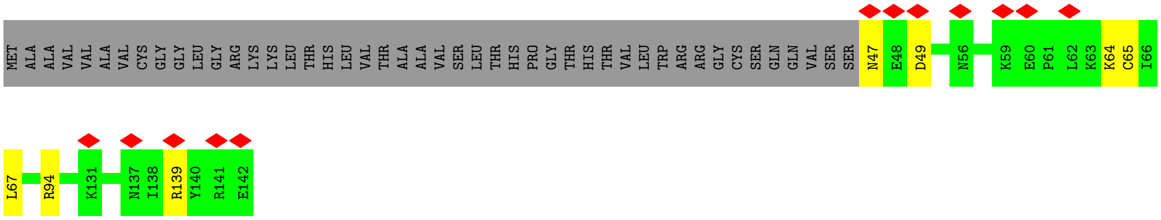
- Molecule 67: 28S ribosomal protein S17, mitochondrial



- Molecule 68: 28S ribosomal protein S18b, mitochondrial

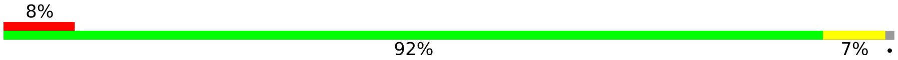


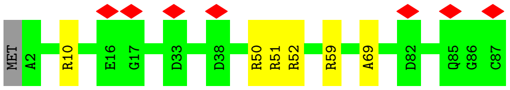
- Molecule 69: 28S ribosomal protein S18c, mitochondrial



- Molecule 70: 28S ribosomal protein S21, mitochondrial

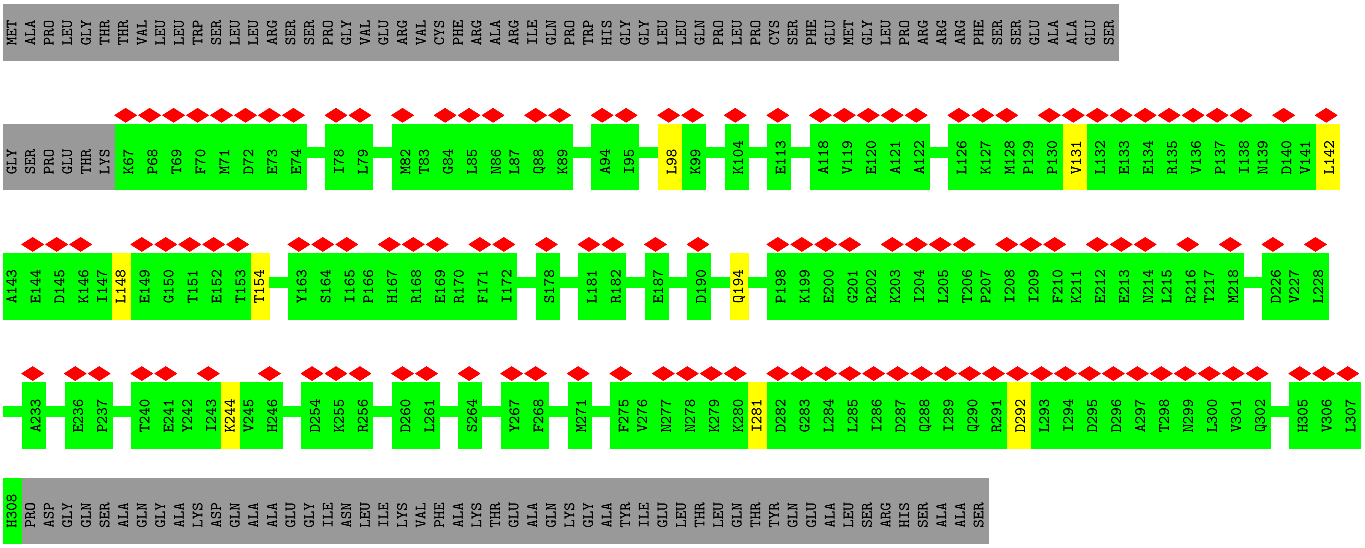
Chain Q6:





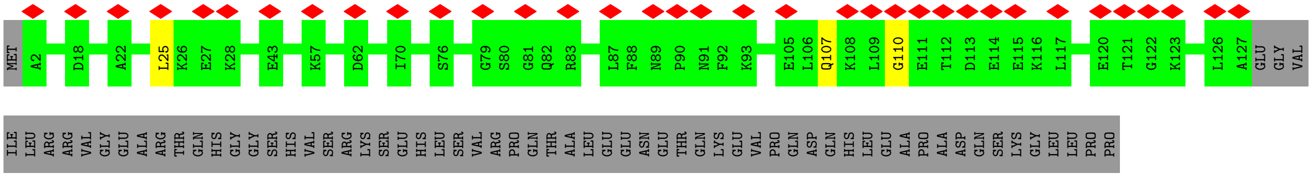
- Molecule 71: 28S ribosomal protein S22, mitochondrial

Chain R6:



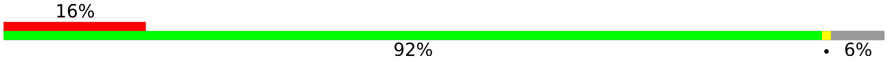
- Molecule 72: 28S ribosomal protein S23, mitochondrial

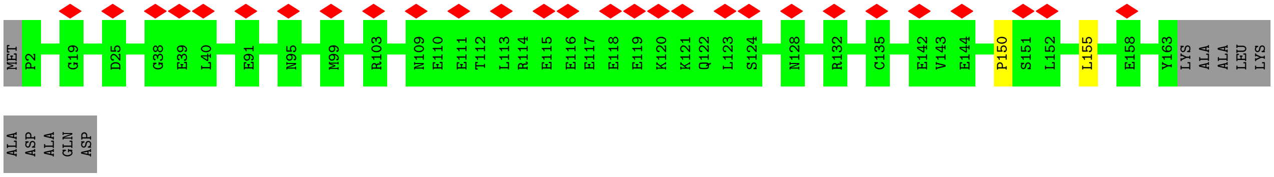
Chain S6:



- Molecule 73: 28S ribosomal protein S25, mitochondrial

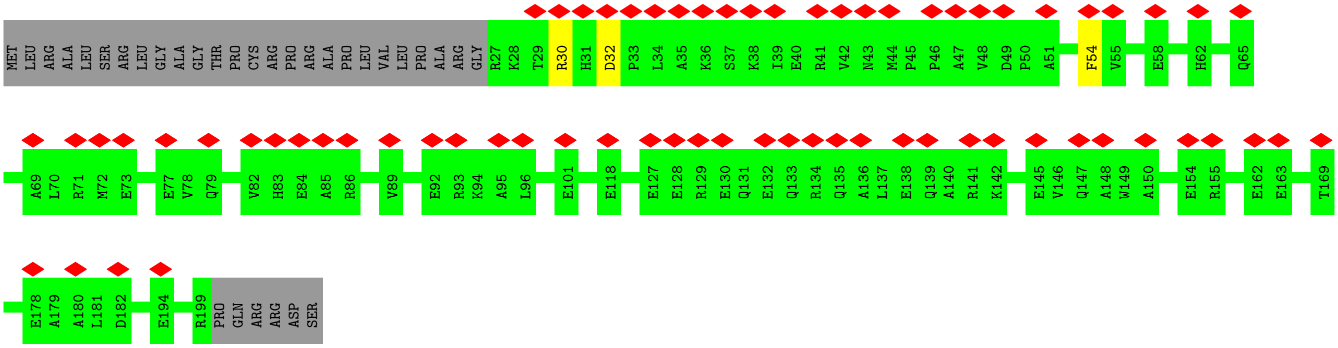
Chain T6:





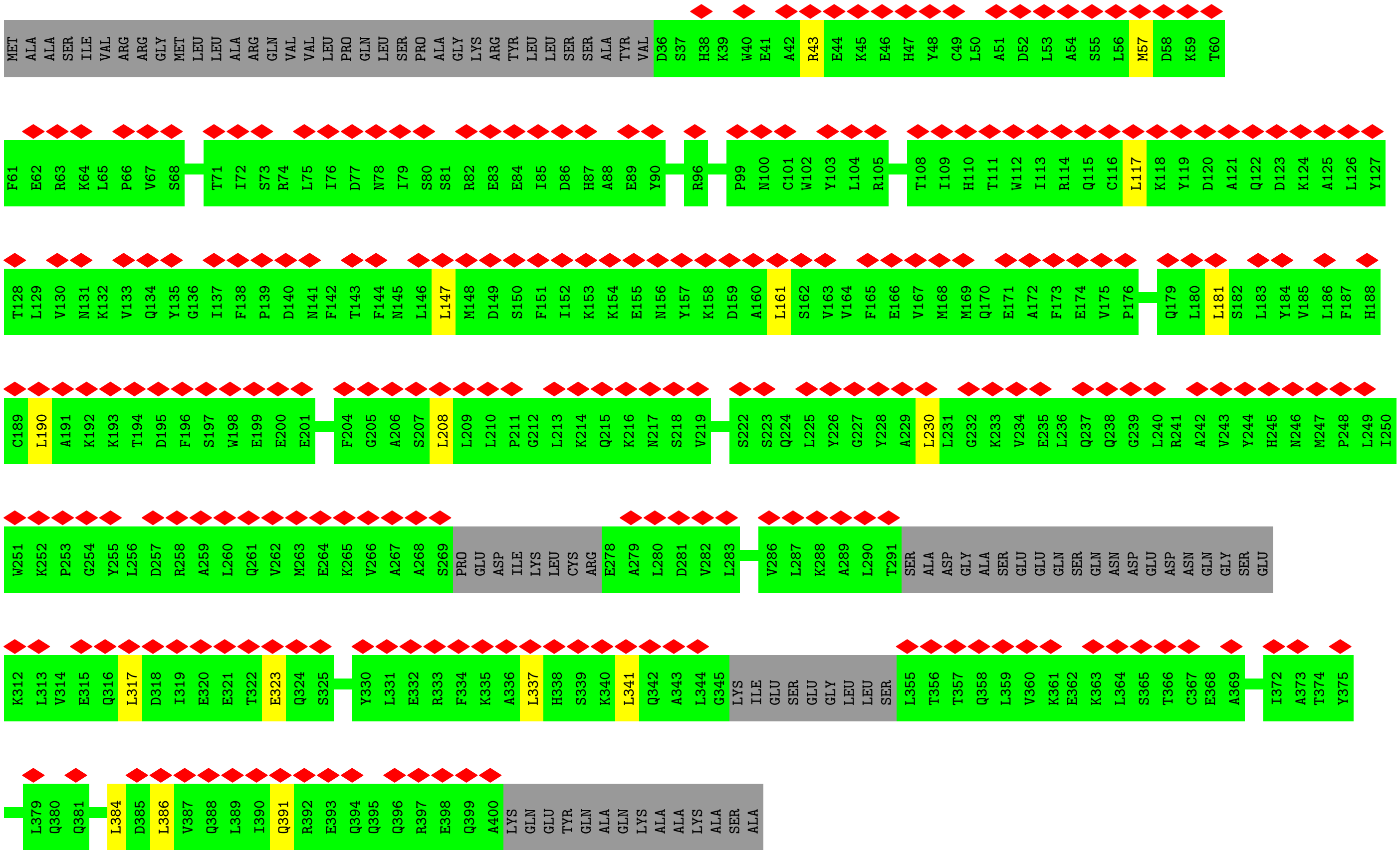
- Molecule 74: 28S ribosomal protein S26, mitochondrial

Chain U6:

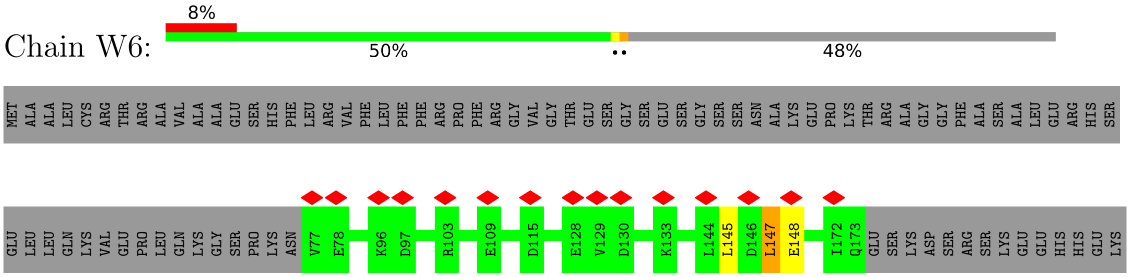


- Molecule 75: 28S ribosomal protein S27, mitochondrial

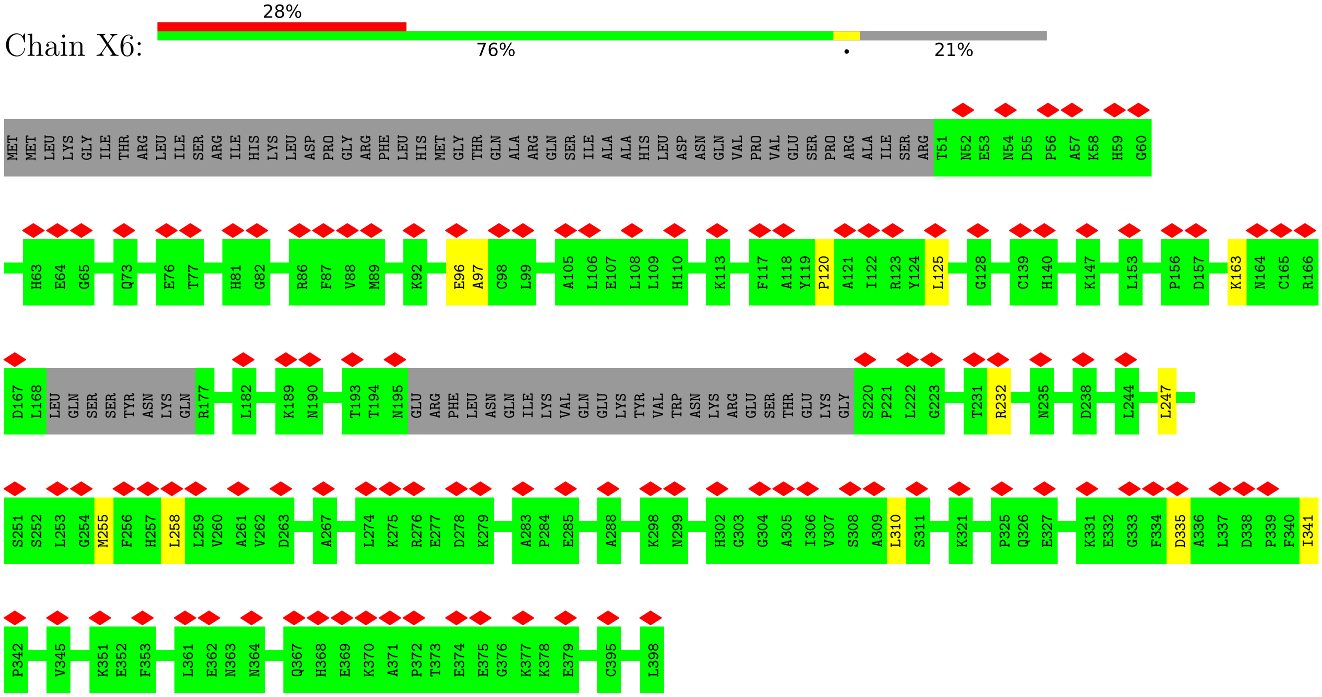
Chain V6:



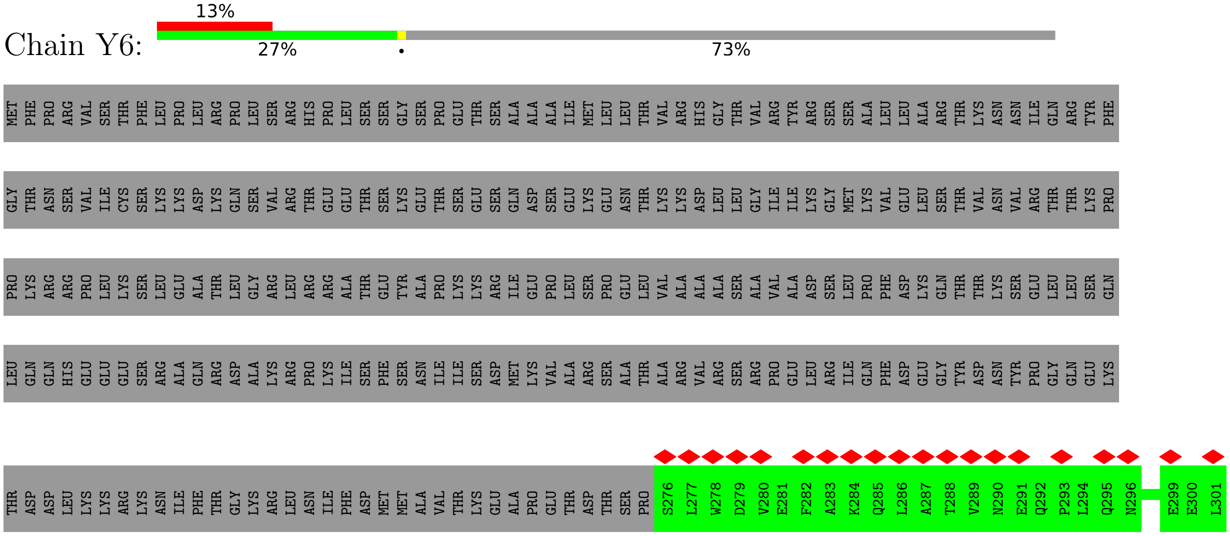
- Molecule 76: 28S ribosomal protein S28, mitochondrial

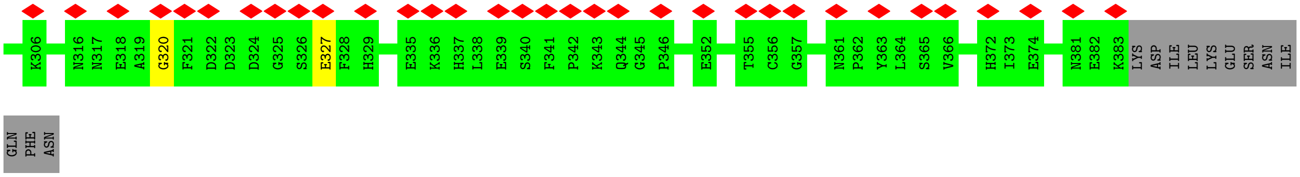


- Molecule 77: 28S ribosomal protein S29, mitochondrial



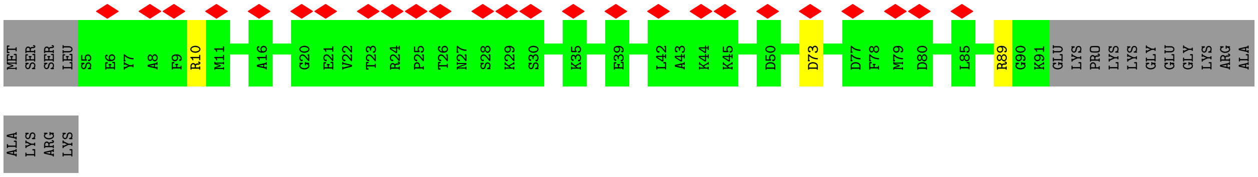
- Molecule 78: 28S ribosomal protein S31, mitochondrial





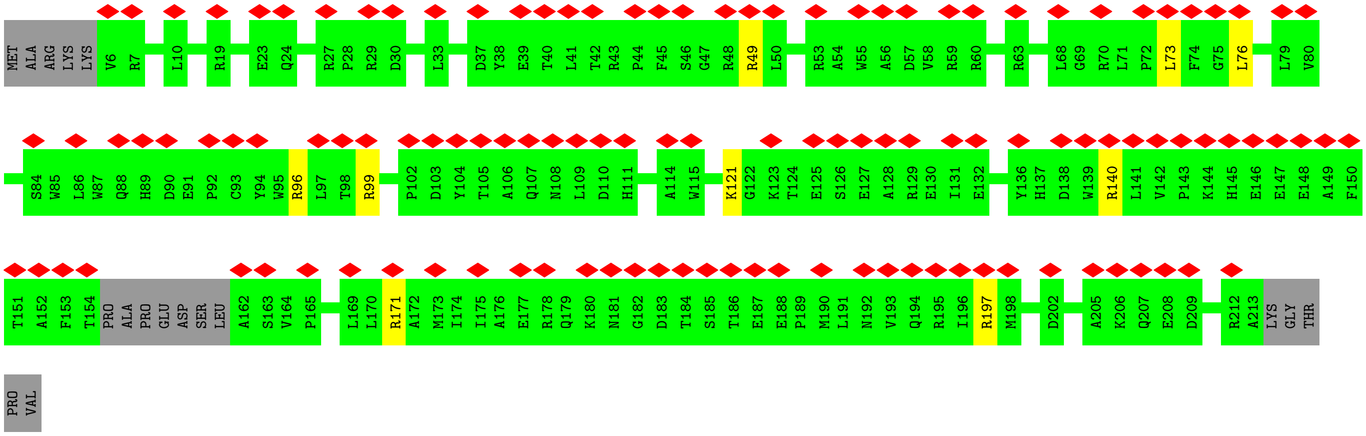
- Molecule 79: 28S ribosomal protein S33, mitochondrial

Chain Z6:



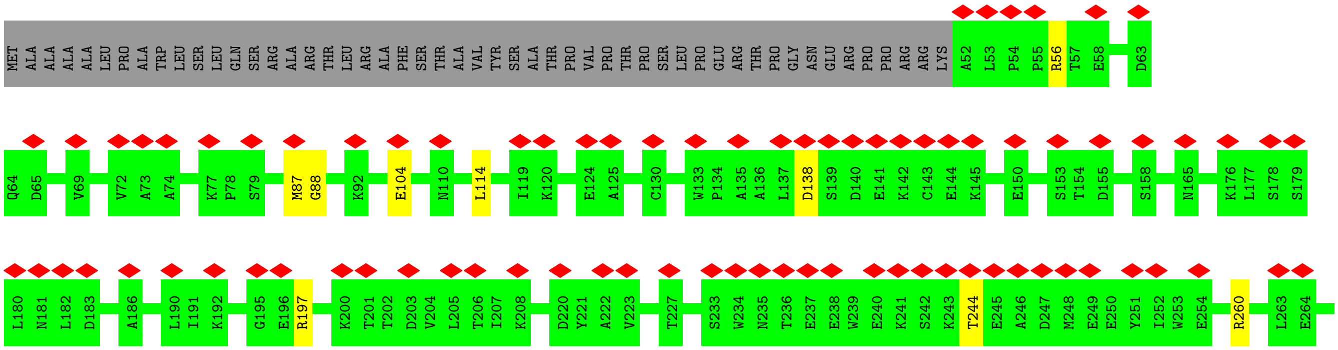
- Molecule 80: 28S ribosomal protein S34, mitochondrial

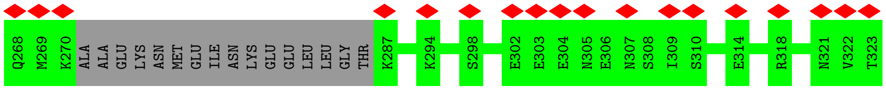
Chain a6:



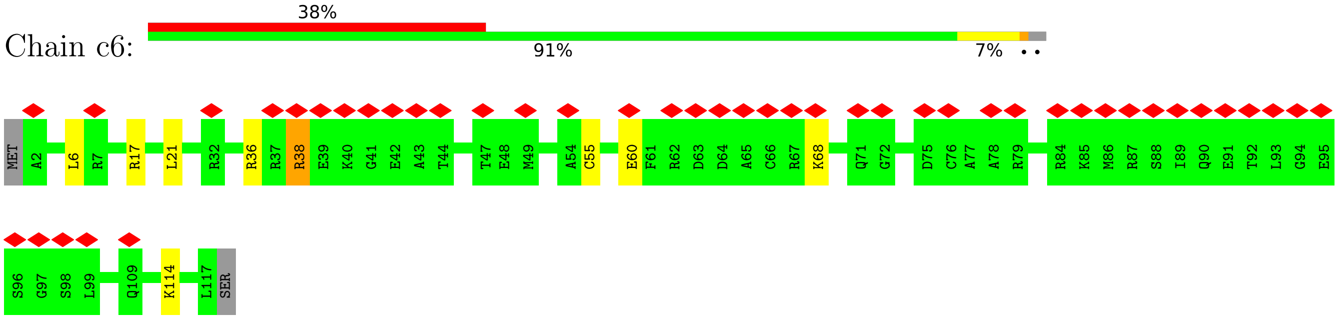
- Molecule 81: 28S ribosomal protein S35, mitochondrial

Chain b6:

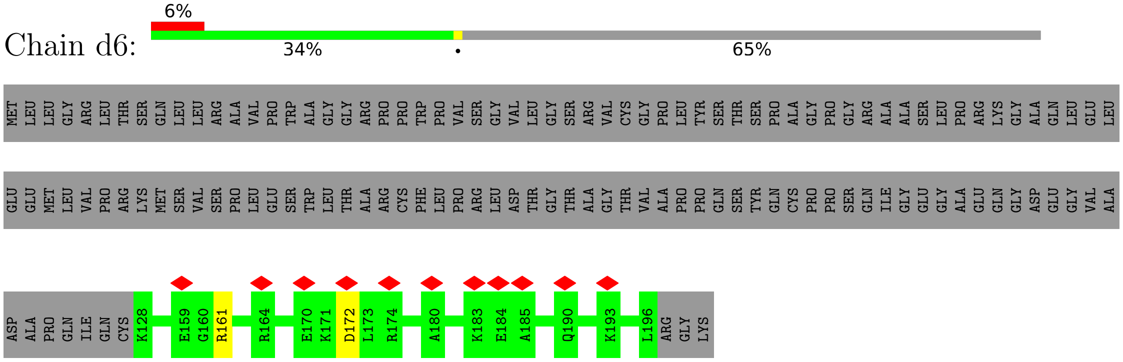




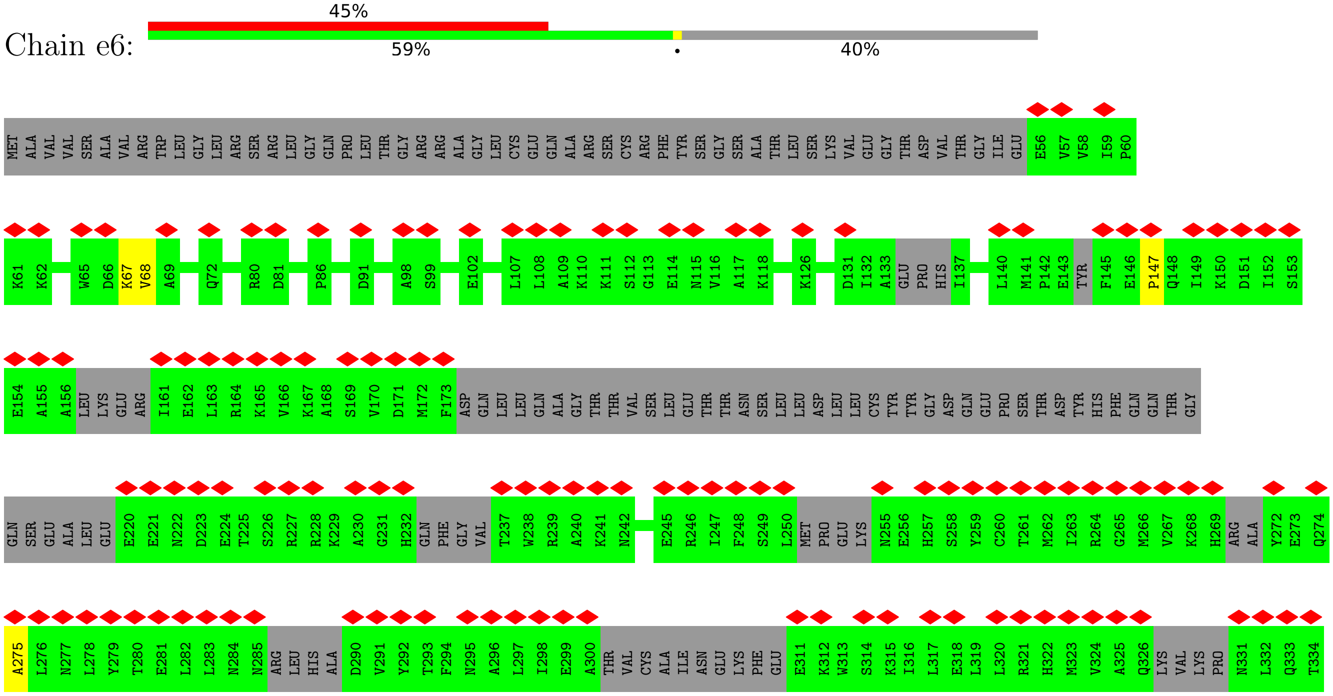
- Molecule 82: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

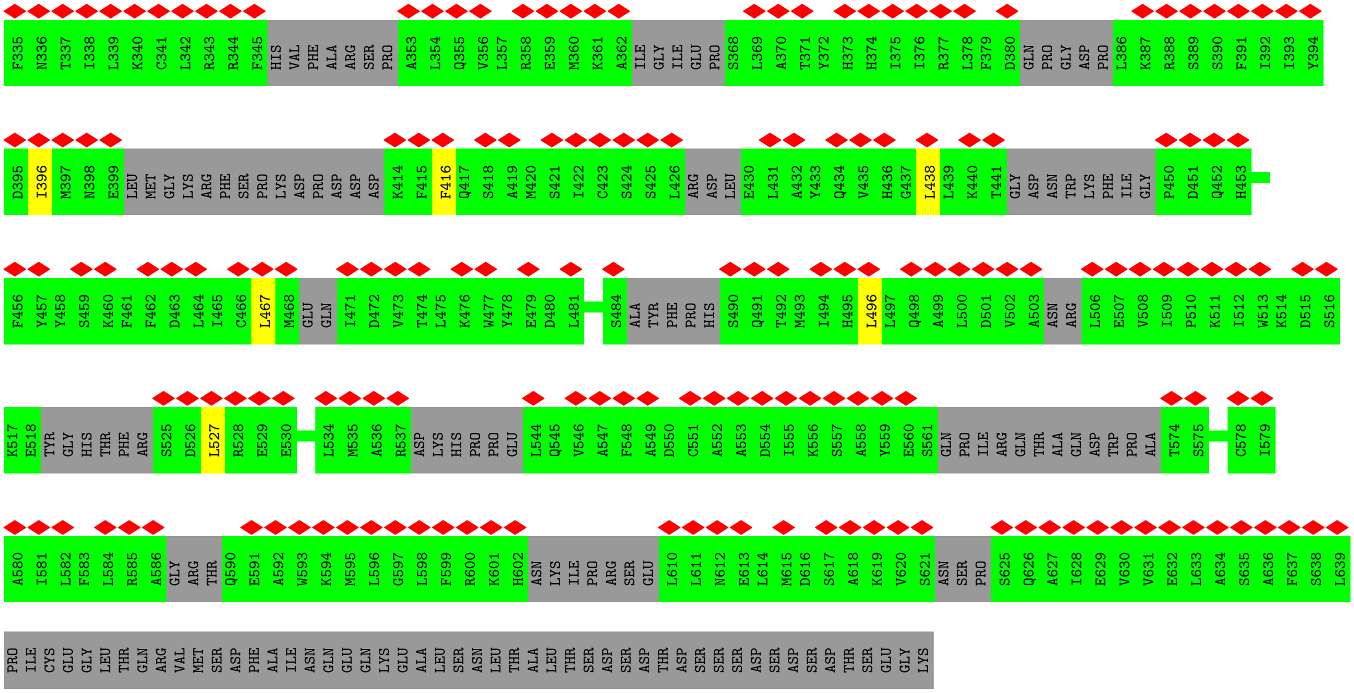


- Molecule 83: Aurora kinase A-interacting protein



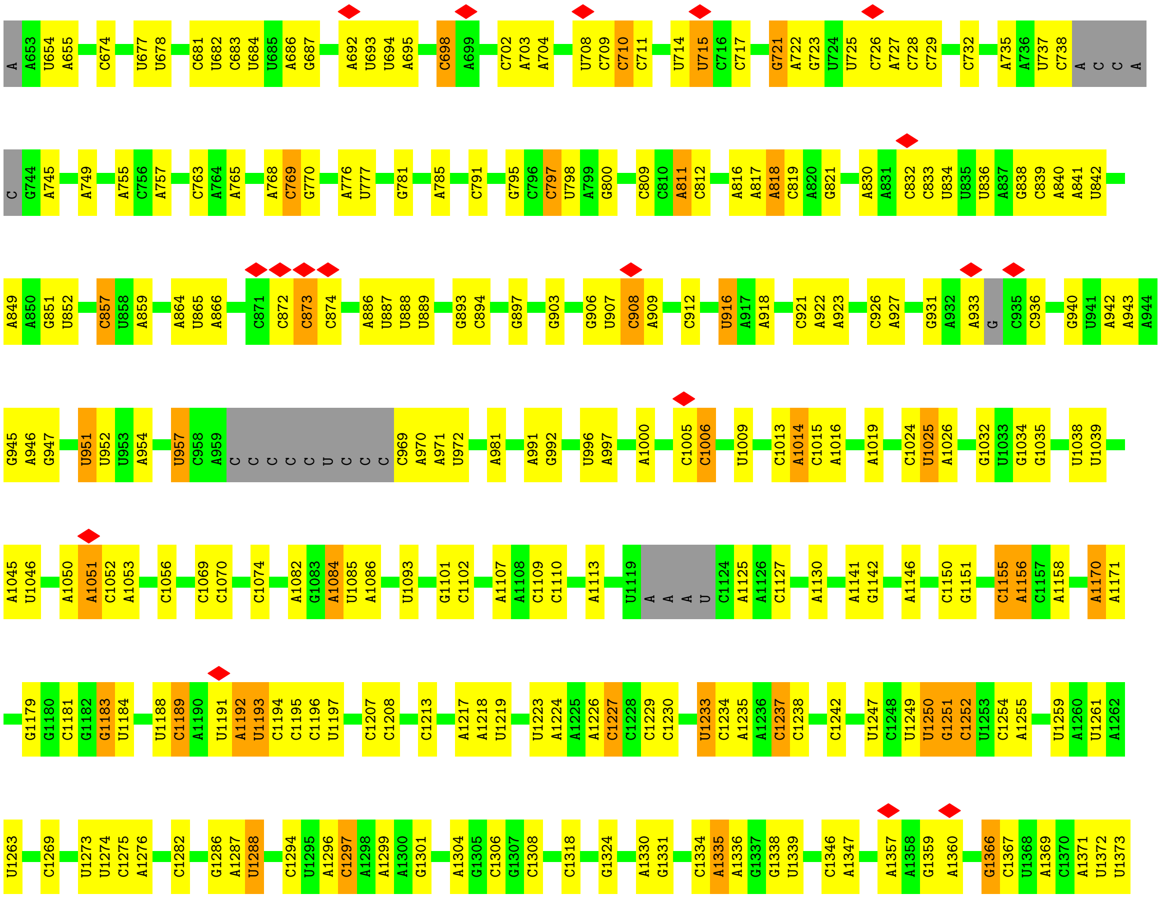
- Molecule 84: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

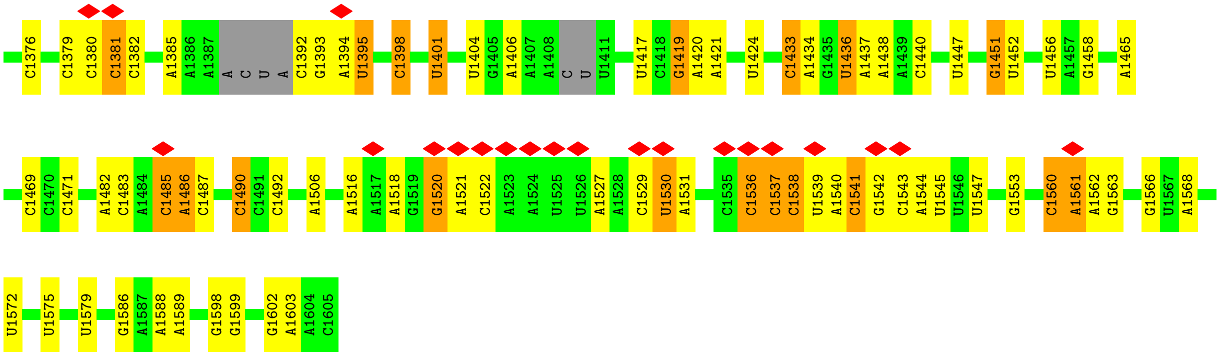




- Molecule 85: 12S rRNA

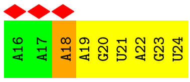
Chain A6:





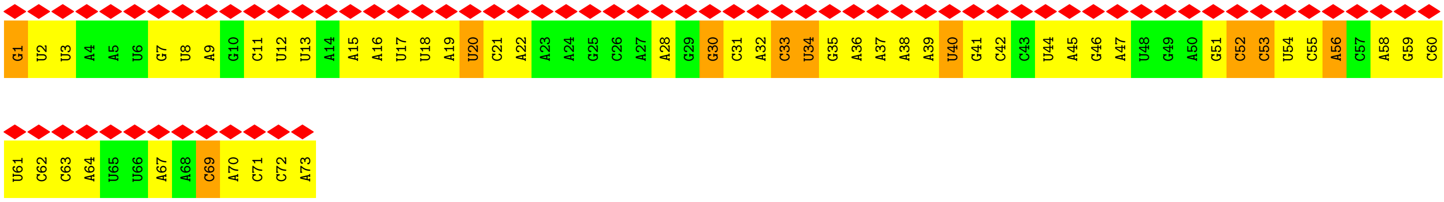
- Molecule 86: mRNA

Chain i4:



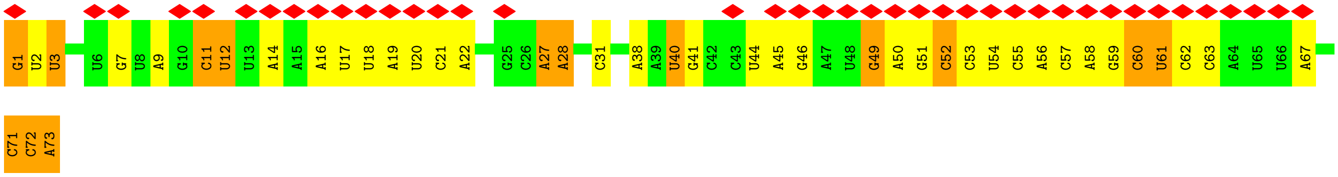
- Molecule 87: mt-tRNA

Chain 99:



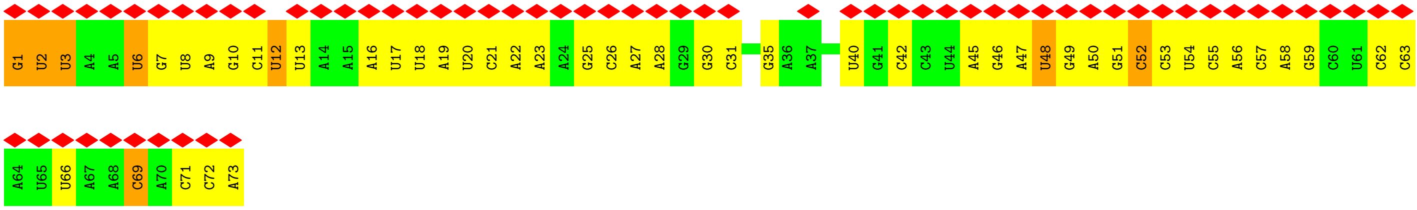
- Molecule 87: mt-tRNA

Chain 94:



- Molecule 87: mt-tRNA

Chain X:



4 Experimental information

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37415	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 ($e^-/\text{Å}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.501	Depositor
Minimum map value	-0.303	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MG, ZN, GDP

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	$\#\|Z\| > 5$
2	A3	1.34	26/35267 (0.1%)	1.40	573/54877 (1.0%)
3	B3	0.72	0/1328	1.30	11/2056 (0.5%)
4	D3	0.68	1/1879 (0.1%)	0.85	6/2527 (0.2%)
5	E3	0.68	1/2433 (0.0%)	0.85	6/3299 (0.2%)
6	F3	0.74	0/2071	0.89	7/2817 (0.2%)
7	H3	0.52	0/798	0.81	1/1073 (0.1%)
8	I3	0.50	0/1308	0.92	12/1761 (0.7%)
9	J3	0.40	0/1077	0.84	1/1452 (0.1%)
10	K3	0.68	1/1495 (0.1%)	0.86	3/2029 (0.1%)
11	L3	0.61	0/904	0.86	5/1218 (0.4%)
12	M3	0.63	0/2359	0.93	10/3185 (0.3%)
13	N3	0.59	0/1697	0.75	1/2281 (0.0%)
14	O3	0.64	0/1269	0.98	6/1708 (0.4%)
15	P3	0.64	0/1103	0.81	0/1491
16	Q3	0.59	0/1863	0.99	11/2509 (0.4%)
17	R3	0.75	1/1174 (0.1%)	0.86	3/1572 (0.2%)
18	S3	0.69	1/1276 (0.1%)	0.91	3/1729 (0.2%)
19	T3	0.71	0/1402	0.83	4/1886 (0.2%)
20	U3	0.68	0/946	0.89	2/1283 (0.2%)
21	V3	0.59	0/1590	0.98	8/2151 (0.4%)
22	W3	0.77	0/893	0.93	4/1204 (0.3%)
23	X3	0.62	1/2081 (0.0%)	0.85	5/2812 (0.2%)
24	Y3	0.62	0/1552	0.84	2/2079 (0.1%)
25	Z3	0.62	0/1003	0.82	2/1354 (0.1%)
26	03	0.59	0/895	0.85	1/1201 (0.1%)
27	13	0.62	0/438	1.02	2/583 (0.3%)
28	23	0.79	0/382	0.86	2/507 (0.4%)
29	33	0.77	0/852	0.87	2/1136 (0.2%)
30	43	0.75	0/329	0.70	0/435
31	53	0.62	1/3154 (0.0%)	0.89	11/4295 (0.3%)
32	63	0.59	0/2722	0.84	10/3709 (0.3%)
33	73	0.54	0/2207	0.82	4/2978 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
34	83	0.49	0/855	0.97	3/1152 (0.3%)
35	93	0.60	0/896	0.83	2/1205 (0.2%)
36	a3	0.66	0/709	0.82	2/963 (0.2%)
37	b3	0.64	0/1202	0.81	4/1626 (0.2%)
38	c3	0.55	0/2264	0.84	7/3059 (0.2%)
39	d3	0.52	0/1385	0.86	3/1877 (0.2%)
40	e3	0.43	0/1797	0.88	4/2422 (0.2%)
41	f3	0.56	0/1055	0.78	1/1427 (0.1%)
42	g3	0.67	1/1102 (0.1%)	0.80	1/1503 (0.1%)
43	h3	0.51	0/847	0.98	5/1150 (0.4%)
44	i3	0.73	0/849	1.00	5/1135 (0.4%)
45	j3	0.55	0/698	0.84	3/940 (0.3%)
46	k3	0.44	0/665	0.89	1/897 (0.1%)
47	l3	0.48	0/226	0.87	1/299 (0.3%)
48	m3	0.54	1/379 (0.3%)	0.85	2/510 (0.4%)
49	o3	0.65	0/818	0.86	4/1097 (0.4%)
50	p3	0.52	0/1071	0.83	4/1433 (0.3%)
51	q3	0.43	0/1107	0.70	0/1498
52	r3	0.63	0/1238	0.86	2/1676 (0.1%)
53	s3	0.63	1/3114 (0.0%)	0.84	10/4225 (0.2%)
55	B6	0.64	1/1811 (0.1%)	0.88	7/2451 (0.3%)
56	C6	0.59	0/1112	0.74	0/1505
57	D6	0.54	0/2607	0.89	9/3498 (0.3%)
58	E6	0.56	0/989	0.90	1/1335 (0.1%)
59	F6	0.50	0/1708	0.83	2/2291 (0.1%)
60	G6	0.49	0/2570	0.88	8/3443 (0.2%)
61	H6	0.62	0/1019	0.97	4/1379 (0.3%)
62	I6	0.55	0/1031	0.74	0/1390
63	J6	0.51	0/854	0.86	0/1148
64	K6	0.69	0/879	1.15	12/1182 (1.0%)
65	L6	0.52	0/1406	0.78	0/1878
66	M6	0.45	0/941	0.96	4/1265 (0.3%)
67	N6	0.58	0/864	0.96	5/1169 (0.4%)
68	O6	0.54	0/1580	0.93	7/2150 (0.3%)
69	P6	0.62	0/791	0.86	3/1062 (0.3%)
70	Q6	0.59	0/752	0.92	3/1001 (0.3%)
71	R6	0.47	0/2050	0.89	5/2770 (0.2%)
72	S6	0.52	0/1069	0.83	1/1441 (0.1%)
73	T6	0.57	0/1361	0.82	1/1829 (0.1%)
74	U6	0.47	0/1482	0.88	1/1987 (0.1%)
75	V6	0.43	0/2758	0.90	13/3724 (0.3%)
76	W6	0.51	0/778	0.83	1/1048 (0.1%)
77	X6	0.48	0/2596	0.92	10/3519 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
78	Y6	0.57	0/943	0.72	0/1274
79	Z6	0.53	0/757	0.97	1/1011 (0.1%)
80	a6	0.50	0/1727	0.96	7/2338 (0.3%)
81	b6	0.52	2/2121 (0.1%)	0.86	6/2873 (0.2%)
82	c6	0.49	0/939	1.01	8/1256 (0.6%)
83	d6	0.67	0/621	0.98	3/820 (0.4%)
84	e6	0.39	0/2859	0.75	5/3864 (0.1%)
85	A6	1.07	3/22053 (0.0%)	1.35	288/34324 (0.8%)
86	i4	0.86	0/220	1.26	1/341 (0.3%)
87	94	0.84	0/1731	1.62	46/2693 (1.7%)
87	99	0.61	0/1731	1.48	32/2693 (1.2%)
87	X	0.65	0/1731	1.47	37/2693 (1.4%)
All	All	0.86	42/172465 (0.0%)	1.11	1313/245936 (0.5%)

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
1	Y2	0	1
4	D3	0	1
5	E3	0	3
7	H3	0	1
8	I3	0	1
9	J3	0	3
10	K3	0	4
11	L3	0	1
12	M3	0	4
14	O3	0	1
16	Q3	0	2
17	R3	0	2
19	T3	0	2
21	V3	0	3
23	X3	0	2
24	Y3	0	1
25	Z3	0	1
26	03	0	2
30	43	0	1
31	53	0	3
32	63	0	6
33	73	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
35	93	0	1
39	d3	0	2
40	e3	0	1
41	f3	0	2
43	h3	0	3
45	j3	0	1
46	k3	0	1
51	q3	0	1
52	r3	0	1
53	s3	0	1
55	B6	0	2
57	D6	0	2
58	E6	0	2
59	F6	0	3
60	G6	0	1
61	H6	0	3
64	K6	0	1
68	O6	0	2
69	P6	0	2
70	Q6	0	1
71	R6	0	2
72	S6	0	1
74	U6	0	2
75	V6	0	2
76	W6	0	1
77	X6	0	2
78	Y6	0	2
79	Z6	0	2
82	c6	0	2
84	e6	0	2
All	All	0	97

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A3	1828	A	N9-C4	-8.08	1.33	1.37
23	X3	5	LYS	C-N	-8.02	1.15	1.34
2	A3	2646	G	N9-C4	-7.20	1.32	1.38
18	S3	57	SER	C-N	-6.92	1.18	1.34
2	A3	2582	A	C8-N7	-6.59	1.26	1.31
5	E3	251	VAL	CB-CG2	-6.25	1.39	1.52
53	s3	266	CYS	CB-SG	-6.22	1.71	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	A6	785	A	N9-C4	-5.92	1.34	1.37
17	R3	109	GLU	CG-CD	-5.85	1.43	1.51
48	m3	51	LEU	C-N	-5.83	1.20	1.34
2	A3	1789	A	N9-C4	-5.81	1.34	1.37
85	A6	1486	A	N9-C4	-5.80	1.34	1.37
2	A3	3029	A	N9-C4	-5.76	1.34	1.37
2	A3	2434	A	N7-C5	-5.72	1.35	1.39
31	53	235	PRO	C-N	-5.67	1.21	1.34
81	b6	88	GLY	C-N	-5.65	1.21	1.34
2	A3	2646	G	C2-N3	-5.55	1.28	1.32
10	K3	144	GLU	C-N	-5.54	1.21	1.34
2	A3	1867	A	N9-C4	-5.52	1.34	1.37
2	A3	2832	A	N7-C5	-5.51	1.35	1.39
2	A3	2646	G	N3-C4	-5.50	1.31	1.35
2	A3	2372	U	N3-C4	-5.49	1.33	1.38
2	A3	2909	G	C8-N7	-5.44	1.27	1.30
2	A3	2132	A	N9-C4	-5.37	1.34	1.37
2	A3	1994	A	N9-C4	-5.36	1.34	1.37
4	D3	134	CYS	CB-SG	-5.33	1.73	1.81
2	A3	2503	A	N9-C4	-5.30	1.34	1.37
2	A3	1885	A	N9-C4	-5.29	1.34	1.37
2	A3	1867	A	N3-C4	-5.25	1.31	1.34
81	b6	104	GLU	CD-OE1	-5.24	1.19	1.25
2	A3	2132	A	C5-C4	-5.24	1.35	1.38
85	A6	1014	A	N9-C4	-5.22	1.34	1.37
2	A3	1984	A	N7-C5	-5.21	1.36	1.39
2	A3	2295	C	N3-C4	-5.17	1.30	1.33
2	A3	2496	G	N7-C5	-5.16	1.36	1.39
2	A3	2694	A	N7-C5	-5.13	1.36	1.39
2	A3	2923	G	N7-C5	-5.12	1.36	1.39
2	A3	2582	A	N7-C5	-5.06	1.36	1.39
2	A3	2102	A	N7-C5	-5.04	1.36	1.39
42	g3	90	ARG	CB-CG	-5.02	1.39	1.52
2	A3	3151	A	N9-C4	-5.00	1.34	1.37
55	B6	165	TYR	CD2-CE2	-5.00	1.31	1.39

All (1313) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	A6	1530	U	N1-C2-O2	14.57	133.00	122.80
2	A3	1732	C	N1-C2-O2	13.36	126.91	118.90
64	K6	33	ARG	NE-CZ-NH1	-12.89	113.86	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	2523	C	N1-C2-O2	12.61	126.47	118.90
2	A3	2523	C	C2-N1-C1'	12.52	132.58	118.80
87	94	11	C	N1-C2-O2	12.38	126.33	118.90
2	A3	1693	C	N1-C2-O2	12.34	126.30	118.90
2	A3	2372	U	N3-C2-O2	-12.28	113.60	122.20
2	A3	1732	C	C2-N1-C1'	11.87	131.86	118.80
2	A3	2960	U	N1-C2-O2	11.73	131.01	122.80
16	Q3	204	MET	C-N-CA	11.60	150.70	121.70
2	A3	1699	C	N1-C2-O2	11.24	125.64	118.90
85	A6	1250	U	N3-C2-O2	-11.17	114.38	122.20
2	A3	3157	C	C2-N1-C1'	11.11	131.02	118.80
2	A3	1693	C	C2-N1-C1'	11.06	130.97	118.80
2	A3	2372	U	N1-C2-O2	11.06	130.54	122.80
2	A3	2522	U	C2-N1-C1'	11.06	130.97	117.70
85	A6	1373	U	N1-C2-O2	11.01	130.50	122.80
2	A3	1732	C	C6-N1-C2	-10.86	115.96	120.30
2	A3	2646	G	N3-C4-N9	-10.77	119.54	126.00
87	94	62	C	N1-C2-O2	10.76	125.36	118.90
2	A3	1699	C	N3-C2-O2	-10.71	114.40	121.90
85	A6	1530	U	N3-C2-O2	-10.68	114.72	122.20
2	A3	2030	U	C5-C6-N1	10.65	128.03	122.70
21	V3	53	ASP	CB-CG-OD1	10.54	127.79	118.30
2	A3	1732	C	N3-C2-O2	-10.51	114.54	121.90
2	A3	1693	C	N3-C2-O2	-10.35	114.65	121.90
2	A3	1837	C	N3-C2-O2	-10.35	114.66	121.90
85	A6	951	U	C5-C6-N1	10.28	127.84	122.70
85	A6	1433	C	C2-N1-C1'	10.25	130.08	118.80
2	A3	2746	U	N1-C2-O2	10.24	129.97	122.80
2	A3	2215	C	N1-C2-O2	10.24	125.04	118.90
85	A6	1250	U	N1-C2-O2	10.19	129.94	122.80
2	A3	2523	C	N3-C2-O2	-10.18	114.77	121.90
2	A3	2484	C	C2-N1-C1'	10.15	129.97	118.80
2	A3	2295	C	N3-C2-O2	-10.08	114.84	121.90
85	A6	709	C	N1-C2-O2	9.99	124.89	118.90
2	A3	1902	C	C2-N1-C1'	9.98	129.78	118.80
2	A3	1902	C	N1-C2-O2	9.98	124.89	118.90
85	A6	1237	C	N3-C2-O2	-9.97	114.92	121.90
2	A3	2960	U	N3-C2-O2	-9.95	115.23	122.20
87	X	11	C	N1-C2-O2	9.90	124.84	118.90
2	A3	1901	C	N1-C2-O2	9.90	124.84	118.90
2	A3	2746	U	N3-C2-O2	-9.89	115.27	122.20
60	G6	389	ARG	CG-CD-NE	-9.87	91.08	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A3	2522	U	N1-C2-O2	9.86	129.70	122.80
85	A6	1025	U	N3-C2-O2	-9.86	115.30	122.20
43	h3	125	ASP	CB-CG-OD1	9.83	127.14	118.30
2	A3	2030	U	C5-C4-O4	-9.81	120.02	125.90
2	A3	3204	C	C2-N1-C1’	9.76	129.53	118.80
2	A3	2582	A	N9-C4-C5	-9.75	101.90	105.80
85	A6	809	C	N1-C2-O2	9.69	124.71	118.90
2	A3	1699	C	C2-N1-C1’	9.68	129.45	118.80
85	A6	1373	U	N3-C2-O2	-9.65	115.45	122.20
2	A3	2284	C	C2-N1-C1’	9.58	129.33	118.80
2	A3	1902	C	N3-C2-O2	-9.52	115.23	121.90
2	A3	3212	C	C2-N1-C1’	9.49	129.24	118.80
2	A3	2952	U	N3-C2-O2	-9.47	115.57	122.20
85	A6	936	C	C2-N1-C1’	9.45	129.19	118.80
2	A3	1875	C	O5’-P-OP1	-9.43	97.21	105.70
60	G6	263	ASP	CB-CG-OD2	9.43	126.78	118.30
2	A3	3212	C	N1-C2-O2	9.42	124.55	118.90
2	A3	2582	A	N3-C4-N9	9.40	134.92	127.40
31	53	276	ASP	CB-CG-OD1	9.37	126.73	118.30
2	A3	2960	U	C2-N1-C1’	9.36	128.94	117.70
2	A3	2005	C	C6-N1-C2	-9.35	116.56	120.30
2	A3	2484	C	N1-C2-O2	9.32	124.49	118.90
2	A3	1807	U	N3-C2-O2	-9.31	115.68	122.20
85	A6	1208	C	C6-N1-C2	-9.31	116.58	120.30
3	B3	1607	U	C2-N1-C1’	9.30	128.86	117.70
85	A6	1541	C	N3-C2-O2	-9.29	115.40	121.90
10	K3	164	ASP	CB-CG-OD1	9.29	126.66	118.30
2	A3	2079	C	C2-N1-C1’	9.28	129.01	118.80
2	A3	1837	C	N1-C2-O2	9.28	124.47	118.90
85	A6	1541	C	C6-N1-C2	-9.25	116.60	120.30
85	A6	717	C	N1-C2-O2	9.23	124.44	118.90
2	A3	1807	U	N1-C2-O2	9.21	129.25	122.80
85	A6	1193	U	C2-N1-C1’	9.20	128.74	117.70
64	K6	67	LEU	CA-CB-CG	9.20	136.46	115.30
87	94	52	C	C5-C6-N1	9.19	125.59	121.00
53	s3	148	ASP	CB-CG-OD2	9.17	126.55	118.30
2	A3	2824	C	C6-N1-C2	-9.16	116.64	120.30
2	A3	2061	C	C2-N1-C1’	9.12	128.83	118.80
85	A6	1433	C	C6-N1-C2	-9.11	116.66	120.30
87	94	52	C	C6-N1-C2	-9.10	116.66	120.30
85	A6	957	U	N3-C2-O2	-9.10	115.83	122.20
2	A3	3077	C	C5-C6-N1	9.08	125.54	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	X6	335	ASP	CB-CG-OD2	9.06	126.45	118.30
2	A3	2329	C	N1-C2-O2	9.05	124.33	118.90
2	A3	2329	C	N3-C2-O2	-9.04	115.57	121.90
61	H6	126	ILE	CG1-CB-CG2	-9.03	91.54	111.40
2	A3	1732	C	C5-C6-N1	9.01	125.51	121.00
2	A3	1707	C	C2-N1-C1’	9.00	128.70	118.80
5	E3	301	ASP	CB-CG-OD2	8.97	126.38	118.30
85	A6	1237	C	N1-C2-O2	8.97	124.28	118.90
85	A6	1433	C	N1-C2-O2	8.94	124.26	118.90
2	A3	2523	C	C6-N1-C1’	-8.93	110.09	120.80
2	A3	2295	C	N1-C2-O2	8.92	124.25	118.90
2	A3	2493	C	C2-N1-C1’	8.91	128.60	118.80
85	A6	1247	U	N3-C2-O2	-8.90	115.97	122.20
2	A3	2224	C	C2-N1-C1’	8.88	128.57	118.80
85	A6	709	C	N3-C2-O2	-8.84	115.71	121.90
85	A6	1282	C	C6-N1-C2	-8.84	116.77	120.30
85	A6	1150	C	C5-C6-N1	8.83	125.42	121.00
2	A3	1901	C	N3-C2-O2	-8.83	115.72	121.90
44	i3	38	LEU	CA-CB-CG	8.81	135.57	115.30
2	A3	3157	C	C6-N1-C1’	-8.80	110.24	120.80
85	A6	769	C	C2-N1-C1’	8.78	128.46	118.80
74	U6	30	ARG	CA-CB-CG	8.76	132.67	113.40
85	A6	1395	U	N3-C2-O2	-8.75	116.08	122.20
85	A6	969	C	N3-C2-O2	-8.73	115.79	121.90
2	A3	2494	C	N3-C2-O2	-8.70	115.81	121.90
10	K3	25	MET	CA-CB-CG	8.69	128.08	113.30
11	L3	71	ASP	CB-CG-OD1	8.69	126.12	118.30
2	A3	2493	C	N1-C2-O2	8.67	124.10	118.90
85	A6	1181	C	C6-N1-C2	-8.66	116.84	120.30
2	A3	2235	C	C2-N1-C1’	8.64	128.31	118.80
85	A6	1150	C	C6-N1-C2	-8.63	116.85	120.30
2	A3	2079	C	N3-C2-O2	-8.60	115.88	121.90
2	A3	3204	C	N3-C2-O2	-8.60	115.88	121.90
87	99	40	U	C2-N1-C1’	8.60	128.01	117.70
85	A6	957	U	N1-C2-O2	8.59	128.81	122.80
14	O3	84	ASP	CB-CG-OD1	8.57	126.01	118.30
2	A3	1837	C	C2-N1-C1’	8.55	128.21	118.80
85	A6	709	C	C2-N1-C1’	8.56	128.21	118.80
85	A6	1541	C	N1-C2-O2	8.54	124.02	118.90
85	A6	710	C	C2-N1-C1’	8.51	128.16	118.80
2	A3	2386	C	C2-N1-C1’	8.51	128.16	118.80
85	A6	1433	C	N3-C2-O2	-8.50	115.95	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	A6	969	C	N1-C2-O2	8.49	124.00	118.90
85	A6	1393	G	C8-N9-C4	-8.49	103.00	106.40
2	A3	1693	C	C6-N1-C2	-8.48	116.91	120.30
85	A6	936	C	N1-C2-O2	8.46	123.98	118.90
2	A3	2211	U	N3-C2-O2	-8.46	116.28	122.20
2	A3	1901	C	C2-N1-C1'	8.45	128.10	118.80
2	A3	2235	C	N3-C2-O2	-8.45	115.99	121.90
2	A3	3228	U	N3-C2-O2	-8.44	116.30	122.20
87	94	62	C	N3-C2-O2	-8.43	116.00	121.90
2	A3	2898	U	N3-C2-O2	-8.41	116.31	122.20
85	A6	1486	A	O4'-C1'-N9	8.40	114.92	108.20
2	A3	2493	C	N3-C2-O2	-8.36	116.05	121.90
12	M3	261	ASP	CB-CG-OD1	8.36	125.82	118.30
16	Q3	162	ILE	CG1-CB-CG2	-8.36	93.01	111.40
2	A3	2080	U	N3-C2-O2	-8.36	116.35	122.20
16	Q3	106	LEU	CA-CB-CG	8.36	134.52	115.30
55	B6	94	LYS	CD-CE-NZ	-8.36	92.48	111.70
87	94	62	C	C2-N1-C1'	8.34	127.98	118.80
2	A3	2909	G	C6-C5-N7	-8.34	125.40	130.40
2	A3	3157	C	C5-C6-N1	8.33	125.17	121.00
79	Z6	73	ASP	CB-CG-OD1	8.33	125.80	118.30
2	A3	2522	U	C6-N1-C1'	-8.33	109.54	121.20
85	A6	1451	G	C4-N9-C1'	8.32	137.31	126.50
87	94	53	C	C6-N1-C2	-8.31	116.97	120.30
2	A3	2578	C	N1-C2-O2	8.31	123.88	118.90
2	A3	2079	C	N1-C2-O2	8.29	123.88	118.90
2	A3	2582	A	C6-C5-N7	-8.29	126.50	132.30
87	94	60	C	N3-C2-O2	-8.28	116.10	121.90
2	A3	1707	C	N1-C2-O2	8.23	123.84	118.90
2	A3	3170	C	N1-C2-O2	8.22	123.83	118.90
71	R6	281	ILE	CG1-CB-CG2	-8.21	93.34	111.40
4	D3	180	ASP	CB-CG-OD1	8.20	125.68	118.30
87	X	52	C	N1-C2-O2	8.20	123.82	118.90
2	A3	2386	C	N1-C2-O2	8.20	123.82	118.90
85	A6	714	U	C2-N1-C1'	8.20	127.53	117.70
85	A6	1417	U	C5-C6-N1	8.19	126.79	122.70
2	A3	2588	C	C6-N1-C2	-8.18	117.03	120.30
85	A6	702	C	C6-N1-C2	-8.14	117.04	120.30
2	A3	2334	C	C5-C6-N1	8.13	125.07	121.00
2	A3	1813	C	N1-C2-O2	8.13	123.78	118.90
87	94	11	C	C2-N3-C4	8.13	123.97	119.90
87	94	60	C	N1-C2-O2	8.12	123.78	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	1530	U	C2-N1-C1’	8.12	127.44	117.70
2	A3	1902	C	C6-N1-C2	-8.11	117.06	120.30
2	A3	3173	G	C8-N9-C4	-8.11	103.16	106.40
2	A3	3151	A	O4’-C1’-N9	8.10	114.68	108.20
85	A6	1193	U	N3-C2-O2	-8.10	116.53	122.20
85	A6	1451	G	C8-N9-C1’	-8.10	116.46	127.00
53	s3	409	ASP	CB-CG-OD1	8.09	125.58	118.30
2	A3	3204	C	C6-N1-C2	-8.09	117.07	120.30
16	Q3	185	ASP	CB-CG-OD1	8.07	125.56	118.30
2	A3	1726	C	C6-N1-C2	-8.07	117.07	120.30
2	A3	3093	C	C5-C6-N1	8.06	125.03	121.00
85	A6	1208	C	N3-C2-O2	-8.06	116.26	121.90
82	c6	6	LEU	CB-CG-CD2	-8.05	97.31	111.00
2	A3	2079	C	C6-N1-C2	-8.03	117.09	120.30
28	23	49	ARG	NE-CZ-NH2	-8.03	116.29	120.30
87	99	11	C	N1-C2-O2	8.03	123.72	118.90
2	A3	3077	C	C6-N1-C2	-8.02	117.09	120.30
60	G6	373	ASP	CB-CG-OD2	8.02	125.51	118.30
2	A3	2557	C	C2-N1-C1’	8.01	127.61	118.80
85	A6	1282	C	C5-C6-N1	7.99	125.00	121.00
2	A3	2190	C	C2-N1-C1’	7.99	127.58	118.80
87	94	53	C	N1-C2-O2	7.98	123.69	118.90
2	A3	2898	U	C2-N1-C1’	7.98	127.28	117.70
2	A3	2898	U	N1-C2-O2	7.98	128.39	122.80
64	K6	105	ARG	NE-CZ-NH2	-7.96	116.32	120.30
3	B3	1607	U	N1-C2-O2	7.96	128.37	122.80
2	A3	2066	C	C2-N1-C1’	7.92	127.51	118.80
87	94	71	C	C5-C6-N1	7.92	124.96	121.00
87	99	31	C	C6-N1-C2	-7.92	117.13	120.30
87	94	53	C	C5-C6-N1	7.91	124.95	121.00
85	A6	1193	U	N1-C2-O2	7.90	128.33	122.80
12	M3	250	ASP	CB-CG-OD1	7.89	125.40	118.30
2	A3	1984	A	C5-N7-C8	-7.89	99.96	103.90
2	A3	1984	A	N7-C8-N9	7.89	117.74	113.80
85	A6	717	C	C2-N1-C1’	7.88	127.46	118.80
2	A3	2581	A	O4’-C1’-N9	7.87	114.50	108.20
2	A3	3192	C	N1-C2-O2	7.87	123.62	118.90
85	A6	936	C	N3-C2-O2	-7.86	116.40	121.90
85	A6	1373	U	C2-N1-C1’	7.84	127.11	117.70
2	A3	1807	U	C2-N1-C1’	7.82	127.09	117.70
85	A6	957	U	C2-N1-C1’	7.82	127.08	117.70
57	D6	410	ASP	CB-CG-OD1	7.81	125.33	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	X	52	C	C2-N1-C1'	7.81	127.39	118.80
2	A3	2165	C	C6-N1-C2	-7.80	117.18	120.30
85	A6	1379	C	C6-N1-C2	-7.80	117.18	120.30
57	D6	171	ASP	CB-CG-OD2	7.80	125.32	118.30
2	A3	2224	C	N1-C2-O2	7.79	123.57	118.90
85	A6	1376	C	C5-C6-N1	7.79	124.89	121.00
22	W3	74	ARG	CB-CG-CD	7.78	131.84	111.60
87	94	71	C	C6-N1-C2	-7.78	117.19	120.30
2	A3	2215	C	N3-C2-O2	-7.77	116.46	121.90
87	94	62	C	C6-N1-C2	-7.77	117.19	120.30
2	A3	2211	U	N1-C2-O2	7.76	128.23	122.80
2	A3	2653	C	C6-N1-C2	-7.75	117.20	120.30
68	O6	143	CYS	CA-CB-SG	7.74	127.94	114.00
2	A3	3170	C	C2-N1-C1'	7.73	127.31	118.80
2	A3	1840	C	C6-N1-C2	-7.73	117.21	120.30
2	A3	2080	U	C2-N1-C1'	7.72	126.97	117.70
85	A6	1471	C	N1-C2-O2	7.72	123.53	118.90
85	A6	1451	G	C6-C5-N7	-7.72	125.77	130.40
87	X	11	C	N3-C2-O2	-7.70	116.51	121.90
2	A3	2557	C	C6-N1-C2	-7.70	117.22	120.30
2	A3	2824	C	C5-C6-N1	7.69	124.85	121.00
23	X3	180	ASP	CB-CG-OD2	7.69	125.22	118.30
16	Q3	84	ARG	CA-CB-CG	7.68	130.30	113.40
85	A6	1451	G	N3-C4-N9	7.68	130.61	126.00
85	A6	951	U	C2-N1-C1'	7.67	126.91	117.70
60	G6	299	ASP	CB-CG-OD1	7.67	125.20	118.30
87	99	33	C	N1-C2-O2	7.67	123.50	118.90
2	A3	3172	C	N1-C2-O2	7.65	123.49	118.90
39	d3	182	ARG	NE-CZ-NH1	7.61	124.11	120.30
77	X6	255	MET	CA-CB-CG	7.61	126.23	113.30
2	A3	1699	C	C6-N1-C2	-7.61	117.26	120.30
85	A6	1490	C	C6-N1-C2	-7.60	117.26	120.30
85	A6	809	C	N3-C2-O2	-7.59	116.58	121.90
85	A6	717	C	N3-C2-O2	-7.58	116.60	121.90
85	A6	1227	C	C5-C6-N1	7.57	124.79	121.00
2	A3	3134	C	N1-C2-O2	7.56	123.44	118.90
87	X	11	C	C2-N1-C1'	7.56	127.11	118.80
2	A3	2215	C	C2-N1-C1'	7.55	127.11	118.80
57	D6	320	ILE	CG1-CB-CG2	-7.55	94.79	111.40
14	O3	71	ARG	NE-CZ-NH1	7.54	124.07	120.30
85	A6	1366	G	N9-C4-C5	7.54	108.42	105.40
85	A6	1376	C	C6-N1-C2	-7.53	117.29	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	M6	68	LEU	CA-CB-CG	7.52	132.60	115.30
85	A6	1227	C	C6-N1-C2	-7.51	117.30	120.30
67	N6	46	ARG	CG-CD-NE	7.50	127.56	111.80
38	c3	119	LEU	CA-CB-CG	7.50	132.55	115.30
87	94	12	U	N1-C2-O2	7.50	128.05	122.80
4	D3	147	ARG	NE-CZ-NH2	7.50	124.05	120.30
2	A3	2284	C	C6-N1-C2	-7.50	117.30	120.30
85	A6	728	C	C6-N1-C2	-7.49	117.30	120.30
2	A3	1810	A	O5'-P-OP1	-7.49	98.96	105.70
2	A3	2646	G	N3-C4-C5	7.45	132.32	128.60
19	T3	204	ARG	NE-CZ-NH1	7.44	124.02	120.30
2	A3	1726	C	C5-C6-N1	7.43	124.72	121.00
2	A3	2523	C	C6-N1-C2	-7.43	117.33	120.30
2	A3	1783	U	N3-C2-O2	-7.43	117.00	122.20
2	A3	2235	C	N1-C2-O2	7.42	123.35	118.90
2	A3	3204	C	N1-C2-O2	7.42	123.35	118.90
2	A3	1828	A	C2-N3-C4	-7.41	106.89	110.60
87	X	63	C	C5-C6-N1	7.41	124.70	121.00
8	I3	174	LEU	CA-CB-CG	7.40	132.32	115.30
82	c6	6	LEU	CA-CB-CG	7.39	132.31	115.30
2	A3	2379	C	N1-C2-O2	7.39	123.33	118.90
87	99	40	U	C5-C6-N1	7.38	126.39	122.70
2	A3	3170	C	N3-C2-O2	-7.37	116.74	121.90
2	A3	2582	A	C4-C5-N7	7.37	114.38	110.70
2	A3	2066	C	N1-C2-O2	7.36	123.32	118.90
22	W3	49	ARG	NE-CZ-NH2	7.36	123.98	120.30
8	I3	177	LEU	CA-CB-CG	7.36	132.22	115.30
87	99	69	C	C2-N1-C1'	7.35	126.88	118.80
2	A3	1813	C	N3-C2-O2	-7.34	116.76	121.90
85	A6	715	U	C2-N1-C1'	7.34	126.51	117.70
2	A3	2215	C	C6-N1-C2	-7.34	117.37	120.30
43	h3	64	GLU	CA-CB-CG	7.34	129.54	113.40
34	83	96	ASP	CB-CG-OD1	7.33	124.90	118.30
85	A6	1367	C	C5-C6-N1	7.33	124.66	121.00
2	A3	2372	U	C5-C6-N1	7.33	126.36	122.70
2	A3	2484	C	C6-N1-C1'	-7.33	112.01	120.80
87	94	52	C	N1-C2-O2	7.32	123.29	118.90
85	A6	1324	G	O4'-C1'-N9	7.31	114.05	108.20
85	A6	1366	G	N1-C6-O6	-7.31	115.52	119.90
2	A3	2474	C	C6-N1-C2	-7.31	117.38	120.30
2	A3	2005	C	C5-C6-N1	7.30	124.65	121.00
2	A3	2900	C	C5-C6-N1	7.30	124.65	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	717	C	C6-N1-C2	-7.29	117.38	120.30
2	A3	1975	U	C5-C6-N1	7.29	126.35	122.70
2	A3	1835	A	O4'-C1'-N9	7.29	114.03	108.20
2	A3	1732	C	C6-N1-C1'	-7.27	112.07	120.80
2	A3	2427	C	C2-N1-C1'	7.26	126.79	118.80
2	A3	2061	C	N1-C2-O2	7.26	123.25	118.90
85	A6	1530	U	C6-N1-C1'	-7.26	111.04	121.20
2	A3	1693	C	C6-N1-C1'	-7.25	112.10	120.80
3	B3	1663	C	C6-N1-C2	-7.25	117.40	120.30
85	A6	1070	C	C6-N1-C2	-7.25	117.40	120.30
2	A3	2684	C	N3-C2-O2	-7.23	116.84	121.90
87	94	71	C	C2-N1-C1'	7.23	126.75	118.80
5	E3	331	ASP	CB-CG-OD1	7.23	124.80	118.30
2	A3	3201	A	OP1-P-O3'	7.22	121.08	105.20
2	A3	1813	C	C2-N1-C1'	7.21	126.73	118.80
2	A3	2557	C	N1-C2-O2	7.21	123.23	118.90
2	A3	2580	U	C5-C6-N1	7.21	126.31	122.70
39	d3	241	ASP	CB-CG-OD1	7.21	124.79	118.30
75	V6	57	MET	CA-CB-CG	7.21	125.55	113.30
85	A6	1395	U	N1-C2-O2	7.20	127.84	122.80
2	A3	3212	C	C6-N1-C2	-7.20	117.42	120.30
64	K6	105	ARG	CB-CG-CD	7.18	130.27	111.60
2	A3	2190	C	C6-N1-C2	-7.17	117.43	120.30
2	A3	2900	C	C6-N1-C2	-7.15	117.44	120.30
2	A3	3173	G	N7-C8-N9	7.12	116.66	113.10
2	A3	3043	C	N1-C2-O2	7.12	123.17	118.90
85	A6	1025	U	P-O3'-C3'	7.12	128.24	119.70
85	A6	852	U	C5-C6-N1	7.12	126.26	122.70
85	A6	1536	C	N1-C2-O2	7.12	123.17	118.90
85	A6	1379	C	C5-C6-N1	7.10	124.55	121.00
16	Q3	152	ARG	NE-CZ-NH1	7.09	123.85	120.30
85	A6	1070	C	C5-C6-N1	7.09	124.55	121.00
16	Q3	271	ARG	NE-CZ-NH1	7.09	123.84	120.30
2	A3	2219	C	C2-N1-C1'	7.09	126.60	118.80
2	A3	2909	G	C4-C5-N7	7.09	113.64	110.80
85	A6	1000	A	N7-C8-N9	7.07	117.34	113.80
2	A3	2329	C	C6-N1-C2	-7.06	117.48	120.30
2	A3	2728	C	C6-N1-C2	-7.05	117.48	120.30
2	A3	2334	C	C6-N1-C2	-7.04	117.48	120.30
2	A3	2484	C	C5-C6-N1	7.04	124.52	121.00
85	A6	1025	U	N1-C2-O2	7.03	127.72	122.80
85	A6	1195	C	C6-N1-C2	-7.03	117.49	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	i3	80	LEU	CB-CG-CD1	7.03	122.95	111.00
2	A3	1806	U	P-O3'-C3'	7.03	128.13	119.70
60	G6	122	ARG	CG-CD-NE	7.02	126.55	111.80
87	X	12	U	C2-N1-C1'	7.01	126.11	117.70
2	A3	3151	A	C5-N7-C8	-7.00	100.40	103.90
21	V3	191	LEU	CA-CB-CG	7.00	131.41	115.30
2	A3	2490	C	C6-N1-C2	-7.00	117.50	120.30
85	A6	1392	C	C2-N1-C1'	7.00	126.50	118.80
42	g3	90	ARG	CG-CD-NE	-7.00	97.10	111.80
49	o3	93	ASP	CB-CG-OD1	7.00	124.60	118.30
2	A3	2952	U	N1-C2-O2	6.99	127.69	122.80
80	a6	49	ARG	NE-CZ-NH1	6.99	123.79	120.30
2	A3	2087	U	C5-C6-N1	6.98	126.19	122.70
2	A3	3212	C	N3-C2-O2	-6.98	117.01	121.90
85	A6	1398	C	C2-N1-C1'	6.98	126.48	118.80
31	53	98	LEU	CA-CB-CG	6.98	131.35	115.30
2	A3	2061	C	N3-C2-O2	-6.98	117.02	121.90
2	A3	2909	G	N7-C8-N9	6.97	116.59	113.10
2	A3	1701	U	C2-N1-C1'	6.97	126.07	117.70
8	I3	131	LEU	CA-CB-CG	6.97	131.34	115.30
85	A6	936	C	C6-N1-C1'	-6.97	112.43	120.80
12	M3	57	ARG	NE-CZ-NH2	6.96	123.78	120.30
77	X6	163	LYS	CA-CB-CG	6.96	128.71	113.40
49	o3	67	ARG	NE-CZ-NH1	-6.94	116.83	120.30
55	B6	100	ARG	CB-CG-CD	-6.94	93.56	111.60
55	B6	88	ARG	NE-CZ-NH1	6.94	123.77	120.30
2	A3	2284	C	N1-C2-O2	6.93	123.06	118.90
2	A3	2522	U	N3-C2-O2	-6.93	117.35	122.20
58	E6	117	LEU	CB-CG-CD1	-6.93	99.22	111.00
85	A6	1530	U	O4'-C1'-N1	6.92	113.73	108.20
2	A3	2379	C	C2-N1-C1'	6.91	126.40	118.80
2	A3	2372	U	C6-N1-C2	-6.91	116.85	121.00
85	A6	1263	U	C2-N1-C1'	6.91	125.99	117.70
2	A3	2698	G	N3-C2-N2	-6.90	115.07	119.90
85	A6	1237	C	C2-N1-C1'	6.90	126.39	118.80
2	A3	1770	G	N3-C2-N2	-6.90	115.07	119.90
53	s3	269	ASP	CB-CG-OD1	6.87	124.49	118.30
44	i3	63	LEU	CA-CB-CG	6.87	131.10	115.30
85	A6	1398	C	C5-C6-N1	6.87	124.44	121.00
85	A6	1395	U	C2-N1-C1'	6.86	125.94	117.70
73	T6	155	LEU	CA-CB-CG	6.86	131.08	115.30
16	Q3	246	ASP	CB-CG-OD1	6.86	124.47	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	1984	A	C4-C5-N7	6.85	114.13	110.70
2	A3	1689	C	C2-N1-C1'	6.85	126.34	118.80
2	A3	3134	C	N3-C2-O2	-6.84	117.11	121.90
2	A3	2646	G	N9-C4-C5	6.83	108.13	105.40
87	94	62	C	C5-C6-N1	6.83	124.41	121.00
53	s3	235	ASP	CB-CG-OD1	6.82	124.44	118.30
2	A3	3169	C	C2-N1-C1'	6.82	126.30	118.80
85	A6	1183	G	N3-C4-N9	-6.82	121.91	126.00
85	A6	1367	C	C6-N1-C2	-6.82	117.57	120.30
22	W3	74	ARG	CA-CB-CG	6.82	128.39	113.40
2	A3	3134	C	C6-N1-C2	-6.81	117.58	120.30
75	V6	230	LEU	CA-CB-CG	6.81	130.96	115.30
2	A3	3009	C	N3-C2-O2	-6.80	117.14	121.90
18	S3	68	ASP	CB-CG-OD2	6.80	124.42	118.30
85	A6	1247	U	N1-C2-O2	6.80	127.56	122.80
87	99	34	U	N3-C2-O2	-6.79	117.45	122.20
87	X	52	C	C5-C6-N1	6.79	124.39	121.00
2	A3	2210	C	C6-N1-C2	-6.78	117.59	120.30
2	A3	2900	C	C2-N1-C1'	6.78	126.26	118.80
75	V6	117	LEU	CA-CB-CG	6.78	130.88	115.30
85	A6	1392	C	N1-C2-O2	6.78	122.97	118.90
59	F6	209	LEU	CA-CB-CG	6.77	130.88	115.30
85	A6	710	C	C6-N1-C1'	-6.77	112.67	120.80
2	A3	3077	C	C2-N1-C1'	6.77	126.25	118.80
71	R6	292	ASP	CB-CG-OD2	6.77	124.39	118.30
2	A3	2066	C	C6-N1-C1'	-6.76	112.69	120.80
85	A6	1393	G	N7-C8-N9	6.75	116.48	113.10
2	A3	3169	C	N1-C2-O2	6.75	122.95	118.90
3	B3	1607	U	C6-N1-C1'	-6.75	111.75	121.20
80	a6	96	ARG	NE-CZ-NH2	6.75	123.68	120.30
2	A3	2961	C	N1-C2-O2	6.75	122.95	118.90
2	A3	2284	C	N3-C2-O2	-6.74	117.18	121.90
85	A6	1093	U	N3-C2-O2	-6.74	117.48	122.20
70	Q6	50	ARG	NE-CZ-NH1	6.74	123.67	120.30
85	A6	1195	C	C2-N1-C1'	6.74	126.21	118.80
85	A6	709	C	C6-N1-C2	-6.73	117.61	120.30
2	A3	2224	C	C6-N1-C2	-6.73	117.61	120.30
2	A3	2113	G	O5'-P-OP2	-6.72	99.65	105.70
2	A3	2235	C	C6-N1-C2	-6.72	117.61	120.30
87	99	69	C	C6-N1-C2	-6.71	117.61	120.30
85	A6	797	C	N1-C2-O2	6.71	122.92	118.90
14	O3	144	LEU	CA-CB-CG	6.71	130.72	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	P6	67	LEU	CA-CB-CG	6.71	130.72	115.30
2	A3	2061	C	C6-N1-C2	-6.70	117.62	120.30
87	94	52	C	C2-N1-C1'	6.70	126.17	118.80
45	j3	53	ASP	CB-CG-OD1	6.69	124.32	118.30
77	X6	232	ARG	NE-CZ-NH1	6.69	123.65	120.30
2	A3	2684	C	N1-C2-O2	6.69	122.91	118.90
85	A6	1433	C	P-O3'-C3'	6.68	127.72	119.70
87	94	72	C	C6-N1-C2	-6.68	117.63	120.30
16	Q3	235	ARG	NE-CZ-NH1	6.68	123.64	120.30
85	A6	873	C	C6-N1-C2	-6.67	117.63	120.30
4	D3	138	ASP	CB-CG-OD1	6.67	124.30	118.30
2	A3	2080	U	N1-C2-O2	6.66	127.47	122.80
2	A3	1840	C	C5-C6-N1	6.66	124.33	121.00
85	A6	951	U	C5-C4-O4	-6.66	121.91	125.90
85	A6	921	C	C6-N1-C2	-6.65	117.64	120.30
2	A3	1901	C	C6-N1-C2	-6.65	117.64	120.30
2	A3	2909	G	N3-C4-N9	6.64	129.99	126.00
6	F3	274	LEU	CB-CG-CD1	-6.64	99.70	111.00
82	c6	38	ARG	NE-CZ-NH1	6.64	123.62	120.30
2	A3	1823	A	P-O3'-C3'	6.64	127.67	119.70
2	A3	2557	C	N3-C2-O2	-6.63	117.26	121.90
2	A3	2522	U	C5-C6-N1	6.63	126.01	122.70
2	A3	3056	C	C6-N1-C2	-6.62	117.65	120.30
85	A6	1052	C	C6-N1-C2	-6.62	117.65	120.30
2	A3	1711	C	C6-N1-C2	-6.61	117.66	120.30
2	A3	2494	C	N1-C2-O2	6.61	122.86	118.90
2	A3	1993	A	C8-N9-C4	-6.60	103.16	105.80
43	h3	66	LEU	CA-CB-CG	6.60	130.48	115.30
2	A3	1689	C	N3-C2-O2	-6.60	117.28	121.90
2	A3	3157	C	N1-C2-O2	6.59	122.86	118.90
85	A6	1366	G	C8-N9-C4	-6.59	103.76	106.40
38	c3	67	ASP	CB-CG-OD1	6.59	124.23	118.30
2	A3	1707	C	C6-N1-C1'	-6.59	112.90	120.80
87	94	11	C	N3-C2-O2	-6.58	117.29	121.90
85	A6	1308	C	C6-N1-C2	-6.58	117.67	120.30
87	99	53	C	C5-C6-N1	6.57	124.28	121.00
2	A3	2684	C	C2-N1-C1'	6.56	126.02	118.80
85	A6	1398	C	C6-N1-C2	-6.56	117.68	120.30
87	99	30	G	O4'-C1'-N9	6.56	113.45	108.20
64	K6	90	ARG	NE-CZ-NH1	-6.55	117.02	120.30
2	A3	3043	C	C5-C6-N1	6.55	124.28	121.00
6	F3	168	LYS	CD-CE-NZ	-6.55	96.63	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	R3	10	LEU	CA-CB-CG	6.55	130.36	115.30
2	A3	1701	U	N3-C2-O2	-6.55	117.62	122.20
2	A3	1732	C	C2-N3-C4	6.54	123.17	119.90
3	B3	1637	C	C6-N1-C2	-6.54	117.68	120.30
85	A6	1189	C	C2-N1-C1'	6.54	126.00	118.80
75	V6	208	LEU	CA-CB-CG	6.54	130.34	115.30
85	A6	721	G	P-O3'-C3'	6.54	127.55	119.70
2	A3	2667	U	N3-C2-O2	-6.54	117.62	122.20
87	94	73	A	C8-N9-C4	-6.54	103.19	105.80
2	A3	3009	C	C2-N1-C1'	6.53	125.99	118.80
38	c3	220	ILE	CG1-CB-CG2	-6.53	97.03	111.40
85	A6	1238	C	C2-N1-C1'	6.53	125.98	118.80
33	73	119	LEU	CA-CB-CG	6.53	130.31	115.30
2	A3	1993	A	N7-C8-N9	6.53	117.06	113.80
2	A3	2386	C	N3-C2-O2	-6.52	117.33	121.90
2	A3	2639	C	C6-N1-C2	-6.52	117.69	120.30
2	A3	3192	C	N3-C2-O2	-6.52	117.33	121.90
2	A3	2728	C	C5-C6-N1	6.52	124.26	121.00
57	D6	180	ASP	CB-CG-OD1	6.52	124.17	118.30
2	A3	3204	C	O4'-C1'-N1	6.52	113.41	108.20
2	A3	2593	G	O4'-C1'-N9	6.51	113.41	108.20
2	A3	2132	A	N1-C6-N6	-6.50	114.70	118.60
2	A3	2243	A	P-O3'-C3'	6.50	127.50	119.70
2	A3	1725	C	C6-N1-C2	-6.49	117.70	120.30
12	M3	100	ARG	NE-CZ-NH1	6.49	123.55	120.30
87	94	12	U	N3-C2-O2	-6.49	117.66	122.20
85	A6	745	A	N9-C4-C5	-6.49	103.21	105.80
2	A3	2559	U	P-O3'-C3'	6.48	127.47	119.70
85	A6	809	C	C2-N1-C1'	6.48	125.93	118.80
85	A6	1000	A	C8-N9-C4	-6.48	103.21	105.80
85	A6	1522	C	N1-C2-O2	6.47	122.78	118.90
8	I3	143	LEU	CA-CB-CG	6.47	130.18	115.30
2	A3	1944	C	C6-N1-C2	-6.46	117.72	120.30
87	X	12	U	N1-C2-O2	6.46	127.32	122.80
8	I3	146	LEU	CA-CB-CG	6.45	130.14	115.30
85	A6	1084	A	O4'-C1'-N9	6.45	113.36	108.20
40	e3	97	ARG	NE-CZ-NH1	6.45	123.52	120.30
2	A3	2224	C	N3-C2-O2	-6.44	117.39	121.90
2	A3	1721	C	N1-C2-O2	6.44	122.76	118.90
33	73	47	LEU	CA-CB-CG	6.44	130.10	115.30
77	X6	163	LYS	CD-CE-NZ	-6.44	96.89	111.70
85	A6	682	U	N3-C2-O2	-6.43	117.70	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	678	U	C5-C6-N1	6.43	125.92	122.70
52	r3	94	ARG	NE-CZ-NH1	6.42	123.51	120.30
2	A3	2569	C	N1-C2-O2	6.41	122.75	118.90
3	B3	1607	U	N3-C2-O2	-6.41	117.72	122.20
2	A3	2030	U	C4-C5-C6	-6.40	115.86	119.70
2	A3	2541	C	C5-C6-N1	6.40	124.20	121.00
85	A6	812	C	N3-C2-O2	-6.40	117.42	121.90
85	A6	769	C	C6-N1-C1'	-6.40	113.12	120.80
20	U3	79	ARG	NE-CZ-NH2	-6.39	117.11	120.30
24	Y3	228	ARG	NE-CZ-NH1	6.38	123.49	120.30
85	A6	1433	C	C6-N1-C1'	-6.38	113.14	120.80
2	A3	2066	C	N3-C2-O2	-6.38	117.43	121.90
85	A6	1039	U	C5-C6-N1	6.38	125.89	122.70
85	A6	1195	C	C5-C6-N1	6.38	124.19	121.00
2	A3	2999	C	C6-N1-C2	-6.37	117.75	120.30
85	A6	1483	C	C6-N1-C2	-6.37	117.75	120.30
2	A3	3103	C	C6-N1-C2	-6.37	117.75	120.30
2	A3	1902	C	C6-N1-C1'	-6.37	113.16	120.80
2	A3	1944	C	C2-N1-C1'	6.36	125.80	118.80
39	d3	182	ARG	NE-CZ-NH2	-6.36	117.12	120.30
85	A6	1238	C	N3-C2-O2	-6.36	117.45	121.90
2	A3	1989	C	C6-N1-C2	-6.36	117.75	120.30
2	A3	3158	A	O4'-C1'-N9	6.36	113.28	108.20
40	e3	86	ASP	CB-CG-OD1	6.36	124.02	118.30
2	A3	2100	C	C6-N1-C2	-6.35	117.76	120.30
2	A3	2326	C	C6-N1-C2	-6.34	117.76	120.30
87	94	3	U	N3-C2-O2	-6.34	117.76	122.20
66	M6	93	LEU	CA-CB-CG	6.34	129.88	115.30
87	99	3	U	N1-C2-O2	6.33	127.23	122.80
80	a6	73	LEU	CA-CB-CG	6.33	129.86	115.30
2	A3	1807	U	P-O3'-C3'	6.33	127.29	119.70
85	A6	1288	U	N3-C2-O2	-6.33	117.77	122.20
2	A3	1752	U	C5-C6-N1	6.32	125.86	122.70
6	F3	142	ARG	NE-CZ-NH1	6.32	123.46	120.30
85	A6	1392	C	C6-N1-C2	-6.32	117.77	120.30
87	X	3	U	C2-N1-C1'	6.32	125.29	117.70
2	A3	2057	C	C6-N1-C2	-6.32	117.77	120.30
85	A6	838	G	C4-C5-N7	6.32	113.33	110.80
2	A3	2698	G	N3-C4-N9	-6.32	122.21	126.00
85	A6	1392	C	N3-C2-O2	-6.32	117.48	121.90
87	99	3	U	C5-C6-N1	6.32	125.86	122.70
2	A3	3201	A	P-O3'-C3'	6.31	127.28	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	3151	A	N7-C8-N9	6.31	116.95	113.80
2	A3	2490	C	N3-C2-O2	-6.31	117.48	121.90
2	A3	3157	C	O4'-C1'-N1	6.31	113.25	108.20
2	A3	2386	C	C6-N1-C2	-6.31	117.78	120.30
2	A3	2544	C	C6-N1-C2	-6.31	117.78	120.30
2	A3	2871	U	C5-C6-N1	6.30	125.85	122.70
2	A3	1721	C	C6-N1-C2	-6.30	117.78	120.30
2	A3	2832	A	N7-C8-N9	6.30	116.95	113.80
35	93	16	ASP	CB-CG-OD1	6.30	123.97	118.30
26	03	139	ARG	NE-CZ-NH1	6.30	123.45	120.30
67	N6	65	LEU	CA-CB-CG	6.29	129.78	115.30
17	R3	11	ARG	NE-CZ-NH1	6.29	123.45	120.30
85	A6	1297	C	C2-N1-C1'	6.29	125.72	118.80
38	c3	105	ARG	NE-CZ-NH1	6.29	123.44	120.30
2	A3	1707	C	N3-C2-O2	-6.29	117.50	121.90
2	A3	2141	U	O5'-P-OP1	-6.28	100.05	105.70
85	A6	1373	U	C6-N1-C1'	-6.28	112.41	121.20
2	A3	2726	C	C6-N1-C2	-6.28	117.79	120.30
85	A6	728	C	C5-C6-N1	6.28	124.14	121.00
11	L3	96	MET	C-N-CA	6.27	137.38	121.70
85	A6	710	C	O4'-C1'-N1	6.27	113.22	108.20
2	A3	1689	C	C6-N1-C2	-6.27	117.79	120.30
2	A3	2960	U	C6-N1-C1'	-6.26	112.43	121.20
85	A6	715	U	N1-C2-O2	6.26	127.19	122.80
2	A3	1699	C	C6-N1-C1'	-6.26	113.28	120.80
87	X	48	U	N1-C2-O2	6.26	127.18	122.80
85	A6	717	C	C5-C6-N1	6.25	124.13	121.00
85	A6	1170	A	P-O3'-C3'	6.25	127.21	119.70
66	M6	29	ARG	NE-CZ-NH1	6.25	123.42	120.30
85	A6	714	U	O4'-C1'-N1	6.25	113.20	108.20
2	A3	3212	C	C6-N1-C1'	-6.25	113.30	120.80
25	Z3	40	ARG	N-CA-CB	6.25	121.84	110.60
2	A3	1711	C	N1-C2-O2	6.24	122.64	118.90
4	D3	251	ASP	CB-CG-OD1	6.24	123.91	118.30
2	A3	2588	C	C5-C6-N1	6.23	124.12	121.00
2	A3	2835	C	N1-C2-O2	6.23	122.64	118.90
85	A6	1192	A	C4-C5-N7	6.23	113.82	110.70
10	K3	38	ARG	NE-CZ-NH1	6.23	123.42	120.30
68	O6	218	ARG	CB-CG-CD	6.23	127.79	111.60
70	Q6	51	ARG	NE-CZ-NH2	6.22	123.41	120.30
87	99	40	U	N1-C2-O2	6.21	127.15	122.80
38	c3	311	ARG	NE-CZ-NH1	6.21	123.40	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	1102	C	C6-N1-C2	-6.21	117.82	120.30
2	A3	2284	C	C6-N1-C1'	-6.20	113.36	120.80
53	s3	229	LEU	CA-CB-CG	6.20	129.57	115.30
87	94	28	A	C6-N1-C2	6.20	122.32	118.60
77	X6	310	LEU	CA-CB-CG	6.20	129.56	115.30
2	A3	3212	C	C5-C6-N1	6.20	124.10	121.00
64	K6	33	ARG	CG-CD-NE	-6.20	98.79	111.80
2	A3	2999	C	C5-C6-N1	6.19	124.09	121.00
87	94	40	U	N3-C2-O2	-6.19	117.87	122.20
2	A3	3043	C	C6-N1-C2	-6.18	117.83	120.30
85	A6	1237	C	C6-N1-C2	-6.18	117.83	120.30
83	d6	161	ARG	CB-CG-CD	-6.18	95.54	111.60
2	A3	2653	C	C5-C6-N1	6.18	124.09	121.00
43	h3	125	ASP	CB-CG-OD2	-6.17	112.74	118.30
85	A6	1242	C	N3-C2-O2	-6.17	117.58	121.90
87	X	25	G	C2-N3-C4	6.17	114.99	111.90
71	R6	148	LEU	CA-CB-CG	6.17	129.49	115.30
3	B3	1624	C	N1-C2-O2	6.17	122.60	118.90
32	63	52	ARG	CG-CD-NE	6.17	124.75	111.80
2	A3	3204	C	C6-N1-C1'	-6.16	113.40	120.80
82	c6	55	CYS	CA-CB-SG	6.16	125.10	114.00
2	A3	2523	C	OP1-P-O3'	6.16	118.76	105.20
85	A6	714	U	C6-N1-C1'	-6.16	112.58	121.20
2	A3	2493	C	C6-N1-C1'	-6.16	113.41	120.80
6	F3	142	ARG	NE-CZ-NH2	-6.15	117.22	120.30
85	A6	1560	C	P-O3'-C3'	6.15	127.08	119.70
2	A3	2372	U	N3-C4-O4	-6.15	115.09	119.40
2	A3	2295	C	C2-N1-C1'	6.14	125.55	118.80
85	A6	681	C	C6-N1-C2	-6.14	117.84	120.30
2	A3	1944	C	N1-C2-O2	6.13	122.58	118.90
85	A6	908	C	N1-C2-O2	6.13	122.58	118.90
85	A6	1263	U	N1-C2-O2	6.13	127.09	122.80
85	A6	1242	C	N1-C2-O2	6.12	122.57	118.90
50	p3	179	ARG	CG-CD-NE	6.12	124.65	111.80
8	I3	117	ARG	NE-CZ-NH1	-6.11	117.24	120.30
85	A6	1233	U	C2-N1-C1'	6.11	125.03	117.70
37	b3	28	ARG	NE-CZ-NH2	6.10	123.35	120.30
2	A3	3043	C	C2-N1-C1'	6.10	125.51	118.80
12	M3	162	LEU	CB-CG-CD2	6.10	121.38	111.00
2	A3	2379	C	N3-C2-O2	-6.10	117.63	121.90
87	94	12	U	C2-N1-C1'	6.10	125.02	117.70
66	M6	91	LEU	CA-CB-CG	6.09	129.31	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	1335	A	P-O3'-C3'	6.09	127.01	119.70
85	A6	1417	U	C2-N1-C1'	6.09	125.01	117.70
87	99	34	U	N1-C2-O2	6.09	127.06	122.80
12	M3	57	ARG	NE-CZ-NH1	-6.08	117.26	120.30
85	A6	1155	C	C2-N1-C1'	6.08	125.48	118.80
2	A3	2364	C	N1-C2-O2	6.07	122.54	118.90
2	A3	2923	G	N3-C4-C5	-6.07	125.56	128.60
2	A3	2150	U	N1-C2-O2	6.06	127.05	122.80
85	A6	715	U	N3-C2-O2	-6.06	117.96	122.20
85	A6	921	C	C5-C6-N1	6.06	124.03	121.00
27	13	19	ARG	NE-CZ-NH2	6.06	123.33	120.30
2	A3	2493	C	C6-N1-C2	-6.05	117.88	120.30
14	O3	48	ARG	NE-CZ-NH1	6.05	123.33	120.30
85	A6	1207	C	N1-C2-O2	6.05	122.53	118.90
85	A6	1193	U	P-O3'-C3'	6.04	126.95	119.70
3	B3	1663	C	C5-C6-N1	6.04	124.02	121.00
2	A3	2061	C	C6-N1-C1'	-6.04	113.55	120.80
2	A3	2096	U	C2-N1-C1'	6.04	124.95	117.70
85	A6	1541	C	P-O3'-C3'	6.04	126.95	119.70
61	H6	157	LEU	CA-CB-CG	6.04	129.18	115.30
82	c6	36	ARG	NE-CZ-NH2	6.04	123.32	120.30
21	V3	117	HIS	C-N-CA	6.03	136.78	121.70
2	A3	2496	G	C4-N9-C1'	6.03	134.34	126.50
2	A3	2515	U	N3-C2-O2	-6.03	117.98	122.20
64	K6	106	LEU	CA-CB-CG	6.03	129.17	115.30
27	13	20	MET	CG-SD-CE	-6.03	90.56	100.20
19	T3	106	LEU	CB-CG-CD1	-6.02	100.76	111.00
2	A3	1725	C	C5-C6-N1	6.02	124.01	121.00
3	B3	1649	C	N1-C2-O2	6.01	122.50	118.90
87	94	3	U	N1-C2-O2	6.00	127.00	122.80
85	A6	1483	C	N1-C2-O2	6.00	122.50	118.90
87	94	53	C	C2-N3-C4	6.00	122.90	119.90
2	A3	2544	C	N1-C2-O2	5.99	122.50	118.90
37	b3	112	VAL	CG1-CB-CG2	-5.99	101.31	110.90
60	G6	302	LEU	CA-CB-CG	5.99	129.07	115.30
87	X	52	C	C6-N1-C2	-5.99	117.90	120.30
2	A3	1701	U	N1-C2-O2	5.99	126.99	122.80
87	X	48	U	C5-C6-N1	5.98	125.69	122.70
2	A3	2756	C	N1-C2-O2	5.98	122.49	118.90
2	A3	2190	C	N1-C2-O2	5.98	122.49	118.90
75	V6	386	LEU	CA-CB-CG	5.98	129.05	115.30
2	A3	1696	C	N1-C2-O2	5.97	122.48	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	2311	U	N1-C2-O2	5.97	126.98	122.80
2	A3	2096	U	O4'-C1'-N1	5.97	112.97	108.20
2	A3	2523	C	C5-C6-N1	5.96	123.98	121.00
2	A3	1839	C	C5-C6-N1	5.96	123.98	121.00
87	X	66	U	C5-C6-N1	5.96	125.68	122.70
2	A3	2057	C	C5-C6-N1	5.96	123.98	121.00
2	A3	2168	U	N1-C2-O2	5.96	126.97	122.80
2	A3	1685	C	N3-C2-O2	-5.96	117.73	121.90
44	i3	45	ASP	CB-CG-OD1	5.95	123.66	118.30
53	s3	188	LEU	CB-CG-CD2	5.95	121.12	111.00
2	A3	2599	U	N3-C2-O2	-5.95	118.04	122.20
68	O6	96	ARG	CG-CD-NE	-5.95	99.31	111.80
2	A3	1783	U	N1-C2-O2	5.95	126.96	122.80
2	A3	2386	C	C5-C6-N1	5.94	123.97	121.00
32	63	161	LEU	CA-CB-CG	5.94	128.97	115.30
85	A6	1456	U	N3-C2-O2	-5.94	118.04	122.20
2	A3	2274	A	O4'-C1'-N9	5.94	112.95	108.20
85	A6	1208	C	N1-C2-N3	5.93	123.35	119.20
57	D6	148	LEU	CA-CB-CG	5.93	128.94	115.30
50	p3	135	LEU	CA-CB-CG	5.93	128.93	115.30
2	A3	2316	U	C5-C6-N1	5.92	125.66	122.70
2	A3	2667	U	N1-C2-O2	5.92	126.94	122.80
2	A3	1689	C	N1-C2-O2	5.91	122.45	118.90
2	A3	2511	C	C2-N1-C1'	5.91	125.30	118.80
68	O6	197	ASP	CB-CG-OD1	5.91	123.61	118.30
75	V6	161	LEU	CA-CB-CG	5.91	128.88	115.30
85	A6	1189	C	N1-C2-O2	5.91	122.44	118.90
85	A6	1000	A	O4'-C1'-N9	5.90	112.92	108.20
57	D6	351	ARG	NE-CZ-NH1	5.90	123.25	120.30
29	33	175	ASP	CB-CG-OD2	5.89	123.60	118.30
2	A3	2599	U	C2-N1-C1'	5.89	124.77	117.70
2	A3	1693	C	C5-C6-N1	5.89	123.94	121.00
2	A3	1711	C	C5-C6-N1	5.89	123.94	121.00
2	A3	2173	G	O5'-P-OP2	-5.89	100.40	105.70
2	A3	2186	C	C6-N1-C2	-5.88	117.95	120.30
53	s3	174	LEU	CA-CB-CG	5.88	128.84	115.30
85	A6	1306	C	C6-N1-C2	-5.88	117.95	120.30
2	A3	1993	A	C4-N9-C1'	5.88	136.89	126.30
85	A6	951	U	C6-N1-C2	-5.88	117.47	121.00
2	A3	2756	C	C5-C6-N1	5.88	123.94	121.00
85	A6	1436	U	N3-C2-O2	-5.88	118.09	122.20
2	A3	1895	C	C6-N1-C2	-5.87	117.95	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	94	63	C	C5-C6-N1	5.87	123.93	121.00
6	F3	172	LEU	CA-CB-CG	5.86	128.78	115.30
85	A6	864	A	C2-N3-C4	5.86	113.53	110.60
81	b6	87	MET	CB-CG-SD	5.86	129.98	112.40
2	A3	1837	C	C6-N1-C1'	-5.86	113.77	120.80
2	A3	2499	U	C2-N1-C1'	5.86	124.73	117.70
85	A6	1381	C	C2-N1-C1'	5.86	125.24	118.80
2	A3	1809	U	P-O3'-C3'	5.86	126.73	119.70
34	83	104	VAL	CG1-CB-CG2	-5.86	101.53	110.90
31	53	381	LEU	CA-CB-CG	5.86	128.77	115.30
2	A3	3124	U	C2-N1-C1'	5.85	124.72	117.70
2	A3	3201	A	O4'-C1'-N9	-5.85	103.52	108.20
2	A3	1716	U	N3-C2-O2	-5.85	118.11	122.20
2	A3	2669	A	N7-C8-N9	5.85	116.72	113.80
75	V6	190	LEU	CA-CB-CG	5.85	128.76	115.30
85	A6	811	A	C5-N7-C8	-5.85	100.98	103.90
87	99	20	U	N1-C2-O2	5.85	126.89	122.80
11	L3	95	ARG	NE-CZ-NH2	-5.85	117.38	120.30
2	A3	2942	C	C6-N1-C2	-5.84	117.96	120.30
2	A3	2540	C	C6-N1-C2	-5.84	117.96	120.30
87	99	61	U	C5-C6-N1	5.84	125.62	122.70
16	Q3	274	ASP	CB-CG-OD1	5.84	123.55	118.30
75	V6	384	LEU	CA-CB-CG	5.83	128.71	115.30
85	A6	908	C	C6-N1-C2	-5.83	117.97	120.30
85	A6	1483	C	C2-N1-C1'	5.83	125.21	118.80
2	A3	2209	G	C4-N9-C1'	5.83	134.08	126.50
2	A3	3009	C	N1-C2-O2	5.83	122.40	118.90
85	A6	1288	U	N1-C2-O2	5.83	126.88	122.80
2	A3	2224	C	C6-N1-C1'	-5.82	113.82	120.80
85	A6	1252	C	C6-N1-C2	-5.82	117.97	120.30
2	A3	1809	U	OP1-P-O3'	5.82	118.00	105.20
87	X	3	U	C5-C6-N1	5.81	125.61	122.70
85	A6	1485	C	C2-N1-C1'	5.81	125.19	118.80
2	A3	2150	U	N3-C2-O2	-5.81	118.13	122.20
85	A6	857	C	C5-C6-N1	5.81	123.91	121.00
87	99	11	C	C2-N1-C1'	5.81	125.19	118.80
2	A3	1839	C	C6-N1-C2	-5.81	117.98	120.30
2	A3	2224	C	C5-C6-N1	5.81	123.90	121.00
77	X6	258	LEU	CB-CG-CD1	-5.81	101.13	111.00
87	99	3	U	C2-N1-C1'	5.80	124.66	117.70
2	A3	2726	C	C2-N1-C1'	5.80	125.18	118.80
2	A3	1750	G	O4'-C1'-N9	5.79	112.83	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	3061	G	C4-C5-N7	5.79	113.12	110.80
2	A3	1995	A	C8-N9-C4	-5.79	103.48	105.80
85	A6	1093	U	N1-C2-O2	5.79	126.85	122.80
2	A3	2252	C	C2-N1-C1'	5.79	125.17	118.80
85	A6	763	C	C6-N1-C2	-5.79	117.99	120.30
2	A3	1993	A	N3-C4-C5	-5.78	122.75	126.80
2	A3	2221	C	OP1-P-O3'	5.78	117.91	105.20
2	A3	2419	C	C6-N1-C2	-5.78	117.99	120.30
85	A6	873	C	C5-C6-N1	5.78	123.89	121.00
2	A3	2611	C	C6-N1-C2	-5.77	117.99	120.30
37	b3	56	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	A3	2245	A	P-O3'-C3'	5.76	126.62	119.70
8	I3	92	ASP	CB-CG-OD1	5.76	123.49	118.30
2	A3	2079	C	C6-N1-C1'	-5.76	113.89	120.80
2	A3	2386	C	C6-N1-C1'	-5.76	113.89	120.80
57	D6	325	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	A3	2219	C	C6-N1-C1'	-5.76	113.89	120.80
87	X	6	U	C2-N1-C1'	5.76	124.61	117.70
2	A3	1782	G	O4'-C1'-N9	5.75	112.80	108.20
69	P6	49	ASP	CB-CG-OD1	5.75	123.48	118.30
2	A3	2211	U	C2-N1-C1'	5.75	124.60	117.70
2	A3	1813	C	C6-N1-C2	-5.75	118.00	120.30
2	A3	2484	C	N3-C2-O2	-5.75	117.88	121.90
2	A3	1837	C	C6-N1-C2	-5.75	118.00	120.30
85	A6	1127	C	C5-C6-N1	5.75	123.87	121.00
2	A3	2922	A	N1-C6-N6	-5.74	115.16	118.60
20	U3	11	ARG	NE-CZ-NH2	5.74	123.17	120.30
2	A3	2186	C	C5-C6-N1	5.74	123.87	121.00
2	A3	2215	C	C5-C6-N1	5.74	123.87	121.00
2	A3	1807	U	C5-C6-N1	5.74	125.57	122.70
2	A3	2484	C	C6-N1-C2	-5.74	118.01	120.30
41	f3	178	LEU	CA-CB-CG	5.74	128.49	115.30
87	X	2	U	N3-C2-O2	-5.74	118.19	122.20
87	94	73	A	N7-C8-N9	5.73	116.66	113.80
2	A3	2646	G	N3-C2-N2	-5.72	115.89	119.90
85	A6	1233	U	N1-C2-O2	5.72	126.81	122.80
2	A3	2544	C	N3-C2-O2	-5.72	117.90	121.90
31	53	293	LEU	CA-CB-CG	5.72	128.45	115.30
85	A6	921	C	C2-N1-C1'	5.72	125.09	118.80
2	A3	2190	C	N3-C2-O2	-5.72	117.90	121.90
85	A6	1483	C	C5-C6-N1	5.72	123.86	121.00
2	A3	2892	A	N1-C6-N6	-5.71	115.17	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	2898	U	C6-N1-C1'	-5.71	113.20	121.20
85	A6	1471	C	N3-C2-O2	-5.71	117.90	121.90
2	A3	1703	C	C6-N1-C2	-5.71	118.02	120.30
38	c3	240	LEU	CA-CB-CG	5.71	128.43	115.30
85	A6	737	U	C5-C4-O4	-5.71	122.47	125.90
87	X	12	U	C5-C6-N1	5.71	125.55	122.70
2	A3	1715	C	C2-N1-C1'	5.71	125.08	118.80
81	b6	114	LEU	CB-CG-CD2	5.71	120.70	111.00
85	A6	745	A	C4-C5-N7	5.71	113.55	110.70
2	A3	2578	C	O5'-P-OP1	-5.70	100.57	105.70
3	B3	1635	C	N1-C2-O2	5.70	122.32	118.90
2	A3	2132	A	C4-C5-C6	-5.70	114.15	117.00
35	93	127	LEU	CA-CB-CG	5.70	128.40	115.30
2	A3	2372	U	C2-N1-C1'	5.69	124.53	117.70
2	A3	2205	U	N1-C2-O2	5.69	126.78	122.80
12	M3	244	LEU	CB-CG-CD1	-5.68	101.33	111.00
87	94	11	C	C2-N1-C1'	5.68	125.05	118.80
2	A3	2311	U	N3-C2-O2	-5.68	118.22	122.20
87	99	11	C	N3-C2-O2	-5.68	117.92	121.90
85	A6	1381	C	N1-C2-O2	5.68	122.31	118.90
36	a3	56	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	A3	1694	U	C2-N1-C1'	5.67	124.51	117.70
2	A3	1993	A	C2-N3-C4	5.67	113.44	110.60
2	A3	2236	C	C2-N1-C1'	5.67	125.04	118.80
85	A6	812	C	C6-N1-C2	-5.67	118.03	120.30
85	A6	838	G	C6-C5-N7	-5.67	127.00	130.40
71	R6	142	LEU	CA-CB-CG	5.67	128.34	115.30
52	r3	88	LEU	CA-CB-CG	5.67	128.34	115.30
75	V6	337	LEU	CA-CB-CG	5.67	128.34	115.30
2	A3	3201	A	C4-N9-C1'	5.66	136.49	126.30
2	A3	1910	C	C6-N1-C2	-5.66	118.04	120.30
2	A3	3102	U	C2-N1-C1'	5.66	124.49	117.70
2	A3	1696	C	N3-C2-O2	-5.66	117.94	121.90
5	E3	187	ILE	CG1-CB-CG2	-5.66	98.96	111.40
87	99	52	C	N1-C2-O2	5.66	122.29	118.90
2	A3	1951	C	C5-C6-N1	5.65	123.83	121.00
2	A3	1995	A	C2-N3-C4	5.65	113.43	110.60
2	A3	2061	C	O4'-C1'-N1	5.65	112.72	108.20
2	A3	3157	C	C4-C5-C6	-5.65	114.58	117.40
2	A3	3066	C	C6-N1-C2	-5.65	118.04	120.30
70	Q6	59	ARG	NE-CZ-NH1	5.64	123.12	120.30
80	a6	140	ARG	NE-CZ-NH1	-5.64	117.48	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	1192	A	C5-N7-C8	-5.64	101.08	103.90
2	A3	2235	C	C6-N1-C1'	-5.63	114.04	120.80
85	A6	951	U	N3-C4-O4	5.63	123.34	119.40
8	I3	174	LEU	CB-CG-CD2	-5.63	101.42	111.00
23	X3	61	ARG	NE-CZ-NH2	-5.62	117.49	120.30
85	A6	711	C	N1-C2-O2	5.62	122.27	118.90
2	A3	2835	C	C2-N1-C1'	5.62	124.98	118.80
2	A3	1975	U	C2-N1-C1'	5.62	124.44	117.70
85	A6	1251	G	O5'-P-OP2	-5.62	100.64	105.70
16	Q3	194	LEU	CA-CB-CG	5.62	128.22	115.30
32	63	233	LEU	CB-CG-CD1	5.62	120.55	111.00
2	A3	2832	A	C5-N7-C8	-5.62	101.09	103.90
81	b6	260	ARG	CA-CB-CG	5.61	125.75	113.40
2	A3	2646	G	C8-N9-C1'	5.61	134.30	127.00
2	A3	2646	G	N1-C6-O6	-5.61	116.53	119.90
2	A3	3061	G	C6-C5-N7	-5.61	127.03	130.40
85	A6	1263	U	C6-N1-C1'	-5.61	113.35	121.20
85	A6	1527	A	C8-N9-C4	-5.61	103.56	105.80
19	T3	204	ARG	NE-CZ-NH2	-5.61	117.50	120.30
60	G6	122	ARG	CB-CG-CD	5.61	126.17	111.60
85	A6	1233	U	N3-C2-O2	-5.61	118.28	122.20
2	A3	2171	U	N3-C2-O2	-5.60	118.28	122.20
85	A6	1395	U	C6-N1-C2	-5.60	117.64	121.00
2	A3	2387	U	N3-C2-O2	-5.60	118.28	122.20
85	A6	1417	U	C6-N1-C2	-5.60	117.64	121.00
7	H3	118	LEU	CA-CB-CG	5.60	128.17	115.30
2	A3	2067	C	C6-N1-C2	-5.59	118.06	120.30
87	99	40	U	N3-C2-O2	-5.59	118.28	122.20
2	A3	3206	C	C2-N1-C1'	5.59	124.95	118.80
6	F3	261	LEU	CA-CB-CG	5.59	128.15	115.30
2	A3	2427	C	C6-N1-C2	-5.58	118.07	120.30
2	A3	1745	U	N3-C2-O2	-5.58	118.30	122.20
80	a6	49	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	A3	2627	G	N3-C4-N9	-5.57	122.66	126.00
2	A3	2665	U	C5-C6-N1	5.57	125.48	122.70
85	A6	1102	C	C2-N1-C1'	5.57	124.93	118.80
85	A6	1247	U	C6-N1-C2	-5.57	117.66	121.00
2	A3	1828	A	N3-C4-C5	5.57	130.70	126.80
25	Z3	134	MET	CA-CB-CG	5.57	122.76	113.30
85	A6	709	C	C6-N1-C1'	-5.57	114.12	120.80
2	A3	1714	C	N1-C2-O2	5.57	122.24	118.90
85	A6	1308	C	C5-C6-N1	5.56	123.78	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	2698	G	N9-C4-C5	5.56	107.62	105.40
2	A3	2396	C	N1-C2-O2	5.56	122.23	118.90
2	A3	2909	G	C4-N9-C1’	5.56	133.72	126.50
85	A6	729	C	C6-N1-C2	-5.56	118.08	120.30
2	A3	2541	C	C6-N1-C2	-5.56	118.08	120.30
5	E3	323	GLY	C-N-CA	5.55	135.57	121.70
87	X	35	G	N3-C4-C5	-5.55	125.83	128.60
2	A3	1721	C	C5-C6-N1	5.55	123.77	121.00
2	A3	2579	C	N1-C2-O2	5.54	122.23	118.90
75	V6	147	LEU	CA-CB-CG	5.54	128.05	115.30
85	A6	1247	U	C2-N1-C1’	5.54	124.35	117.70
68	O6	78	ARG	CA-CB-CG	5.54	125.59	113.40
85	A6	683	C	N1-C2-O2	5.54	122.22	118.90
85	A6	1436	U	N1-C2-O2	5.54	126.68	122.80
2	A3	2511	C	O4’-C1’-N1	5.54	112.63	108.20
2	A3	3201	A	C8-N9-C1’	-5.53	117.74	127.70
85	A6	1193	U	C6-N1-C1’	-5.53	113.45	121.20
2	A3	3228	U	N1-C2-O2	5.53	126.67	122.80
2	A3	2746	U	C2-N1-C1’	5.53	124.33	117.70
80	a6	76	LEU	CA-CB-CG	5.53	128.02	115.30
87	94	49	G	P-O3’-C3’	5.53	126.33	119.70
18	S3	122	LEU	CB-CG-CD2	-5.53	101.60	111.00
85	A6	970	A	O5’-P-OP1	-5.53	100.72	105.70
2	A3	3217	A	OP1-P-O3’	5.52	117.35	105.20
2	A3	2190	C	C5-C6-N1	5.52	123.76	121.00
2	A3	2221	C	P-O3’-C3’	5.52	126.32	119.70
82	c6	17	ARG	NE-CZ-NH1	-5.52	117.54	120.30
49	o3	41	ILE	CG1-CB-CG2	-5.52	99.26	111.40
87	X	11	C	C6-N1-C1’	-5.52	114.18	120.80
2	A3	2284	C	C5-C6-N1	5.51	123.76	121.00
85	A6	1366	G	C5-C6-O6	5.51	131.91	128.60
87	94	53	C	N3-C2-O2	-5.51	118.04	121.90
87	X	52	C	O4’-C1’-N1	5.51	112.61	108.20
85	A6	714	U	N1-C2-O2	5.51	126.66	122.80
85	A6	1051	A	C2-N3-C4	5.51	113.36	110.60
57	D6	368	LEU	CA-CB-CG	5.50	127.96	115.30
81	b6	56	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	A3	2628	U	P-O3’-C3’	5.50	126.31	119.70
85	A6	818	A	C4-N9-C1’	5.50	136.21	126.30
2	A3	3122	U	C2-N1-C1’	5.50	124.30	117.70
85	A6	1156	A	C4-N9-C1’	5.50	136.20	126.30
64	K6	33	ARG	NE-CZ-NH2	5.50	123.05	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A3	2530	A	P-O3'-C3'	5.49	126.29	119.70
87	X	66	U	C5-C4-O4	-5.49	122.60	125.90
31	53	315	LEU	CA-CB-CG	5.49	127.93	115.30
2	A3	3093	C	C6-N1-C2	-5.49	118.11	120.30
12	M3	184	LEU	CB-CG-CD1	-5.49	101.67	111.00
2	A3	2960	U	C5-C6-N1	5.49	125.44	122.70
2	A3	2205	U	N3-C2-O2	-5.47	118.37	122.20
2	A3	2490	C	C5-C4-N4	5.47	124.03	120.20
31	53	48	ARG	CB-CG-CD	5.47	125.84	111.60
72	S6	25	LEU	CA-CB-CG	5.47	127.89	115.30
85	A6	1127	C	C6-N1-C2	-5.47	118.11	120.30
87	99	72	C	C5-C6-N1	5.47	123.74	121.00
85	A6	811	A	N7-C8-N9	5.47	116.54	113.80
2	A3	1730	U	N3-C2-O2	-5.47	118.37	122.20
64	K6	90	ARG	NE-CZ-NH2	5.47	123.03	120.30
85	A6	906	G	C4-C5-N7	5.47	112.99	110.80
21	V3	128	ARG	NE-CZ-NH1	5.47	123.03	120.30
2	A3	3134	C	C2-N1-C1'	5.47	124.81	118.80
31	53	215	ARG	NE-CZ-NH1	-5.47	117.57	120.30
87	X	52	C	N3-C2-O2	-5.47	118.07	121.90
2	A3	2017	U	N3-C2-O2	-5.46	118.38	122.20
8	I3	80	ARG	NE-CZ-NH1	5.46	123.03	120.30
36	a3	128	ARG	CB-CG-CD	5.46	125.80	111.60
85	A6	1000	A	C5-N7-C8	-5.46	101.17	103.90
85	A6	812	C	N1-C2-O2	5.46	122.18	118.90
87	X	6	U	N3-C2-O2	-5.46	118.38	122.20
85	A6	1074	C	N1-C2-O2	5.46	122.17	118.90
2	A3	1973	G	N3-C4-C5	5.45	131.33	128.60
40	e3	66	LEU	CA-CB-CG	5.45	127.84	115.30
85	A6	842	U	N3-C2-O2	-5.45	118.38	122.20
2	A3	1984	A	C6-C5-N7	-5.45	128.48	132.30
2	A3	2186	C	N1-C2-O2	5.45	122.17	118.90
2	A3	2447	A	N7-C8-N9	5.45	116.53	113.80
5	E3	50	ASP	CB-CG-OD2	5.45	123.20	118.30
32	63	233	LEU	CA-CB-CG	5.45	127.84	115.30
61	H6	79	LEU	CA-CB-CG	5.45	127.84	115.30
2	A3	1901	C	C6-N1-C1'	-5.45	114.26	120.80
2	A3	2812	U	C2-N1-C1'	5.45	124.24	117.70
85	A6	1379	C	N1-C2-O2	5.45	122.17	118.90
2	A3	2445	U	N1-C2-O2	5.44	126.61	122.80
2	A3	2215	C	C2-N3-C4	5.44	122.62	119.90
2	A3	2132	A	C5-C6-N1	5.44	120.42	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	1903	C	C6-N1-C2	-5.44	118.12	120.30
2	A3	2168	U	N3-C2-O2	-5.43	118.40	122.20
2	A3	2415	C	C6-N1-C2	-5.43	118.13	120.30
2	A3	2540	C	C5-C6-N1	5.43	123.72	121.00
85	A6	908	C	C5-C6-N1	5.43	123.72	121.00
85	A6	1196	C	N1-C2-O2	5.43	122.16	118.90
2	A3	1902	C	C5-C6-N1	5.43	123.72	121.00
2	A3	3134	C	C5-C6-N1	5.43	123.72	121.00
85	A6	1522	C	N3-C2-O2	-5.43	118.10	121.90
87	X	10	G	C5-C6-O6	-5.43	125.34	128.60
2	A3	2344	C	N3-C2-O2	-5.43	118.10	121.90
24	Y3	213	ARG	NE-CZ-NH1	5.43	123.02	120.30
2	A3	2057	C	C2-N1-C1'	5.43	124.77	118.80
2	A3	1745	U	C5-C6-N1	5.42	125.41	122.70
2	A3	2726	C	N3-C2-O2	-5.42	118.10	121.90
2	A3	2646	G	C5-C6-O6	5.42	131.85	128.60
85	A6	1156	A	C2-N3-C4	5.42	113.31	110.60
75	V6	341	LEU	CA-CB-CG	5.42	127.77	115.30
85	A6	1006	C	C6-N1-C2	-5.42	118.13	120.30
8	I3	78	LEU	CA-CB-CG	5.42	127.75	115.30
2	A3	2575	U	N3-C4-C5	5.41	117.85	114.60
87	99	56	A	C2-N3-C4	5.41	113.31	110.60
2	A3	2209	G	C8-N9-C1'	-5.41	119.96	127.00
2	A3	2364	C	N3-C2-O2	-5.41	118.11	121.90
85	A6	1492	C	C6-N1-C2	-5.41	118.14	120.30
40	e3	83	LEU	CA-CB-CG	5.41	127.74	115.30
38	c3	290	LEU	CA-CB-CG	5.41	127.73	115.30
87	94	3	U	C2-N1-C1'	5.40	124.19	117.70
2	A3	3041	U	OP1-P-O3'	5.40	117.09	105.20
2	A3	2947	U	N1-C2-O2	5.40	126.58	122.80
21	V3	41	ARG	NE-CZ-NH1	-5.40	117.60	120.30
32	63	334	LEU	CA-CB-CG	5.40	127.72	115.30
85	A6	1193	U	C6-N1-C2	-5.40	117.76	121.00
85	A6	1013	C	C5-C6-N1	5.40	123.70	121.00
85	A6	1447	U	C2-N1-C1'	5.40	124.18	117.70
2	A3	3187	C	C6-N1-C2	-5.40	118.14	120.30
2	A3	2948	C	N1-C2-O2	5.39	122.14	118.90
64	K6	33	ARG	CA-CB-CG	-5.39	101.53	113.40
57	D6	93	LEU	CA-CB-CG	5.39	127.70	115.30
85	A6	1006	C	C5-C6-N1	5.39	123.69	121.00
2	A3	2001	C	N3-C4-C5	5.39	124.05	121.90
2	A3	1833	C	C6-N1-C2	-5.38	118.15	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	e6	147	PRO	N-CA-CB	5.38	109.76	103.30
2	A3	3170	C	C6-N1-C1'	-5.38	114.34	120.80
86	i4	18	A	O4'-C1'-N9	5.38	112.51	108.20
2	A3	1989	C	C5-C6-N1	5.38	123.69	121.00
64	K6	41	ARG	NE-CZ-NH1	5.38	122.99	120.30
87	X	48	U	N3-C2-O2	-5.38	118.43	122.20
2	A3	1884	G	C8-N9-C4	5.38	108.55	106.40
5	E3	232	GLY	N-CA-C	-5.38	99.65	113.10
85	A6	1440	C	C6-N1-C2	-5.38	118.15	120.30
2	A3	2661	U	N3-C2-O2	-5.38	118.44	122.20
76	W6	147	LEU	CA-CB-CG	5.38	127.67	115.30
85	A6	677	U	C5-C6-N1	5.38	125.39	122.70
12	M3	220	ARG	NE-CZ-NH1	5.37	122.99	120.30
31	53	309	LEU	CB-CG-CD2	-5.37	101.87	111.00
68	O6	218	ARG	CG-CD-NE	-5.37	100.52	111.80
67	N6	53	ASP	CB-CG-OD1	5.37	123.13	118.30
33	73	227	LEU	CA-CB-CG	5.37	127.65	115.30
11	L3	95	ARG	CA-CB-CG	-5.36	101.61	113.40
2	A3	1984	A	C4-N9-C1'	5.36	135.94	126.30
85	A6	1433	C	C5-C6-N1	5.35	123.68	121.00
2	A3	2387	U	N1-C2-O2	5.35	126.55	122.80
2	A3	2961	C	N3-C2-O2	-5.35	118.15	121.90
2	A3	2494	C	C6-N1-C2	-5.35	118.16	120.30
71	R6	98	LEU	CA-CB-CG	5.35	127.60	115.30
69	P6	94	ARG	NE-CZ-NH1	5.35	122.97	120.30
2	A3	2557	C	C5-C6-N1	5.34	123.67	121.00
85	A6	1419	G	P-O3'-C3'	5.34	126.11	119.70
87	99	40	U	C6-N1-C1'	-5.34	113.72	121.20
2	A3	2168	U	C2-N1-C1'	5.34	124.11	117.70
2	A3	2909	G	C5-N7-C8	-5.34	101.63	104.30
85	A6	1250	U	P-O3'-C3'	5.33	126.10	119.70
2	A3	2282	C	N1-C2-O2	5.33	122.10	118.90
2	A3	2193	U	C5-C6-N1	5.33	125.36	122.70
44	i3	80	LEU	CB-CG-CD2	-5.33	101.94	111.00
23	X3	193	GLU	CA-CB-CG	5.33	125.12	113.40
85	A6	1193	U	C5-C6-N1	5.33	125.36	122.70
2	A3	1745	U	C6-N1-C2	-5.33	117.80	121.00
2	A3	2101	C	C6-N1-C2	-5.33	118.17	120.30
53	s3	270	LYS	CD-CE-NZ	-5.32	99.46	111.70
85	A6	1485	C	N1-C2-O2	5.32	122.09	118.90
14	O3	50	ASP	CB-CG-OD1	5.32	123.09	118.30
2	A3	2540	C	N1-C2-O2	5.32	122.09	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	3055	U	C5-C6-N1	5.32	125.36	122.70
33	73	143	TRP	CA-CB-CG	5.32	123.80	113.70
87	99	61	U	C6-N1-C2	-5.32	117.81	121.00
87	X	12	U	N3-C2-O2	-5.32	118.48	122.20
2	A3	3187	C	C2-N1-C1’	5.32	124.65	118.80
3	B3	1627	C	C6-N1-C2	-5.32	118.17	120.30
87	X	26	C	N1-C2-O2	5.32	122.09	118.90
2	A3	2372	U	C5-C4-O4	5.31	129.09	125.90
2	A3	3191	A	N1-C6-N6	-5.31	115.41	118.60
31	53	327	LEU	CA-CB-CG	5.31	127.52	115.30
2	A3	2507	A	P-O3’-C3’	5.30	126.07	119.70
2	A3	2576	A	C5-C6-N1	5.30	120.35	117.70
85	A6	1189	C	C6-N1-C1’	-5.30	114.43	120.80
85	A6	1195	C	N1-C2-O2	5.30	122.08	118.90
28	23	49	ARG	CG-CD-NE	-5.30	100.67	111.80
85	A6	1156	A	C8-N9-C1’	-5.30	118.16	127.70
87	X	42	C	C5-C6-N1	5.30	123.65	121.00
2	A3	2222	U	OP1-P-OP2	-5.30	111.66	119.60
2	A3	2135	A	C4-N9-C1’	5.29	135.83	126.30
21	V3	194	LEU	CA-CB-CG	5.29	127.48	115.30
60	G6	150	LEU	CA-CB-CG	5.29	127.48	115.30
2	A3	2699	C	N1-C2-O2	5.29	122.07	118.90
2	A3	1745	U	N1-C2-O2	5.29	126.50	122.80
87	99	33	C	N3-C2-O2	-5.29	118.20	121.90
87	94	61	U	N1-C2-O2	5.28	126.50	122.80
2	A3	2889	C	C6-N1-C2	-5.28	118.19	120.30
2	A3	2911	C	O4’-C1’-N1	-5.28	103.97	108.20
2	A3	2989	G	P-O3’-C3’	5.28	126.04	119.70
34	83	147	LEU	CA-CB-CG	5.28	127.45	115.30
48	m3	50	ARG	NE-CZ-NH1	5.28	122.94	120.30
85	A6	769	C	N1-C2-O2	5.28	122.07	118.90
85	A6	1318	C	C6-N1-C2	-5.28	118.19	120.30
81	b6	197	ARG	NE-CZ-NH1	-5.28	117.66	120.30
85	A6	1189	C	C5-C6-N1	5.28	123.64	121.00
80	a6	99	ARG	CD-NE-CZ	5.27	130.98	123.60
2	A3	2479	C	N3-C2-O2	-5.27	118.21	121.90
87	99	1	G	P-O3’-C3’	5.27	126.03	119.70
2	A3	2832	A	C8-N9-C4	-5.27	103.69	105.80
82	c6	21	LEU	CA-CB-CG	5.27	127.42	115.30
4	D3	147	ARG	NE-CZ-NH1	-5.27	117.67	120.30
85	A6	732	C	C6-N1-C2	-5.27	118.19	120.30
2	A3	2419	C	C5-C6-N1	5.27	123.63	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	d6	172	ASP	CB-CG-OD1	5.27	123.04	118.30
55	B6	215	MET	CG-SD-CE	5.26	108.62	100.20
2	A3	1671	G	O4'-C1'-N9	5.26	112.41	108.20
85	A6	738	C	C6-N1-C2	-5.26	118.20	120.30
85	A6	1537	C	C5-C6-N1	5.26	123.63	121.00
77	X6	247	LEU	CA-CB-CG	5.25	127.39	115.30
2	A3	2909	G	C8-N9-C4	-5.25	104.30	106.40
13	N3	250	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	A3	1743	U	N3-C2-O2	-5.25	118.53	122.20
32	63	41	ASP	CB-CG-OD2	5.25	123.03	118.30
47	l3	122	ARG	CG-CD-NE	-5.25	100.77	111.80
2	A3	2119	U	N3-C2-O2	-5.25	118.53	122.20
2	A3	2287	U	C5-C6-N1	5.25	125.32	122.70
31	53	412	ARG	NE-CZ-NH1	5.25	122.92	120.30
87	94	62	C	C2-N3-C4	5.25	122.52	119.90
2	A3	2315	A	C5-N7-C8	-5.24	101.28	103.90
87	94	72	C	C5-C6-N1	5.24	123.62	121.00
85	A6	1013	C	N1-C2-O2	5.24	122.04	118.90
87	X	52	C	C6-N1-C1'	-5.24	114.52	120.80
2	A3	2794	C	N1-C2-O2	5.23	122.04	118.90
18	S3	204	LEU	CA-CB-CG	5.23	127.34	115.30
45	j3	40	TYR	CB-CG-CD2	-5.23	117.86	121.00
2	A3	2100	C	C5-C6-N1	5.23	123.61	121.00
85	A6	1282	C	C2-N1-C1'	5.23	124.55	118.80
2	A3	1973	G	N3-C4-N9	-5.22	122.86	126.00
87	94	52	C	N3-C2-O2	-5.22	118.24	121.90
85	A6	1230	C	N3-C2-O2	-5.22	118.24	121.90
87	94	28	A	N1-C2-N3	-5.22	126.69	129.30
2	A3	2515	U	C6-N1-C2	-5.22	117.87	121.00
2	A3	1714	C	N3-C2-O2	-5.22	118.25	121.90
2	A3	2582	A	C4-N9-C1'	5.22	135.69	126.30
64	K6	96	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	A3	2538	C	C6-N1-C2	-5.21	118.21	120.30
19	T3	161	ARG	N-CA-C	-5.21	96.93	111.00
85	A6	1259	U	N1-C2-O2	5.21	126.45	122.80
2	A3	1711	C	N3-C2-O2	-5.21	118.25	121.90
84	e6	467	LEU	CA-CB-CG	5.21	127.28	115.30
2	A3	3172	C	C2-N1-C1'	5.20	124.53	118.80
49	o3	56	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	A3	3222	C	C6-N1-C2	-5.20	118.22	120.30
43	h3	104	LEU	CA-CB-CG	5.20	127.27	115.30
48	m3	56	LEU	CA-CB-CG	5.20	127.26	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	99	52	C	C2-N1-C1'	5.20	124.52	118.80
2	A3	2080	U	C6-N1-C2	-5.20	117.88	121.00
2	A3	3192	C	C6-N1-C2	-5.20	118.22	120.30
84	e6	496	LEU	CA-CB-CG	5.20	127.25	115.30
85	A6	1398	C	N1-C2-O2	5.19	122.02	118.90
2	A3	2474	C	C5-C6-N1	5.19	123.59	121.00
2	A3	2948	C	C2-N1-C1'	5.19	124.51	118.80
2	A3	2579	C	C2-N1-C1'	5.19	124.51	118.80
85	A6	1263	U	N3-C2-O2	-5.19	118.57	122.20
2	A3	2079	C	C5-C6-N1	5.18	123.59	121.00
45	j3	80	LEU	CA-CB-CG	5.18	127.22	115.30
85	A6	957	U	C6-N1-C1'	-5.18	113.94	121.20
2	A3	2582	A	N3-C4-C5	-5.18	123.17	126.80
68	O6	235	MET	CG-SD-CE	5.18	108.48	100.20
87	99	60	C	N1-C2-O2	5.18	122.01	118.90
2	A3	2025	C	N1-C2-O2	5.18	122.01	118.90
67	N6	81	LEU	CA-CB-CG	5.18	127.21	115.30
85	A6	972	U	C6-N1-C2	-5.18	117.89	121.00
85	A6	1451	G	N1-C6-O6	5.18	123.01	119.90
2	A3	2507	A	C2'-C3'-O3'	5.17	121.98	113.70
2	A3	3169	C	N3-C2-O2	-5.17	118.28	121.90
29	33	154	GLN	CA-CB-CG	5.17	124.78	113.40
2	A3	2578	C	N3-C2-O2	-5.17	118.28	121.90
2	A3	3172	C	N3-C2-O2	-5.17	118.28	121.90
32	63	370	ARG	NE-CZ-NH1	5.17	122.89	120.30
85	A6	1238	C	N1-C2-O2	5.17	122.00	118.90
83	d6	161	ARG	CA-CB-CG	5.17	124.77	113.40
2	A3	1745	U	C2-N1-C1'	5.17	123.90	117.70
2	A3	1707	C	C6-N1-C2	-5.17	118.23	120.30
55	B6	127	LEU	CA-CB-CG	5.17	127.18	115.30
2	A3	3173	G	C2-N3-C4	-5.16	109.32	111.90
2	A3	2241	A	C4-N9-C1'	5.16	135.59	126.30
50	p3	56	ASP	CB-CG-OD2	5.16	122.94	118.30
87	X	25	G	N3-C4-C5	-5.16	126.02	128.60
85	A6	972	U	C5-C6-N1	5.16	125.28	122.70
2	A3	2496	G	C6-C5-N7	-5.15	127.31	130.40
87	94	61	U	N3-C2-O2	-5.15	118.59	122.20
2	A3	1786	C	C6-N1-C2	-5.15	118.24	120.30
85	A6	1538	C	N3-C2-O2	-5.15	118.30	121.90
87	X	1	G	P-O3'-C3'	5.15	125.88	119.70
2	A3	2947	U	N3-C2-O2	-5.15	118.60	122.20
4	D3	220	VAL	CA-CB-CG1	5.15	118.62	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W3	49	ARG	NE-CZ-NH1	-5.15	117.73	120.30
85	A6	1579	U	C5-C6-N1	5.15	125.27	122.70
2	A3	2646	G	C6-C5-N7	5.15	133.49	130.40
61	H6	180	LEU	CA-CB-CG	5.14	127.13	115.30
85	A6	1156	A	N3-C4-N9	5.14	131.52	127.40
2	A3	1895	C	C5-C6-N1	5.14	123.57	121.00
14	O3	135	LEU	CB-CG-CD1	-5.14	102.26	111.00
82	c6	38	ARG	NE-CZ-NH2	-5.14	117.73	120.30
85	A6	1561	A	O5'-P-OP1	-5.14	101.07	105.70
2	A3	1685	C	C5-C4-N4	5.14	123.80	120.20
2	A3	2252	C	C5-C6-N1	5.14	123.57	121.00
2	A3	2689	C	C5-C6-N1	5.14	123.57	121.00
77	X6	96	GLU	C-N-CA	5.14	134.55	121.70
85	A6	916	U	C5-C6-N1	5.14	125.27	122.70
87	X	2	U	C2-N1-C1'	5.14	123.87	117.70
17	R3	16	ASP	CB-CG-OD1	5.13	122.92	118.30
85	A6	1242	C	C6-N1-C2	-5.13	118.25	120.30
85	A6	1451	G	N9-C4-C5	-5.13	103.35	105.40
2	A3	2132	A	C6-C5-N7	5.13	135.89	132.30
2	A3	2246	A	O5'-P-OP2	-5.13	101.08	105.70
2	A3	2569	C	N3-C2-O2	-5.13	118.31	121.90
85	A6	1297	C	C6-N1-C1'	-5.13	114.64	120.80
2	A3	2344	C	C6-N1-C2	-5.13	118.25	120.30
2	A3	2124	A	N1-C2-N3	-5.13	126.73	129.30
2	A3	3077	C	N1-C2-O2	5.13	121.98	118.90
2	A3	2030	U	C6-N1-C2	-5.13	117.92	121.00
21	V3	53	ASP	CB-CG-OD2	-5.12	113.69	118.30
85	A6	1013	C	C6-N1-C2	-5.12	118.25	120.30
50	p3	174	LYS	CB-CG-CD	-5.12	98.28	111.60
85	A6	698	C	N1-C2-O2	5.12	121.97	118.90
53	s3	100	LEU	CB-CG-CD2	-5.12	102.30	111.00
85	A6	1250	U	C2-N1-C1'	5.12	123.84	117.70
85	A6	1451	G	N3-C4-C5	-5.12	126.04	128.60
75	V6	181	LEU	CB-CG-CD2	-5.12	102.31	111.00
2	A3	2158	U	C2-N1-C1'	5.11	123.83	117.70
2	A3	2814	G	N3-C4-C5	-5.11	126.04	128.60
67	N6	13	ILE	CG1-CB-CG2	-5.11	100.15	111.40
87	X	63	C	C6-N1-C2	-5.11	118.25	120.30
2	A3	1993	A	N3-C4-N9	5.11	131.49	127.40
2	A3	1721	C	N3-C2-O2	-5.11	118.33	121.90
85	A6	1183	G	N3-C4-C5	5.11	131.15	128.60
23	X3	54	PRO	C-N-CA	5.11	134.47	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	s3	304	ASP	CB-CG-OD2	5.11	122.89	118.30
2	A3	3201	A	N3-C4-N9	5.10	131.48	127.40
31	53	348	ASP	CB-CG-OD2	5.10	122.89	118.30
2	A3	2603	C	N3-C2-O2	-5.10	118.33	121.90
12	M3	27	LEU	C-N-CA	5.10	134.45	121.70
77	X6	163	LYS	CB-CA-C	5.10	120.60	110.40
2	A3	2136	C	C5-C6-N1	5.10	123.55	121.00
2	A3	3061	G	C5-C6-O6	-5.10	125.54	128.60
87	X	69	C	N3-C2-O2	-5.10	118.33	121.90
85	A6	811	A	C4-C5-N7	5.10	113.25	110.70
85	A6	1250	U	C6-N1-C2	-5.09	117.94	121.00
2	A3	3102	U	C5-C6-N1	5.09	125.25	122.70
87	94	11	C	C5-C6-N1	5.09	123.55	121.00
2	A3	2280	C	N1-C2-O2	5.09	121.95	118.90
85	A6	1471	C	C2-N1-C1’	5.09	124.40	118.80
8	I3	197	LEU	CA-CB-CG	5.09	127.00	115.30
55	B6	224	ASP	CB-CA-C	5.09	120.57	110.40
23	X3	176	LEU	CB-CG-CD2	-5.08	102.36	111.00
87	94	27	A	N1-C2-N3	-5.08	126.76	129.30
87	99	1	G	O4’-C1’-N9	5.08	112.27	108.20
87	99	63	C	C5-C6-N1	5.08	123.54	121.00
2	A3	2502	C	C5-C6-N1	5.08	123.54	121.00
2	A3	1984	A	C8-N9-C4	-5.08	103.77	105.80
87	94	1	G	P-O3’-C3’	5.08	125.79	119.70
84	e6	438	LEU	CA-CB-CG	5.07	126.97	115.30
2	A3	2168	U	C5-C6-N1	5.07	125.23	122.70
2	A3	2447	A	C5-N7-C8	-5.07	101.36	103.90
2	A3	2584	C	C6-N1-C2	-5.07	118.27	120.30
2	A3	2852	C	C2-N1-C1’	5.07	124.37	118.80
55	B6	189	LEU	CA-CB-CG	5.07	126.96	115.30
2	A3	1868	G	N1-C6-O6	-5.07	116.86	119.90
85	A6	1039	U	C6-N1-C2	-5.06	117.96	121.00
85	A6	1401	U	C2-N1-C1’	5.06	123.77	117.70
2	A3	1839	C	C2-N1-C1’	5.06	124.37	118.80
32	63	44	ASN	CB-CA-C	5.06	120.52	110.40
2	A3	2756	C	C2-N1-C1’	5.06	124.36	118.80
81	b6	138	ASP	C-N-CA	5.05	134.34	121.70
2	A3	2596	G	C4-N9-C1’	5.05	133.07	126.50
2	A3	1709	G	C8-N9-C4	-5.05	104.38	106.40
85	A6	674	C	C6-N1-C2	-5.05	118.28	120.30
2	A3	2254	C	C6-N1-C2	-5.05	118.28	120.30
2	A3	2627	G	C8-N9-C1’	5.05	133.56	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	1672	C	N1-C2-O2	5.05	121.93	118.90
2	A3	2582	A	C8-N9-C1'	-5.05	118.61	127.70
2	A3	2075	U	C5-C6-N1	5.04	125.22	122.70
2	A3	3041	U	P-O3'-C3'	5.04	125.75	119.70
2	A3	3157	C	C5-C4-N4	-5.04	116.67	120.20
2	A3	3169	C	C6-N1-C1'	-5.04	114.75	120.80
11	L3	56	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	A3	3192	C	C2-N1-C1'	5.04	124.34	118.80
2	A3	2445	U	C2-N1-C1'	5.04	123.75	117.70
85	A6	677	U	C2-N1-C1'	5.03	123.74	117.70
85	A6	678	U	C5-C4-O4	-5.03	122.88	125.90
85	A6	711	C	C2-N1-C1'	5.03	124.34	118.80
2	A3	1994	A	C5-N7-C8	-5.03	101.38	103.90
2	A3	1835	A	C2-N3-C4	-5.03	108.08	110.60
2	A3	1758	U	N3-C2-O2	-5.03	118.68	122.20
87	99	20	U	C5-C6-N1	5.03	125.21	122.70
2	A3	2496	G	C4-C5-N7	5.03	112.81	110.80
2	A3	2905	A	P-O3'-C3'	5.03	125.73	119.70
85	A6	1213	C	C5-C6-N1	5.03	123.51	121.00
8	I3	148	VAL	CG1-CB-CG2	-5.02	102.86	110.90
2	A3	2627	G	C4-N9-C1'	-5.02	119.97	126.50
37	b3	65	VAL	CG1-CB-CG2	-5.02	102.87	110.90
85	A6	809	C	C6-N1-C2	-5.02	118.29	120.30
6	F3	128	TRP	CA-CB-CG	5.02	123.24	113.70
32	63	59	ARG	NE-CZ-NH1	5.02	122.81	120.30
59	F6	182	LEU	CA-CB-CG	5.02	126.84	115.30
84	e6	527	LEU	CA-CB-CG	5.02	126.84	115.30
87	X	6	U	N1-C2-O2	5.02	126.31	122.80
2	A3	1714	C	C2-N1-C1'	5.01	124.31	118.80
2	A3	3061	G	N3-C4-N9	5.01	129.01	126.00
9	J3	142	ARG	NE-CZ-NH2	-5.01	117.79	120.30
2	A3	2484	C	C2-N3-C4	5.01	122.41	119.90
2	A3	2473	A	N1-C6-N6	-5.01	115.59	118.60
32	63	52	ARG	CA-CB-CG	5.01	124.42	113.40
75	V6	43	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	A3	2871	U	C6-N1-C2	-5.01	117.99	121.00
2	A3	3151	A	C4-C5-N7	5.01	113.20	110.70
2	A3	3228	U	C5-C4-O4	5.01	128.91	125.90
46	k3	74	LEU	CA-CB-CG	5.01	126.82	115.30
85	A6	738	C	C5-C6-N1	5.01	123.50	121.00
85	A6	922	A	N1-C6-N6	-5.01	115.59	118.60
85	A6	1520	G	N3-C4-N9	5.01	129.00	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	2434	A	N7-C8-N9	5.00	116.30	113.80
85	A6	912	C	C6-N1-C2	-5.00	118.30	120.30
85	A6	951	U	N1-C2-O2	5.00	126.30	122.80
2	A3	2730	A	OP2-P-O3'	5.00	116.20	105.20
21	V3	53	ASP	CB-CA-C	5.00	120.40	110.40
85	A6	1324	G	C4-N9-C1'	5.00	133.00	126.50
85	A6	1492	C	C5-C6-N1	5.00	123.50	121.00
87	94	62	C	C6-N1-C1'	-5.00	114.80	120.80

There are no chirality outliers.

All (97) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	03	150	LYS	Peptide
26	03	177	ARG	Peptide
30	43	78	ASP	Peptide
31	53	346	GLY	Peptide
31	53	347	THR	Peptide
31	53	348	ASP	Peptide
32	63	222	ASP	Peptide
32	63	223	GLY	Peptide
32	63	304	TYR	Peptide
32	63	372	SER	Peptide
32	63	49	GLU	Peptide
32	63	51	TYR	Peptide
33	73	118	PRO	Peptide
35	93	132	PRO	Peptide
55	B6	164	GLU	Peptide
55	B6	229	PRO	Peptide
4	D3	206	TYR	Peptide
57	D6	136	ARG	Peptide
57	D6	286	GLU	Peptide
5	E3	169	GLY	Peptide
5	E3	244	ALA	Peptide
5	E3	85	TRP	Peptide
58	E6	11	LYS	Peptide
58	E6	13	MET	Peptide
59	F6	129	ALA	Peptide
59	F6	131	ALA	Peptide
59	F6	162	LEU	Peptide
60	G6	251	GLU	Peptide
7	H3	63	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
61	H6	169	ALA	Peptide
61	H6	181	PRO	Peptide
61	H6	70	ASP	Peptide
8	I3	181	ILE	Peptide
9	J3	133	GLN	Peptide
9	J3	33	PRO	Peptide
9	J3	48	GLN	Peptide
10	K3	158	TYR	Peptide
10	K3	159	THR	Peptide
10	K3	3	SER	Peptide
10	K3	5	SER	Peptide
64	K6	88	ARG	Peptide
11	L3	94	PRO	Peptide
12	M3	18	GLY	Peptide
12	M3	279	ASP	Peptide
12	M3	28	LYS	Peptide
12	M3	286	THR	Peptide
14	O3	127	GLY	Peptide
68	O6	232	PRO	Peptide
68	O6	78	ARG	Peptide
69	P6	139	ARG	Peptide
69	P6	64	LYS	Peptide
16	Q3	182	ARG	Peptide
16	Q3	83	ARG	Peptide
70	Q6	69	ALA	Peptide
17	R3	137	GLU	Peptide
17	R3	142	PHE	Peptide
71	R6	131	VAL	Peptide
71	R6	154	THR	Peptide
72	S6	110	GLY	Peptide
19	T3	163	ARG	Peptide
19	T3	94	ILE	Peptide
74	U6	32	ASP	Peptide
74	U6	54	PHE	Peptide
21	V3	100	LYS	Peptide
21	V3	151	GLY	Peptide
21	V3	170	TRP	Peptide
75	V6	317	LEU	Peptide
75	V6	323	GLU	Peptide
76	W6	145	LEU	Peptide
23	X3	222	ASP	Peptide
23	X3	51	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
77	X6	125	LEU	Peptide
77	X6	341	ILE	Peptide
1	Y2	22	UNK	Peptide
24	Y3	181	PHE	Peptide
78	Y6	320	GLY	Peptide
78	Y6	327	GLU	Peptide
25	Z3	141	SER	Peptide
79	Z6	10	ARG	Peptide
79	Z6	89	ARG	Peptide
82	c6	38	ARG	Peptide
82	c6	60	GLU	Peptide
39	d3	230	ARG	Peptide
39	d3	268	PRO	Peptide
40	e3	265	LYS	Peptide
84	e6	416	PHE	Peptide
84	e6	67	LYS	Peptide
41	f3	189	HIS	Peptide
41	f3	85	ASP	Peptide
43	h3	138	SER	Peptide
43	h3	63	PRO	Peptide
43	h3	65	ASP	Peptide
45	j3	25	GLY	Peptide
46	k3	82	THR	Peptide
51	q3	78	SER	Peptide
52	r3	189	ARG	Peptide
53	s3	270	LYS	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D3	234/305 (77%)	212 (91%)	21 (9%)	1 (0%)	34	69
5	E3	296/348 (85%)	265 (90%)	29 (10%)	2 (1%)	22	59
6	F3	248/311 (80%)	226 (91%)	20 (8%)	2 (1%)	19	56
7	H3	93/267 (35%)	83 (89%)	10 (11%)	0	100	100
8	I3	154/261 (59%)	139 (90%)	15 (10%)	0	100	100
9	J3	138/192 (72%)	122 (88%)	15 (11%)	1 (1%)	22	59
10	K3	175/178 (98%)	151 (86%)	23 (13%)	1 (1%)	25	62
11	L3	113/145 (78%)	100 (88%)	13 (12%)	0	100	100
12	M3	285/296 (96%)	254 (89%)	31 (11%)	0	100	100
13	N3	203/251 (81%)	188 (93%)	14 (7%)	1 (0%)	29	66
14	O3	150/175 (86%)	129 (86%)	20 (13%)	1 (1%)	22	59
15	P3	129/179 (72%)	123 (95%)	6 (5%)	0	100	100
16	Q3	217/292 (74%)	193 (89%)	24 (11%)	0	100	100
17	R3	138/149 (93%)	128 (93%)	10 (7%)	0	100	100
18	S3	154/205 (75%)	144 (94%)	10 (6%)	0	100	100
19	T3	164/212 (77%)	154 (94%)	10 (6%)	0	100	100
20	U3	109/153 (71%)	98 (90%)	11 (10%)	0	100	100
21	V3	183/216 (85%)	150 (82%)	30 (16%)	3 (2%)	9	43
22	W3	109/148 (74%)	103 (94%)	6 (6%)	0	100	100
23	X3	241/256 (94%)	217 (90%)	23 (10%)	1 (0%)	34	69
24	Y3	174/250 (70%)	162 (93%)	11 (6%)	1 (1%)	25	62
25	Z3	118/161 (73%)	109 (92%)	9 (8%)	0	100	100
26	03	106/188 (56%)	97 (92%)	8 (8%)	1 (1%)	17	54
27	13	50/65 (77%)	45 (90%)	5 (10%)	0	100	100
28	23	44/92 (48%)	42 (96%)	2 (4%)	0	100	100
29	33	93/188 (50%)	84 (90%)	9 (10%)	0	100	100
30	43	34/103 (33%)	32 (94%)	2 (6%)	0	100	100
31	53	368/423 (87%)	320 (87%)	45 (12%)	3 (1%)	19	56
32	63	313/380 (82%)	268 (86%)	44 (14%)	1 (0%)	41	74
33	73	258/338 (76%)	235 (91%)	23 (9%)	0	100	100
34	83	97/206 (47%)	88 (91%)	9 (9%)	0	100	100
35	93	105/137 (77%)	91 (87%)	14 (13%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	a3	78/142 (55%)	74 (95%)	4 (5%)	0	100	100
37	b3	146/155 (94%)	134 (92%)	12 (8%)	0	100	100
38	c3	271/332 (82%)	253 (93%)	18 (7%)	0	100	100
39	d3	156/306 (51%)	137 (88%)	17 (11%)	2 (1%)	12	47
40	e3	211/279 (76%)	186 (88%)	25 (12%)	0	100	100
41	f3	125/194 (64%)	114 (91%)	11 (9%)	0	100	100
42	g3	127/166 (76%)	116 (91%)	11 (9%)	0	100	100
43	h3	96/158 (61%)	78 (81%)	16 (17%)	2 (2%)	7	38
44	i3	95/128 (74%)	86 (90%)	9 (10%)	0	100	100
45	j3	83/123 (68%)	75 (90%)	8 (10%)	0	100	100
46	k3	82/112 (73%)	67 (82%)	15 (18%)	0	100	100
47	l3	21/138 (15%)	21 (100%)	0	0	100	100
48	m3	43/128 (34%)	40 (93%)	3 (7%)	0	100	100
49	o3	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
50	p3	119/206 (58%)	109 (92%)	10 (8%)	0	100	100
51	q3	126/222 (57%)	115 (91%)	8 (6%)	3 (2%)	6	35
52	r3	140/196 (71%)	126 (90%)	14 (10%)	0	100	100
53	s3	366/439 (83%)	332 (91%)	34 (9%)	0	100	100
55	B6	215/296 (73%)	198 (92%)	17 (8%)	0	100	100
56	C6	130/167 (78%)	117 (90%)	13 (10%)	0	100	100
57	D6	316/430 (74%)	286 (90%)	30 (10%)	0	100	100
58	E6	120/125 (96%)	108 (90%)	11 (9%)	1 (1%)	19	56
59	F6	197/242 (81%)	181 (92%)	16 (8%)	0	100	100
60	G6	301/396 (76%)	270 (90%)	31 (10%)	0	100	100
61	H6	120/201 (60%)	102 (85%)	17 (14%)	1 (1%)	19	56
62	I6	134/194 (69%)	121 (90%)	13 (10%)	0	100	100
63	J6	106/138 (77%)	91 (86%)	15 (14%)	0	100	100
64	K6	99/128 (77%)	94 (95%)	4 (4%)	1 (1%)	15	51
65	L6	162/257 (63%)	150 (93%)	12 (7%)	0	100	100
66	M6	114/137 (83%)	106 (93%)	8 (7%)	0	100	100
67	N6	105/130 (81%)	90 (86%)	15 (14%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	O6	183/258 (71%)	162 (88%)	21 (12%)	0	100	100
69	P6	94/142 (66%)	85 (90%)	8 (8%)	1 (1%)	14	50
70	Q6	84/87 (97%)	72 (86%)	12 (14%)	0	100	100
71	R6	240/360 (67%)	204 (85%)	36 (15%)	0	100	100
72	S6	124/190 (65%)	115 (93%)	9 (7%)	0	100	100
73	T6	160/173 (92%)	146 (91%)	13 (8%)	1 (1%)	25	62
74	U6	171/205 (83%)	160 (94%)	11 (6%)	0	100	100
75	V6	320/414 (77%)	280 (88%)	40 (12%)	0	100	100
76	W6	95/187 (51%)	83 (87%)	10 (10%)	2 (2%)	7	38
77	X6	310/398 (78%)	271 (87%)	37 (12%)	2 (1%)	25	62
78	Y6	106/395 (27%)	92 (87%)	14 (13%)	0	100	100
79	Z6	85/106 (80%)	74 (87%)	11 (13%)	0	100	100
80	a6	197/218 (90%)	173 (88%)	24 (12%)	0	100	100
81	b6	252/323 (78%)	210 (83%)	41 (16%)	1 (0%)	34	69
82	c6	114/118 (97%)	98 (86%)	16 (14%)	0	100	100
83	d6	67/199 (34%)	62 (92%)	5 (8%)	0	100	100
84	e6	362/689 (52%)	317 (88%)	42 (12%)	3 (1%)	19	56
All	All	12753/17899 (71%)	11421 (90%)	1293 (10%)	39 (0%)	44	74

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	V3	101	THR
21	V3	194	LEU
61	H6	126	ILE
84	e6	68	VAL
4	D3	207	ILE
10	K3	160	GLN
23	X3	52	ILE
31	53	349	GLY
39	d3	231	LEU
51	q3	43	GLU
76	W6	147	LEU
21	V3	193	THR
43	h3	138	SER
69	P6	65	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	W6	148	GLU
31	53	270	ILE
51	q3	42	PRO
77	X6	97	ALA
84	e6	275	ALA
5	E3	245	THR
6	F3	291	SER
13	N3	238	LYS
26	03	178	ASP
64	K6	105	ARG
81	b6	244	THR
31	53	269	ASN
39	d3	164	VAL
43	h3	66	LEU
5	E3	246	GLY
14	O3	111	PRO
9	J3	33	PRO
24	Y3	202	LEU
32	63	351	HIS
84	e6	396	ILE
6	F3	128	TRP
73	T6	150	PRO
51	q3	79	PRO
58	E6	15	ARG
77	X6	120	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D3	190/245 (78%)	190 (100%)	0	100	100
5	E3	255/290 (88%)	255 (100%)	0	100	100
6	F3	217/262 (83%)	216 (100%)	1 (0%)	88	94
7	H3	86/228 (38%)	85 (99%)	1 (1%)	71	84
8	I3	145/232 (62%)	142 (98%)	3 (2%)	53	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J3	113/150 (75%)	112 (99%)	1 (1%)	78	88
10	K3	155/156 (99%)	155 (100%)	0	100	100
11	L3	98/124 (79%)	98 (100%)	0	100	100
12	M3	245/249 (98%)	243 (99%)	2 (1%)	81	89
13	N3	172/211 (82%)	170 (99%)	2 (1%)	71	84
14	O3	133/150 (89%)	133 (100%)	0	100	100
15	P3	115/154 (75%)	114 (99%)	1 (1%)	78	88
16	Q3	201/256 (78%)	200 (100%)	1 (0%)	88	94
17	R3	118/126 (94%)	118 (100%)	0	100	100
18	S3	141/180 (78%)	140 (99%)	1 (1%)	84	91
19	T3	146/182 (80%)	144 (99%)	2 (1%)	67	82
20	U3	99/135 (73%)	99 (100%)	0	100	100
21	V3	169/191 (88%)	168 (99%)	1 (1%)	86	93
22	W3	91/119 (76%)	91 (100%)	0	100	100
23	X3	217/227 (96%)	217 (100%)	0	100	100
24	Y3	159/223 (71%)	159 (100%)	0	100	100
25	Z3	111/147 (76%)	111 (100%)	0	100	100
26	03	97/164 (59%)	97 (100%)	0	100	100
27	13	49/60 (82%)	48 (98%)	1 (2%)	55	74
28	23	40/72 (56%)	40 (100%)	0	100	100
29	33	88/166 (53%)	88 (100%)	0	100	100
30	43	35/89 (39%)	35 (100%)	0	100	100
31	53	337/368 (92%)	335 (99%)	2 (1%)	86	93
32	63	266/332 (80%)	264 (99%)	2 (1%)	81	89
33	73	242/303 (80%)	241 (100%)	1 (0%)	91	95
34	83	91/190 (48%)	90 (99%)	1 (1%)	73	85
35	93	91/112 (81%)	90 (99%)	1 (1%)	73	85
36	a3	78/133 (59%)	78 (100%)	0	100	100
37	b3	130/135 (96%)	129 (99%)	1 (1%)	81	89
38	c3	241/288 (84%)	239 (99%)	2 (1%)	81	89
39	d3	151/274 (55%)	151 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	e3	188/236 (80%)	187 (100%)	1 (0%)	88	94
41	f3	117/173 (68%)	117 (100%)	0	100	100
42	g3	119/148 (80%)	119 (100%)	0	100	100
43	h3	95/148 (64%)	95 (100%)	0	100	100
44	i3	86/110 (78%)	85 (99%)	1 (1%)	71	84
45	j3	68/97 (70%)	68 (100%)	0	100	100
46	k3	74/90 (82%)	73 (99%)	1 (1%)	67	82
47	l3	23/116 (20%)	23 (100%)	0	100	100
48	m3	40/113 (35%)	39 (98%)	1 (2%)	47	70
49	o3	80/87 (92%)	80 (100%)	0	100	100
50	p3	117/181 (65%)	117 (100%)	0	100	100
51	q3	110/178 (62%)	109 (99%)	1 (1%)	78	88
52	r3	133/169 (79%)	133 (100%)	0	100	100
53	s3	326/381 (86%)	324 (99%)	2 (1%)	86	93
55	B6	191/249 (77%)	191 (100%)	0	100	100
56	C6	115/143 (80%)	114 (99%)	1 (1%)	78	88
57	D6	269/357 (75%)	266 (99%)	3 (1%)	73	85
58	E6	104/107 (97%)	104 (100%)	0	100	100
59	F6	178/209 (85%)	178 (100%)	0	100	100
60	G6	265/342 (78%)	264 (100%)	1 (0%)	91	95
61	H6	112/180 (62%)	111 (99%)	1 (1%)	78	88
62	I6	104/147 (71%)	104 (100%)	0	100	100
63	J6	93/118 (79%)	91 (98%)	2 (2%)	52	72
64	K6	91/113 (80%)	90 (99%)	1 (1%)	73	85
65	L6	152/226 (67%)	151 (99%)	1 (1%)	84	91
66	M6	95/113 (84%)	94 (99%)	1 (1%)	73	85
67	N6	93/115 (81%)	93 (100%)	0	100	100
68	O6	166/230 (72%)	166 (100%)	0	100	100
69	P6	87/123 (71%)	86 (99%)	1 (1%)	73	85
70	Q6	78/79 (99%)	76 (97%)	2 (3%)	46	69
71	R6	224/318 (70%)	222 (99%)	2 (1%)	78	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	S6	109/164 (66%)	108 (99%)	1 (1%)	78	88
73	T6	150/157 (96%)	150 (100%)	0	100	100
74	U6	149/174 (86%)	149 (100%)	0	100	100
75	V6	295/364 (81%)	294 (100%)	1 (0%)	92	96
76	W6	84/158 (53%)	84 (100%)	0	100	100
77	X6	275/351 (78%)	275 (100%)	0	100	100
78	Y6	99/357 (28%)	99 (100%)	0	100	100
79	Z6	80/95 (84%)	80 (100%)	0	100	100
80	a6	176/190 (93%)	173 (98%)	3 (2%)	60	79
81	b6	237/291 (81%)	237 (100%)	0	100	100
82	c6	99/101 (98%)	97 (98%)	2 (2%)	55	74
83	d6	63/166 (38%)	63 (100%)	0	100	100
84	e6	226/609 (37%)	226 (100%)	0	100	100
All	All	11347/15496 (73%)	11290 (100%)	57 (0%)	89	94

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F3	49	ARG
7	H3	136	ASN
8	I3	43	GLN
8	I3	84	ARG
8	I3	189	GLN
9	J3	133	GLN
12	M3	47	ARG
12	M3	134	ARG
13	N3	178	GLN
13	N3	222	ASN
15	P3	120	ASN
16	Q3	252	GLN
18	S3	118	ASN
19	T3	133	ASN
19	T3	195	HIS
21	V3	209	LYS
27	13	61	LYS
31	53	269	ASN
31	53	326	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	63	47	ARG
32	63	299	ARG
33	73	50	LYS
34	83	164	ARG
35	93	134	ASN
37	b3	66	ASN
38	c3	192	GLN
38	c3	247	LYS
40	e3	132	LYS
44	i3	65	ASN
46	k3	15	GLN
48	m3	42	ARG
51	q3	120	HIS
53	s3	246	GLN
53	s3	315	ASN
56	C6	57	HIS
57	D6	145	ASN
57	D6	181	ARG
57	D6	365	LYS
60	G6	90	ASN
61	H6	131	ARG
63	J6	43	LYS
63	J6	84	ARG
64	K6	40	ARG
65	L6	100	LYS
66	M6	112	ARG
69	P6	47	ASN
70	Q6	10	ARG
70	Q6	52	ARG
71	R6	194	GLN
71	R6	244	LYS
72	S6	107	GLN
75	V6	391	GLN
80	a6	121	LYS
80	a6	171	ARG
80	a6	197	ARG
82	c6	68	LYS
82	c6	114	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
6	F3	103	GLN
6	F3	241	ASN
6	F3	276	GLN
10	K3	48	HIS
13	N3	110	ASN
14	O3	109	GLN
20	U3	35	GLN
22	W3	41	ASN
24	Y3	88	GLN
31	53	289	HIS
31	53	353	HIS
31	53	380	GLN
33	73	45	ASN
34	83	143	GLN
38	c3	42	GLN
40	e3	67	GLN
40	e3	175	GLN
58	E6	58	HIS
59	F6	169	GLN
60	G6	127	HIS
70	Q6	4	HIS
71	R6	76	GLN
71	R6	224	HIS
71	R6	277	ASN
71	R6	278	ASN
73	T6	20	ASN
79	Z6	75	HIS
81	b6	321	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A3	1473/1559 (94%)	464 (31%)	25 (1%)
3	B3	51/73 (69%)	15 (29%)	0
85	A6	921/954 (96%)	251 (27%)	16 (1%)
86	i4	8/9 (88%)	7 (87%)	0
87	94	73/73 (100%)	39 (53%)	2 (2%)
87	99	73/73 (100%)	46 (63%)	1 (1%)
87	X	73/73 (100%)	40 (54%)	2 (2%)
All	All	2672/2814 (94%)	862 (32%)	46 (1%)

All (862) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A3	1674	A
2	A3	1676	A
2	A3	1677	C
2	A3	1678	C
2	A3	1679	U
2	A3	1680	A
2	A3	1681	G
2	A3	1684	C
2	A3	1685	C
2	A3	1687	A
2	A3	1689	C
2	A3	1690	C
2	A3	1693	C
2	A3	1694	U
2	A3	1699	C
2	A3	1700	U
2	A3	1701	U
2	A3	1703	C
2	A3	1704	U
2	A3	1707	C
2	A3	1708	A
2	A3	1709	G
2	A3	1712	A
2	A3	1713	A
2	A3	1714	C
2	A3	1715	C
2	A3	1716	U
2	A3	1717	U
2	A3	1724	A
2	A3	1727	A
2	A3	1728	U
2	A3	1732	C
2	A3	1741	A
2	A3	1748	G
2	A3	1750	G
2	A3	1751	A
2	A3	1757	A
2	A3	1760	G
2	A3	1767	G
2	A3	1770	G
2	A3	1774	U
2	A3	1777	A
2	A3	1779	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A3	1781	A
2	A3	1791	G
2	A3	1794	A
2	A3	1797	G
2	A3	1803	A
2	A3	1804	A
2	A3	1805	A
2	A3	1806	U
2	A3	1807	U
2	A3	1808	A
2	A3	1809	U
2	A3	1810	A
2	A3	1812	C
2	A3	1813	C
2	A3	1817	C
2	A3	1821	A
2	A3	1824	U
2	A3	1827	C
2	A3	1828	A
2	A3	1829	A
2	A3	1832	A
2	A3	1836	A
2	A3	1844	A
2	A3	1849	C
2	A3	1850	U
2	A3	1854	U
2	A3	1856	A
2	A3	1867	A
2	A3	1869	A
2	A3	1870	A
2	A3	1871	A
2	A3	1872	U
2	A3	1873	A
2	A3	1874	A
2	A3	1879	G
2	A3	1882	A
2	A3	1883	G
2	A3	1888	G
2	A3	1890	C
2	A3	1892	A
2	A3	1893	A
2	A3	1901	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A3	1902	C
2	A3	1903	C
2	A3	1909	A
2	A3	1918	G
2	A3	1927	G
2	A3	1939	G
2	A3	1940	A
2	A3	1944	C
2	A3	1958	G
2	A3	1959	C
2	A3	1966	G
2	A3	1968	G
2	A3	1974	A
2	A3	1975	U
2	A3	1985	G
2	A3	1986	A
2	A3	1987	G
2	A3	1992	C
2	A3	1993	A
2	A3	1994	A
2	A3	1995	A
2	A3	2000	C
2	A3	2001	C
2	A3	2002	G
2	A3	2003	A
2	A3	2009	G
2	A3	2015	G
2	A3	2016	C
2	A3	2021	U
2	A3	2022	G
2	A3	2029	A
2	A3	2031	A
2	A3	2032	G
2	A3	2034	A
2	A3	2036	C
2	A3	2037	U
2	A3	2039	A
2	A3	2053	U
2	A3	2055	U
2	A3	2057	C
2	A3	2060	A
2	A3	2065	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A3	2074	A
2	A3	2079	C
2	A3	2083	U
2	A3	2093	U
2	A3	2096	U
2	A3	2097	A
2	A3	2098	G
2	A3	2105	G
2	A3	2113	G
2	A3	2124	A
2	A3	2125	C
2	A3	2135	A
2	A3	2141	U
2	A3	2142	A
2	A3	2147	G
2	A3	2154	A
2	A3	2158	U
2	A3	2159	U
2	A3	2160	A
2	A3	2163	A
2	A3	2166	C
2	A3	2168	U
2	A3	2169	A
2	A3	2171	U
2	A3	2172	A
2	A3	2173	G
2	A3	2174	G
2	A3	2175	C
2	A3	2180	A
2	A3	2181	A
2	A3	2182	G
2	A3	2183	C
2	A3	2184	A
2	A3	2186	C
2	A3	2187	C
2	A3	2193	U
2	A3	2194	U
2	A3	2195	A
2	A3	2197	G
2	A3	2198	A
2	A3	2199	A
2	A3	2200	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A3	2202	C
2	A3	2203	G
2	A3	2204	U
2	A3	2208	A
2	A3	2209	G
2	A3	2210	C
2	A3	2216	A
2	A3	2218	C
2	A3	2220	A
2	A3	2221	C
2	A3	2222	U
2	A3	2223	A
2	A3	2225	C
2	A3	2227	A
2	A3	2228	A
2	A3	2229	A
2	A3	2230	A
2	A3	2231	A
2	A3	2232	A
2	A3	2233	U
2	A3	2234	C
2	A3	2237	A
2	A3	2239	A
2	A3	2241	A
2	A3	2242	U
2	A3	2243	A
2	A3	2244	U
2	A3	2245	A
2	A3	2246	A
2	A3	2252	C
2	A3	2260	A
2	A3	2262	C
2	A3	2263	C
2	A3	2269	G
2	A3	2282	C
2	A3	2283	C
2	A3	2284	C
2	A3	2290	A
2	A3	2296	U
2	A3	2297	A
2	A3	2299	U
2	A3	2300	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A3	2309	A
2	A3	2315	A
2	A3	2321	A
2	A3	2322	C
2	A3	2323	A
2	A3	2324	U
2	A3	2331	C
2	A3	2332	C
2	A3	2342	U
2	A3	2345	G
2	A3	2358	A
2	A3	2364	C
2	A3	2371	U
2	A3	2372	U
2	A3	2381	A
2	A3	2384	A
2	A3	2387	U
2	A3	2388	A
2	A3	2389	C
2	A3	2390	A
2	A3	2392	U
2	A3	2393	C
2	A3	2397	C
2	A3	2401	A
2	A3	2402	A
2	A3	2404	U
2	A3	2407	U
2	A3	2414	C
2	A3	2415	C
2	A3	2416	U
2	A3	2417	C
2	A3	2425	A
2	A3	2426	C
2	A3	2433	C
2	A3	2434	A
2	A3	2435	G
2	A3	2441	C
2	A3	2443	C
2	A3	2444	A
2	A3	2447	A
2	A3	2449	G
2	A3	2471	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A3	2476	C
2	A3	2478	G
2	A3	2479	C
2	A3	2480	A
2	A3	2484	C
2	A3	2485	U
2	A3	2489	C
2	A3	2493	C
2	A3	2500	A
2	A3	2501	C
2	A3	2502	C
2	A3	2504	A
2	A3	2506	A
2	A3	2507	A
2	A3	2508	C
2	A3	2511	C
2	A3	2512	A
2	A3	2516	C
2	A3	2520	C
2	A3	2521	A
2	A3	2522	U
2	A3	2523	C
2	A3	2524	A
2	A3	2526	C
2	A3	2527	A
2	A3	2530	A
2	A3	2531	U
2	A3	2540	C
2	A3	2546	G
2	A3	2550	A
2	A3	2557	C
2	A3	2558	A
2	A3	2559	U
2	A3	2560	G
2	A3	2563	U
2	A3	2564	A
2	A3	2570	C
2	A3	2577	C
2	A3	2578	C
2	A3	2579	C
2	A3	2581	A
2	A3	2582	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A3	2585	G
2	A3	2587	G
2	A3	2590	A
2	A3	2592	G
2	A3	2593	G
2	A3	2596	G
2	A3	2601	A
2	A3	2603	C
2	A3	2606	U
2	A3	2618	U
2	A3	2626	U
2	A3	2628	U
2	A3	2629	A
2	A3	2630	U
2	A3	2632	A
2	A3	2633	A
2	A3	2634	U
2	A3	2635	G
2	A3	2645	G
2	A3	2652	G
2	A3	2654	U
2	A3	2655	G
2	A3	2656	U
2	A3	2659	C
2	A3	2660	U
2	A3	2676	A
2	A3	2683	C
2	A3	2684	C
2	A3	2686	G
2	A3	2694	A
2	A3	2695	G
2	A3	2696	A
2	A3	2697	G
2	A3	2698	G
2	A3	2706	A
2	A3	2708	C
2	A3	2709	A
2	A3	2718	C
2	A3	2719	G
2	A3	2722	A
2	A3	2723	A
2	A3	2724	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A3	2725	A
2	A3	2726	C
2	A3	2732	G
2	A3	2733	G
2	A3	2740	A
2	A3	2743	U
2	A3	2744	U
2	A3	2745	A
2	A3	2747	U
2	A3	2750	U
2	A3	2751	G
2	A3	2753	A
2	A3	2756	C
2	A3	2757	A
2	A3	2759	U
2	A3	2793	C
2	A3	2794	C
2	A3	2803	A
2	A3	2804	A
2	A3	2810	G
2	A3	2814	G
2	A3	2815	G
2	A3	2831	G
2	A3	2832	A
2	A3	2833	A
2	A3	2844	G
2	A3	2847	C
2	A3	2850	U
2	A3	2851	A
2	A3	2852	C
2	A3	2854	U
2	A3	2861	A
2	A3	2864	U
2	A3	2865	C
2	A3	2870	G
2	A3	2871	U
2	A3	2880	A
2	A3	2881	C
2	A3	2892	A
2	A3	2893	A
2	A3	2895	U
2	A3	2896	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A3	2901	A
2	A3	2906	C
2	A3	2909	G
2	A3	2910	A
2	A3	2911	C
2	A3	2912	C
2	A3	2913	A
2	A3	2917	G
2	A3	2919	A
2	A3	2922	A
2	A3	2926	A
2	A3	2928	C
2	A3	2932	G
2	A3	2935	A
2	A3	2946	A
2	A3	2955	U
2	A3	2956	A
2	A3	2963	A
2	A3	2964	U
2	A3	2971	A
2	A3	2977	G
2	A3	2981	A
2	A3	2985	C
2	A3	2989	G
2	A3	2990	A
2	A3	2991	U
2	A3	2992	G
2	A3	2993	U
2	A3	2995	G
2	A3	3005	A
2	A3	3016	G
2	A3	3018	A
2	A3	3019	G
2	A3	3041	U
2	A3	3042	U
2	A3	3043	C
2	A3	3049	U
2	A3	3053	A
2	A3	3054	G
2	A3	3056	C
2	A3	3060	C
2	A3	3063	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A3	3065	U
2	A3	3077	C
2	A3	3078	C
2	A3	3086	U
2	A3	3089	A
2	A3	3093	C
2	A3	3096	U
2	A3	3098	U
2	A3	3100	U
2	A3	3102	U
2	A3	3108	U
2	A3	3114	U
2	A3	3116	C
2	A3	3123	G
2	A3	3124	U
2	A3	3127	G
2	A3	3128	A
2	A3	3129	A
2	A3	3131	G
2	A3	3134	C
2	A3	3141	A
2	A3	3150	U
2	A3	3155	C
2	A3	3157	C
2	A3	3158	A
2	A3	3159	A
2	A3	3160	A
2	A3	3161	G
2	A3	3162	C
2	A3	3168	C
2	A3	3169	C
2	A3	3172	C
2	A3	3176	A
2	A3	3183	U
2	A3	3184	C
2	A3	3185	A
2	A3	3189	C
2	A3	3190	A
2	A3	3202	U
2	A3	3207	A
2	A3	3217	A
2	A3	3218	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A3	3228	U
3	B3	1604	G
3	B3	1608	G
3	B3	1609	U
3	B3	1610	A
3	B3	1613	U
3	B3	1614	U
3	B3	1615	A
3	B3	1622	A
3	B3	1631	C
3	B3	1632	U
3	B3	1637	C
3	B3	1641	G
3	B3	1644	G
3	B3	1645	A
3	B3	1646	U
85	A6	654	U
85	A6	655	A
85	A6	684	U
85	A6	686	A
85	A6	687	G
85	A6	692	A
85	A6	693	U
85	A6	694	U
85	A6	695	A
85	A6	698	C
85	A6	703	A
85	A6	704	A
85	A6	708	U
85	A6	710	C
85	A6	715	U
85	A6	722	A
85	A6	723	G
85	A6	725	U
85	A6	726	C
85	A6	727	A
85	A6	735	A
85	A6	749	A
85	A6	755	A
85	A6	757	A
85	A6	765	A
85	A6	768	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	A6	769	C
85	A6	770	G
85	A6	776	A
85	A6	777	U
85	A6	781	G
85	A6	791	C
85	A6	795	G
85	A6	797	C
85	A6	798	U
85	A6	800	G
85	A6	811	A
85	A6	816	A
85	A6	817	A
85	A6	818	A
85	A6	819	C
85	A6	821	G
85	A6	830	A
85	A6	832	C
85	A6	833	C
85	A6	834	U
85	A6	836	U
85	A6	839	C
85	A6	840	A
85	A6	841	A
85	A6	849	A
85	A6	851	G
85	A6	857	C
85	A6	859	A
85	A6	865	U
85	A6	866	A
85	A6	872	C
85	A6	873	C
85	A6	874	C
85	A6	886	A
85	A6	887	U
85	A6	888	U
85	A6	889	U
85	A6	893	G
85	A6	894	C
85	A6	897	G
85	A6	903	G
85	A6	907	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	A6	908	C
85	A6	909	A
85	A6	916	U
85	A6	918	A
85	A6	923	A
85	A6	926	C
85	A6	927	A
85	A6	931	G
85	A6	933	A
85	A6	940	G
85	A6	942	A
85	A6	943	A
85	A6	945	G
85	A6	946	A
85	A6	947	G
85	A6	951	U
85	A6	952	U
85	A6	954	A
85	A6	957	U
85	A6	971	A
85	A6	981	A
85	A6	991	A
85	A6	992	G
85	A6	996	U
85	A6	997	A
85	A6	1005	C
85	A6	1006	C
85	A6	1009	U
85	A6	1014	A
85	A6	1015	C
85	A6	1016	A
85	A6	1019	A
85	A6	1024	C
85	A6	1025	U
85	A6	1026	A
85	A6	1032	G
85	A6	1035	G
85	A6	1038	U
85	A6	1046	U
85	A6	1050	A
85	A6	1051	A
85	A6	1053	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	A6	1056	C
85	A6	1069	C
85	A6	1082	A
85	A6	1084	A
85	A6	1085	U
85	A6	1086	A
85	A6	1101	G
85	A6	1107	A
85	A6	1109	C
85	A6	1110	C
85	A6	1113	A
85	A6	1125	A
85	A6	1130	A
85	A6	1141	A
85	A6	1142	G
85	A6	1146	A
85	A6	1151	G
85	A6	1155	C
85	A6	1156	A
85	A6	1158	A
85	A6	1170	A
85	A6	1171	A
85	A6	1179	G
85	A6	1183	G
85	A6	1184	U
85	A6	1188	U
85	A6	1189	C
85	A6	1191	U
85	A6	1192	A
85	A6	1193	U
85	A6	1194	C
85	A6	1197	U
85	A6	1217	A
85	A6	1218	A
85	A6	1219	U
85	A6	1223	U
85	A6	1224	A
85	A6	1226	A
85	A6	1227	C
85	A6	1229	C
85	A6	1233	U
85	A6	1234	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	A6	1235	A
85	A6	1237	C
85	A6	1249	U
85	A6	1250	U
85	A6	1251	G
85	A6	1252	C
85	A6	1254	C
85	A6	1255	A
85	A6	1261	U
85	A6	1269	C
85	A6	1273	U
85	A6	1274	U
85	A6	1275	C
85	A6	1276	A
85	A6	1286	G
85	A6	1287	A
85	A6	1288	U
85	A6	1294	C
85	A6	1296	A
85	A6	1297	C
85	A6	1299	A
85	A6	1301	G
85	A6	1304	A
85	A6	1330	A
85	A6	1331	G
85	A6	1334	C
85	A6	1336	A
85	A6	1338	G
85	A6	1339	U
85	A6	1346	C
85	A6	1347	A
85	A6	1357	A
85	A6	1359	G
85	A6	1360	A
85	A6	1366	G
85	A6	1369	A
85	A6	1371	A
85	A6	1372	U
85	A6	1380	C
85	A6	1381	C
85	A6	1382	C
85	A6	1385	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	A6	1394	A
85	A6	1395	U
85	A6	1398	C
85	A6	1401	U
85	A6	1404	U
85	A6	1406	A
85	A6	1420	A
85	A6	1421	A
85	A6	1424	U
85	A6	1434	A
85	A6	1436	U
85	A6	1437	A
85	A6	1438	A
85	A6	1451	G
85	A6	1452	U
85	A6	1458	G
85	A6	1465	A
85	A6	1469	C
85	A6	1482	A
85	A6	1485	C
85	A6	1486	A
85	A6	1487	C
85	A6	1490	C
85	A6	1506	A
85	A6	1516	A
85	A6	1518	A
85	A6	1520	G
85	A6	1521	A
85	A6	1529	C
85	A6	1530	U
85	A6	1531	A
85	A6	1536	C
85	A6	1537	C
85	A6	1538	C
85	A6	1539	U
85	A6	1540	A
85	A6	1541	C
85	A6	1542	G
85	A6	1543	C
85	A6	1544	A
85	A6	1545	U
85	A6	1547	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	A6	1553	G
85	A6	1561	A
85	A6	1562	A
85	A6	1563	G
85	A6	1566	G
85	A6	1568	A
85	A6	1572	U
85	A6	1575	U
85	A6	1586	G
85	A6	1588	A
85	A6	1589	A
85	A6	1598	G
85	A6	1599	G
85	A6	1602	G
85	A6	1603	A
86	i4	18	A
86	i4	19	A
86	i4	20	G
86	i4	21	U
86	i4	22	A
86	i4	23	G
86	i4	24	U
87	99	2	U
87	99	7	G
87	99	8	U
87	99	9	A
87	99	12	U
87	99	13	U
87	99	15	A
87	99	16	A
87	99	17	U
87	99	18	U
87	99	19	A
87	99	20	U
87	99	21	C
87	99	22	A
87	99	28	A
87	99	30	G
87	99	32	A
87	99	33	C
87	99	34	U
87	99	35	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	99	36	A
87	99	37	A
87	99	38	A
87	99	39	A
87	99	40	U
87	99	41	G
87	99	42	C
87	99	44	U
87	99	45	A
87	99	46	G
87	99	47	A
87	99	51	G
87	99	52	C
87	99	53	C
87	99	54	U
87	99	55	C
87	99	56	A
87	99	58	A
87	99	59	G
87	99	62	C
87	99	64	A
87	99	67	A
87	99	69	C
87	99	70	A
87	99	71	C
87	99	73	A
87	94	2	U
87	94	3	U
87	94	7	G
87	94	9	A
87	94	11	C
87	94	12	U
87	94	14	A
87	94	16	A
87	94	17	U
87	94	18	U
87	94	19	A
87	94	20	U
87	94	21	C
87	94	22	A
87	94	27	A
87	94	28	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	94	31	C
87	94	38	A
87	94	40	U
87	94	41	G
87	94	44	U
87	94	45	A
87	94	46	G
87	94	49	G
87	94	50	A
87	94	51	G
87	94	52	C
87	94	54	U
87	94	55	C
87	94	56	A
87	94	57	C
87	94	58	A
87	94	59	G
87	94	60	C
87	94	61	U
87	94	67	A
87	94	71	C
87	94	72	C
87	94	73	A
87	X	2	U
87	X	3	U
87	X	6	U
87	X	7	G
87	X	8	U
87	X	9	A
87	X	12	U
87	X	13	U
87	X	16	A
87	X	17	U
87	X	18	U
87	X	19	A
87	X	20	U
87	X	21	C
87	X	22	A
87	X	23	A
87	X	27	A
87	X	28	A
87	X	30	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	X	31	C
87	X	40	U
87	X	45	A
87	X	46	G
87	X	47	A
87	X	48	U
87	X	50	A
87	X	51	G
87	X	52	C
87	X	53	C
87	X	54	U
87	X	55	C
87	X	56	A
87	X	57	C
87	X	58	A
87	X	59	G
87	X	62	C
87	X	69	C
87	X	71	C
87	X	72	C
87	X	73	A

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A3	1703	C
2	A3	1805	A
2	A3	1806	U
2	A3	1807	U
2	A3	1809	U
2	A3	1823	A
2	A3	1871	A
2	A3	1901	C
2	A3	2165	C
2	A3	2172	A
2	A3	2186	C
2	A3	2221	C
2	A3	2243	A
2	A3	2245	A
2	A3	2507	A
2	A3	2523	C
2	A3	2530	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A3	2559	U
2	A3	2628	U
2	A3	2653	C
2	A3	2905	A
2	A3	2989	G
2	A3	3041	U
2	A3	3092	U
2	A3	3201	A
85	A6	721	G
85	A6	886	A
85	A6	1025	U
85	A6	1034	G
85	A6	1045	A
85	A6	1170	A
85	A6	1193	U
85	A6	1250	U
85	A6	1287	A
85	A6	1299	A
85	A6	1335	A
85	A6	1419	G
85	A6	1433	C
85	A6	1538	C
85	A6	1541	C
85	A6	1560	C
87	99	1	G
87	94	1	G
87	94	49	G
87	X	1	G
87	X	49	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 136 ligands modelled in this entry, 135 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
91	GDP	X6	500	-	24,30,30	0.95	1 (4%)	30,47,47	1.60	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	GDP	X6	500	-	-	4/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	X6	500	GDP	C6-N1	-2.57	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	X6	500	GDP	PA-O3A-PB	-5.56	113.73	132.83
91	X6	500	GDP	C3'-C2'-C1'	3.57	106.35	100.98
91	X6	500	GDP	O2B-PB-O3A	2.25	112.17	104.64
91	X6	500	GDP	O4'-C1'-C2'	-2.10	103.86	106.93
91	X6	500	GDP	C8-N7-C5	2.03	106.86	102.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

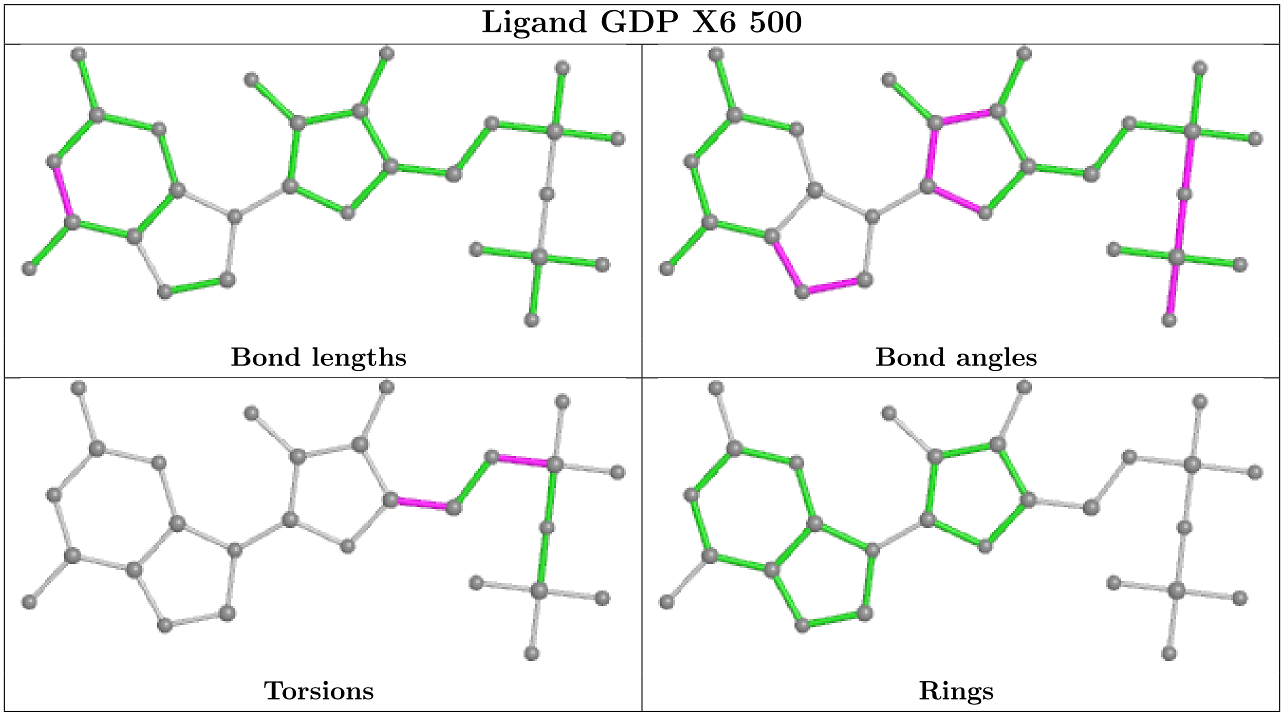
Mol	Chain	Res	Type	Atoms
91	X6	500	GDP	C5'-O5'-PA-O3A
91	X6	500	GDP	C3'-C4'-C5'-O5'
91	X6	500	GDP	O4'-C4'-C5'-O5'
91	X6	500	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GDP X6 500



Bond lengths **Bond angles**

Torsions **Rings**

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	S3	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
23	X3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S3	57:SER	C	58:SER	N	1.18
1	X3	5:LYS	C	6:TYR	N	1.15

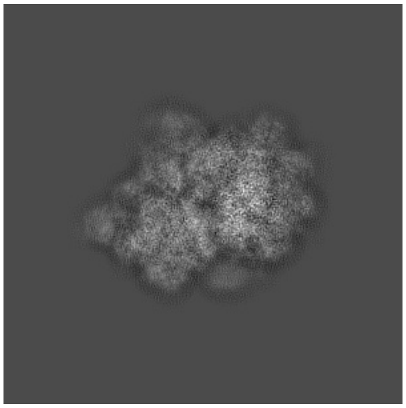
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11644. These allow visual inspection of the internal detail of the map and identification of artifacts.

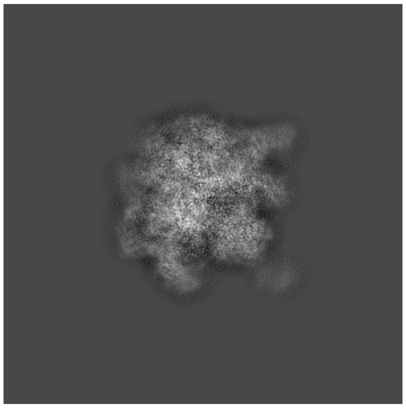
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

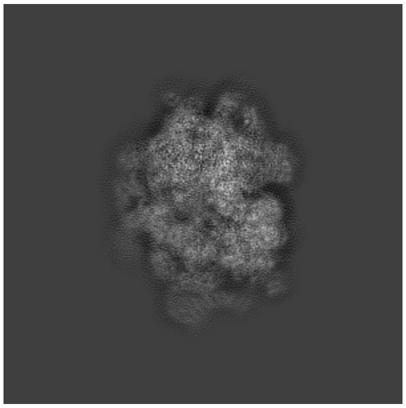
6.1.1 Primary map



X

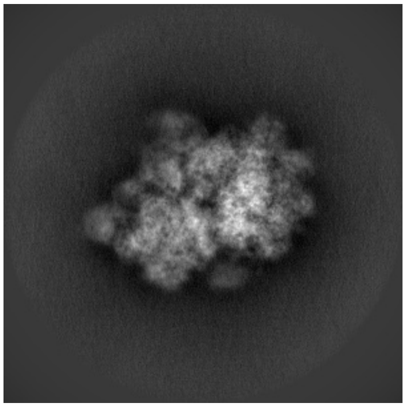


Y

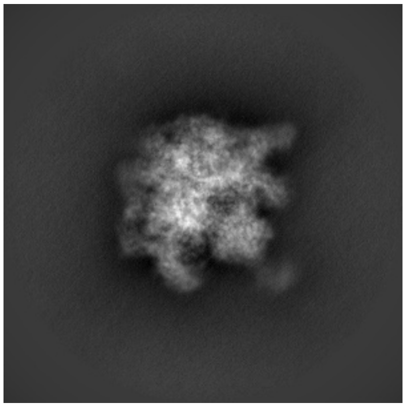


Z

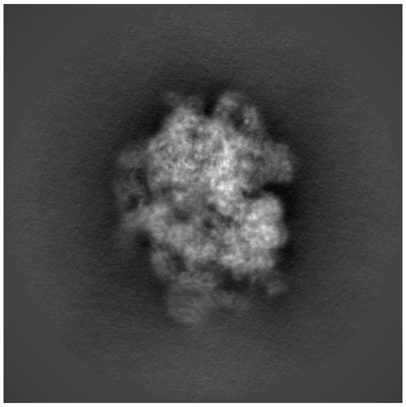
6.1.2 Raw map



X



Y

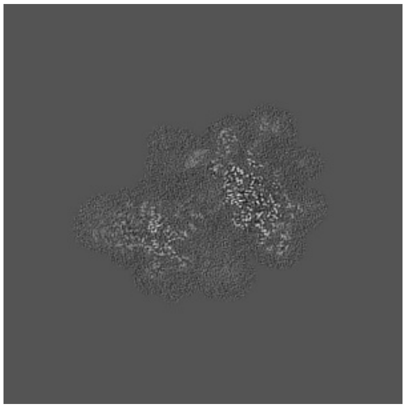


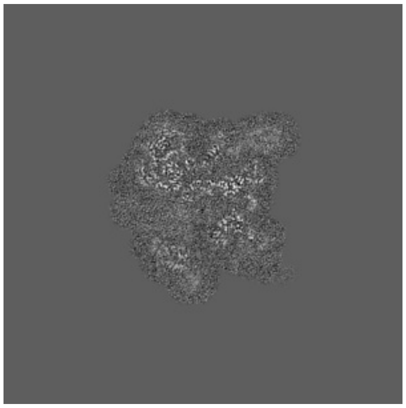
Z

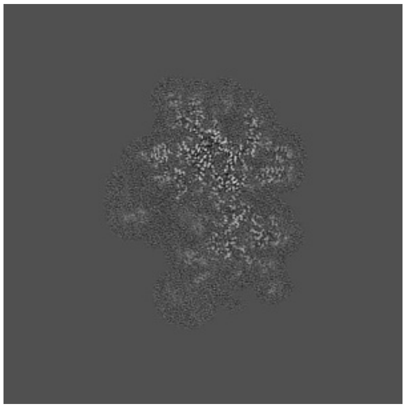
The images above show the map projected in three orthogonal directions.

6.2 Central slices

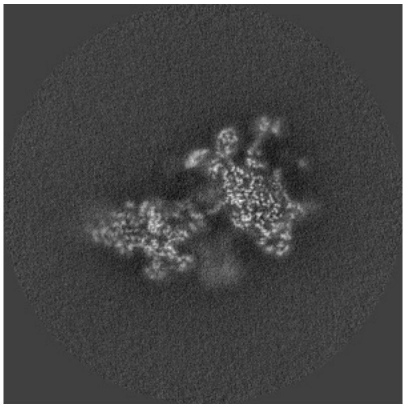
6.2.1 Primary map

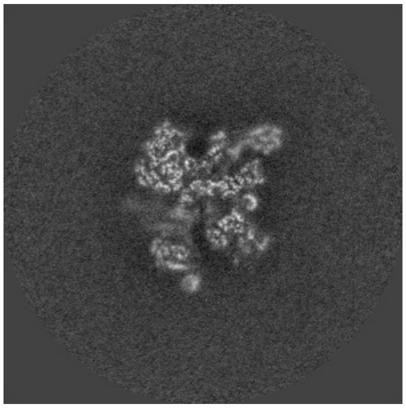

X Index: 256

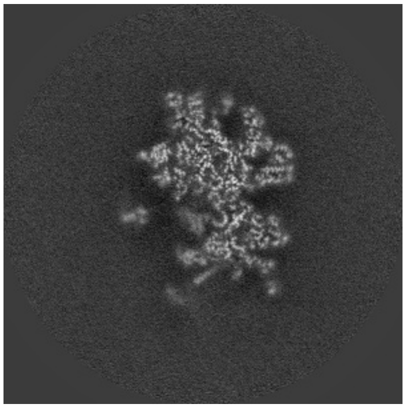

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

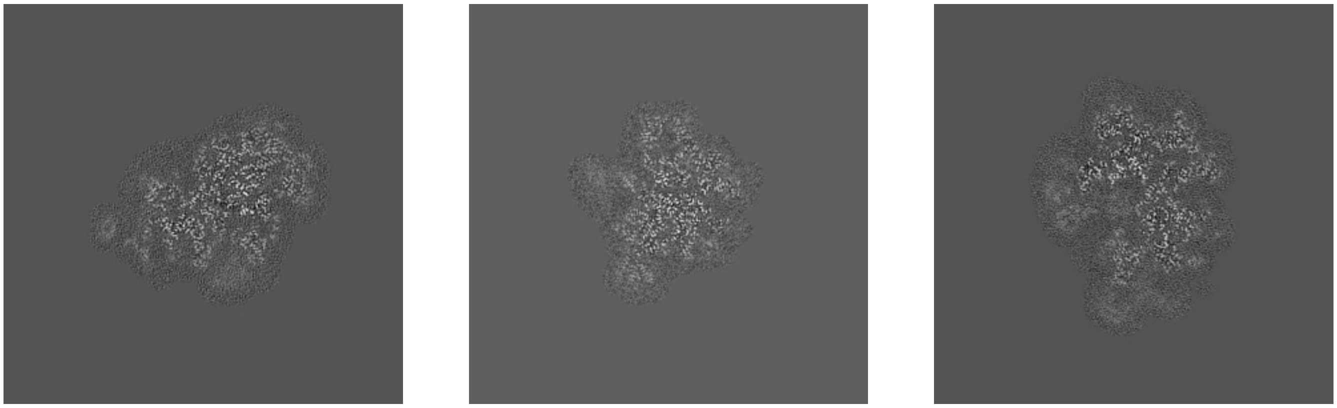

Y Index: 256


Z Index: 256

The images above show central slices of the map in three orthogonal directions.

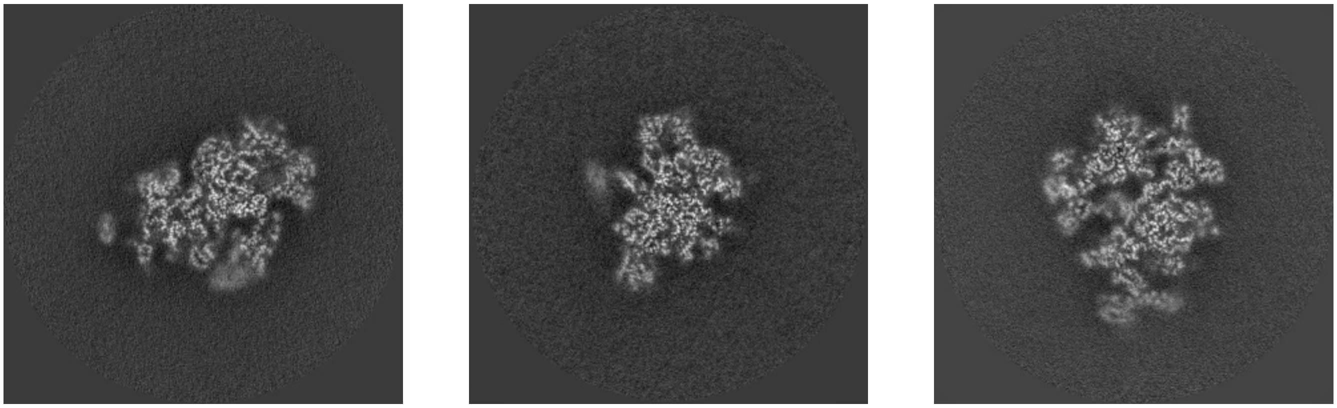
6.3 Largest variance slices ⓘ

6.3.1 Primary map



X Index: 283 Y Index: 305 Z Index: 236

6.3.2 Raw map



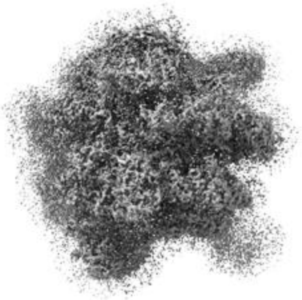
X Index: 287 Y Index: 305 Z Index: 228

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X

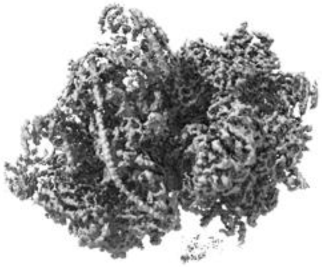


Y

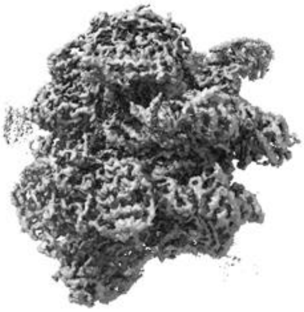
Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

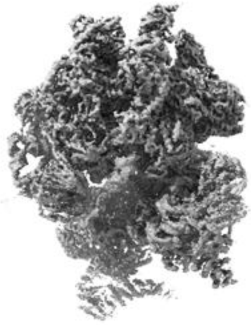
6.4.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

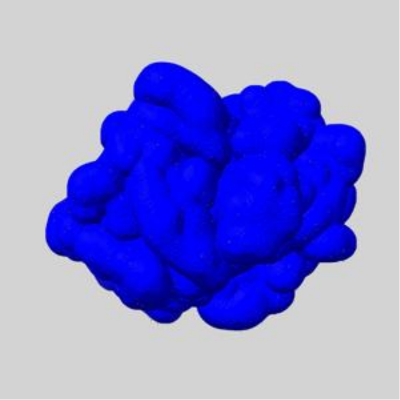
6.5 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

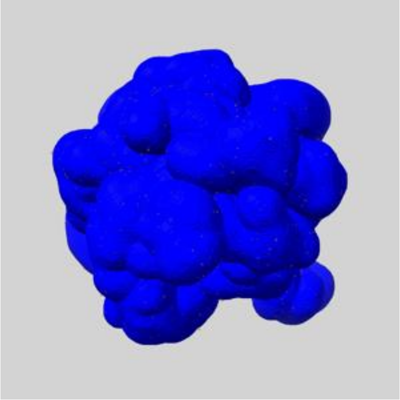
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

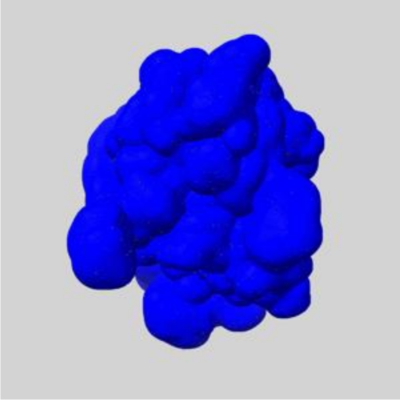
6.5.1 emd_11644_msk_1.map



X



Y

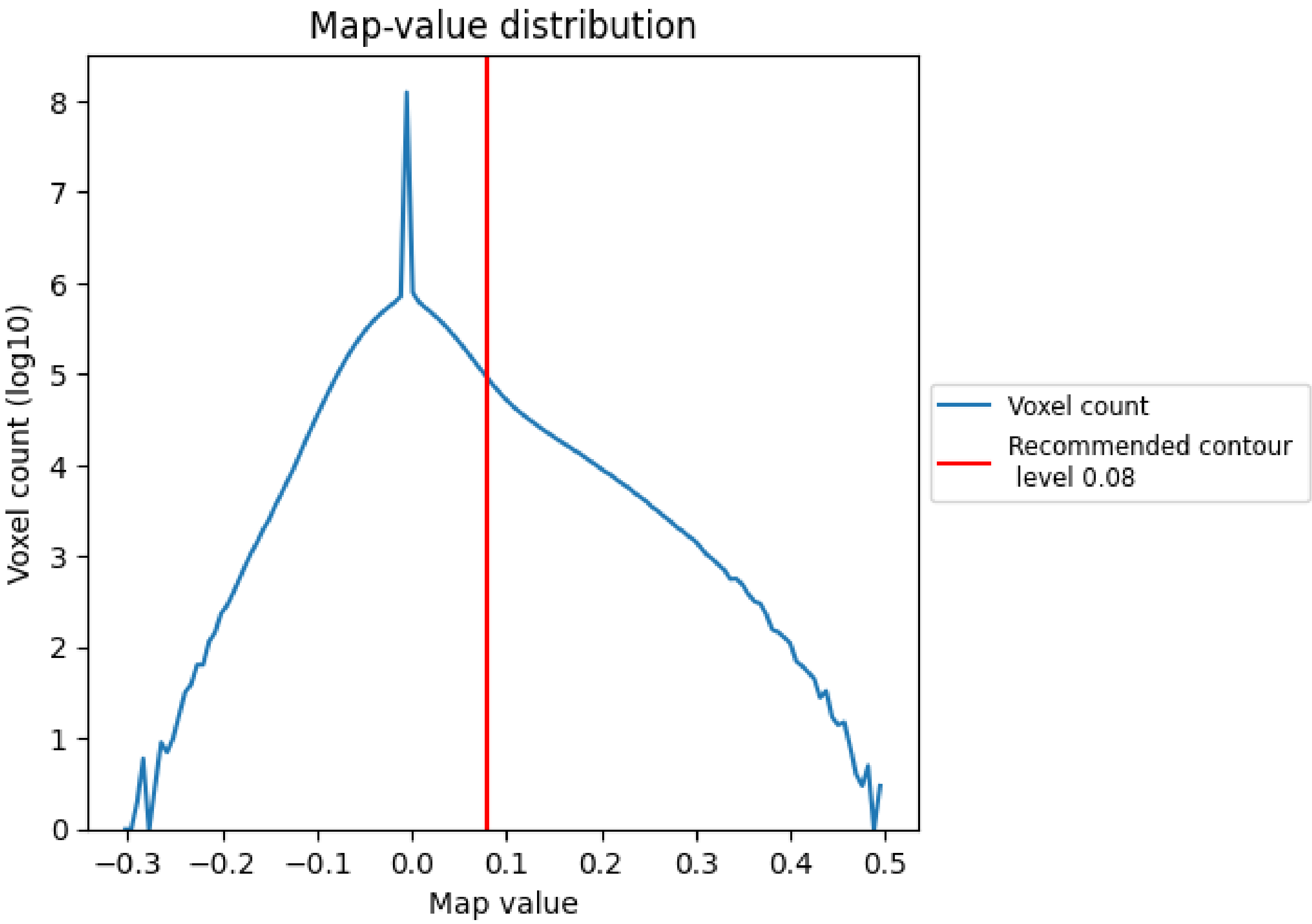


Z

7 Map analysis ⓘ

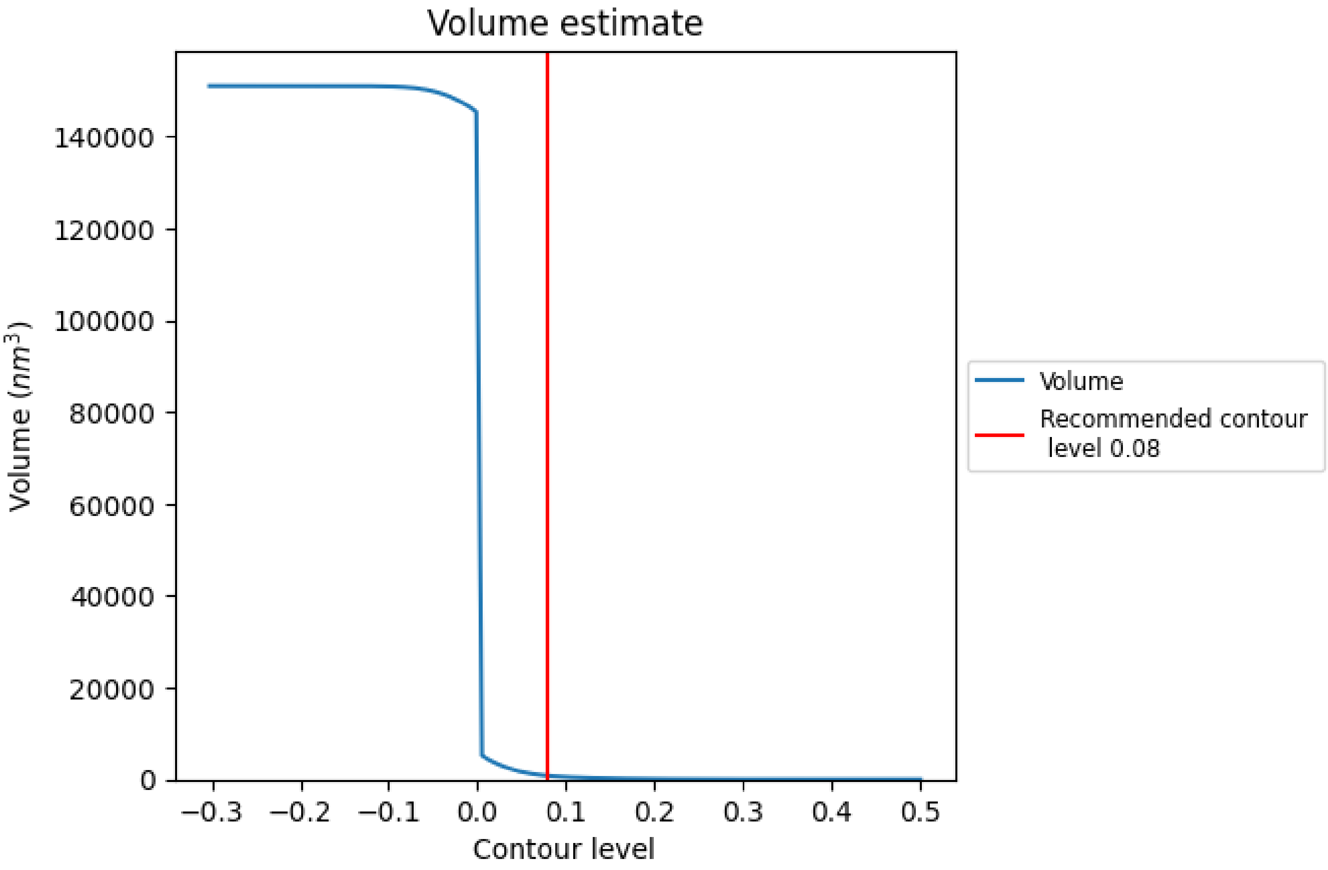
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

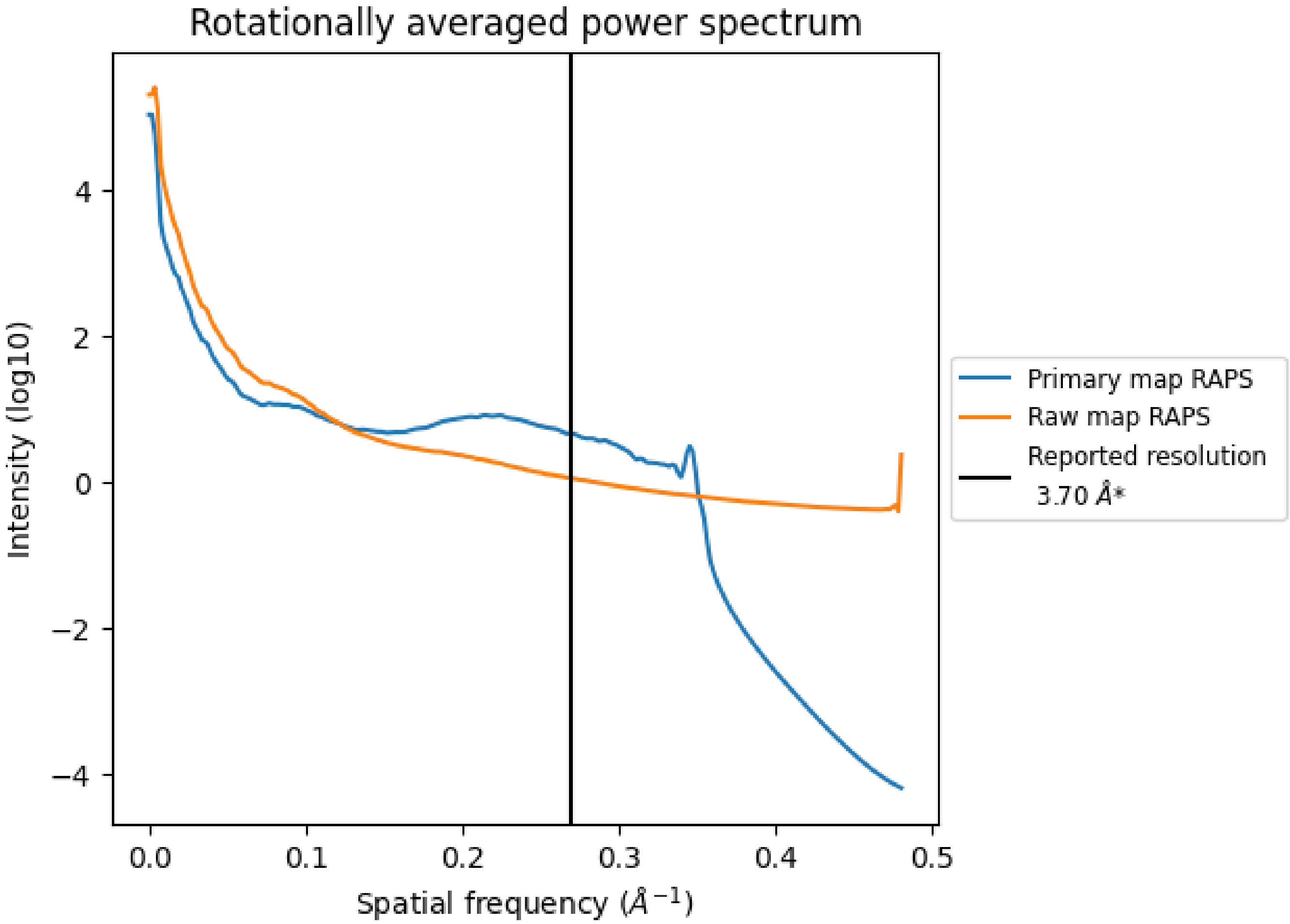
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 802 nm^3; this corresponds to an approximate mass of 725 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

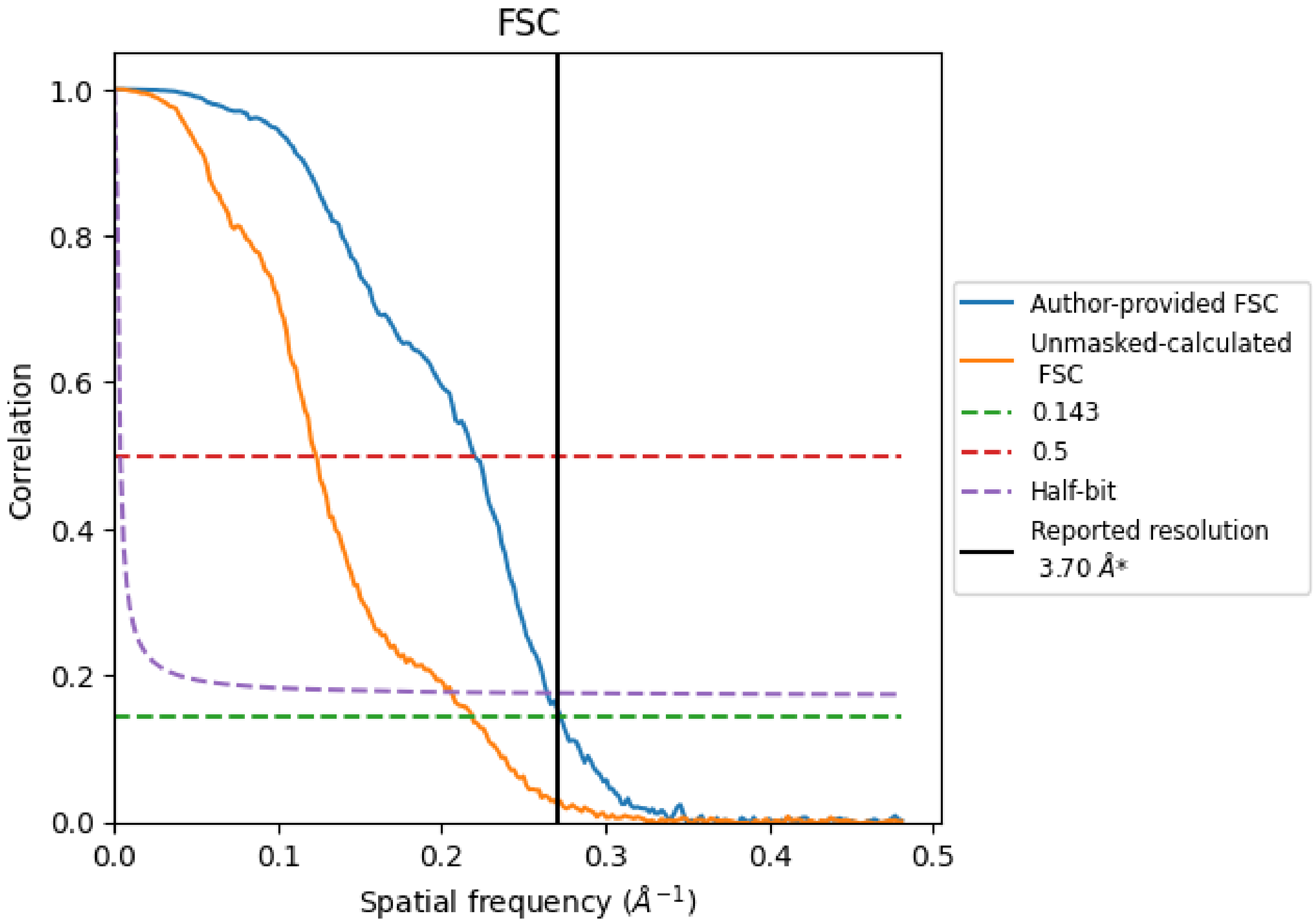


*Reported resolution corresponds to spatial frequency of 0.270 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 $\AA^{-1}$

8.2 Resolution estimates ⓘ

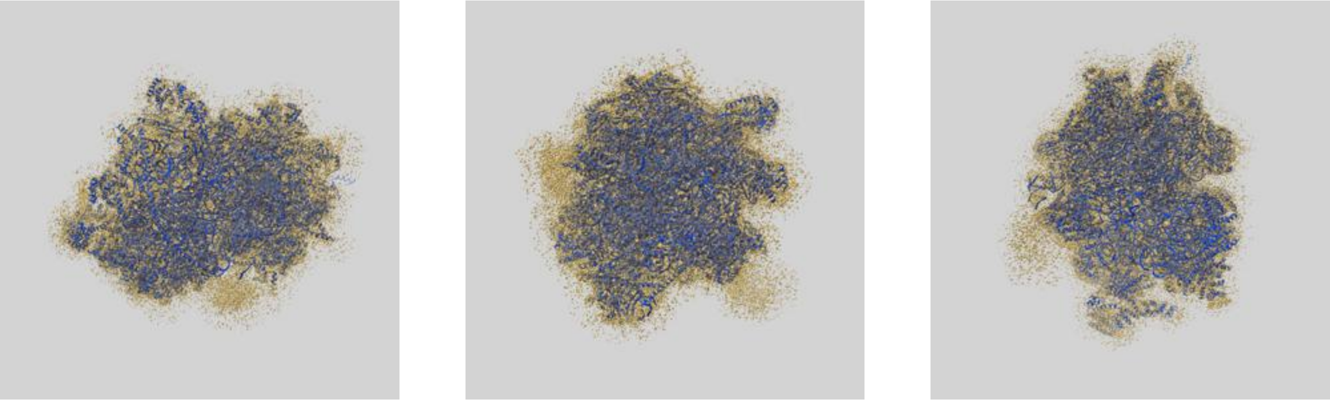
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.67	4.55	3.78
Unmasked-calculated*	4.57	8.12	4.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.57 differs from the reported value 3.7 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-11644 and PDB model 7A5I. Per-residue inclusion information can be found in section 3 on page 22.

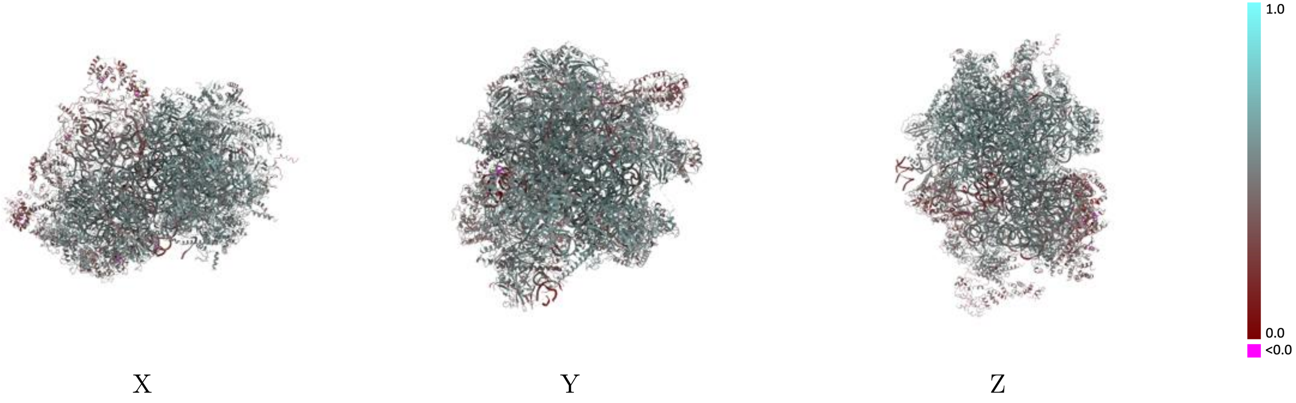
9.1 Map-model overlay ⓘ



X Y Z

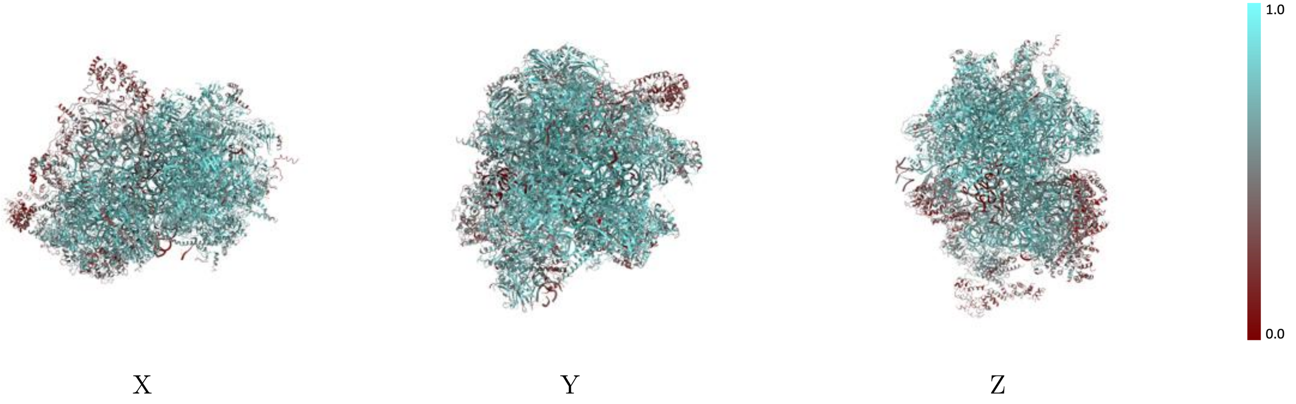
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



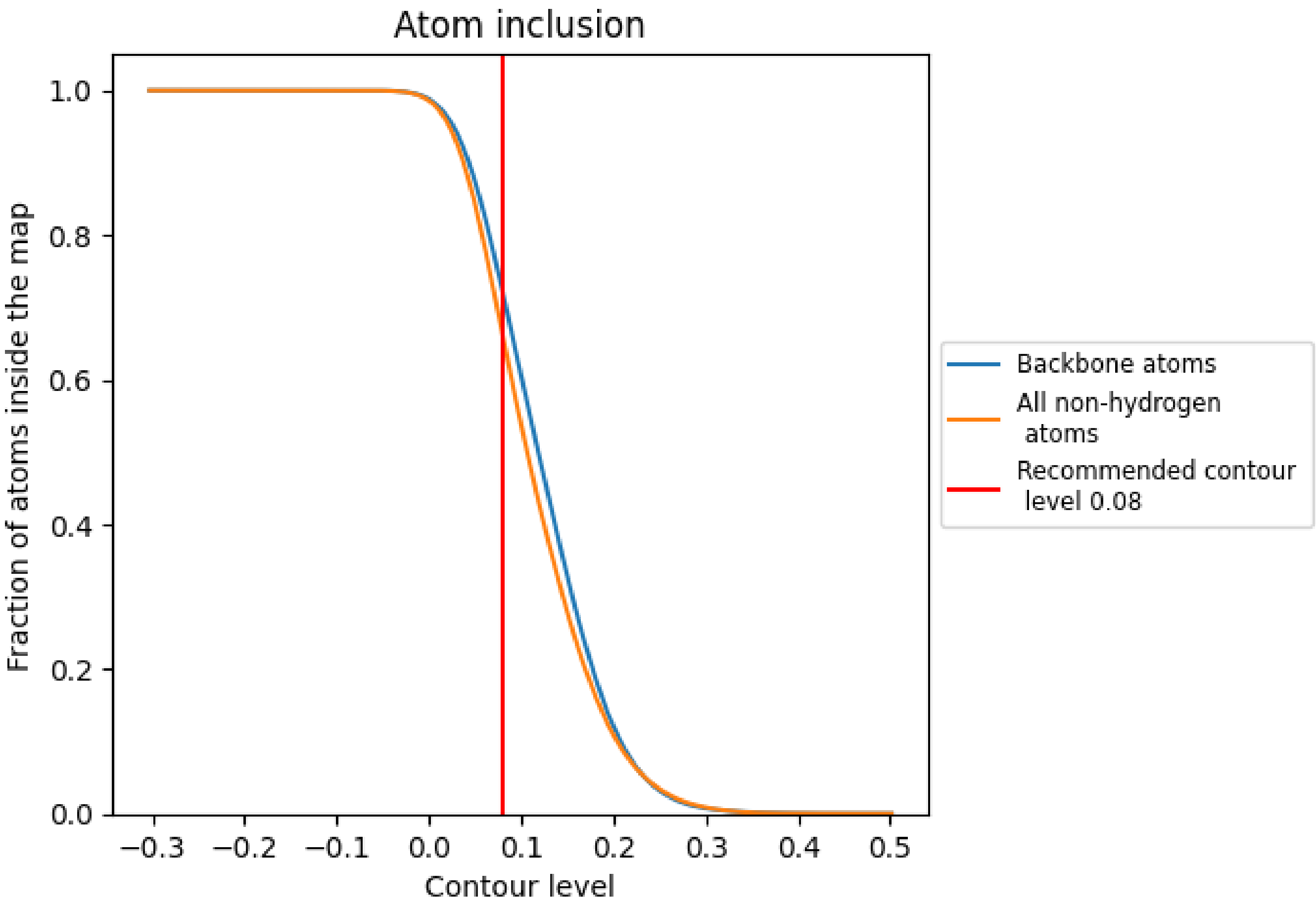
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model ⓘ



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion ⓘ



At the recommended contour level, 72% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6612	0.4940
03	0.6882	0.5250
13	0.7000	0.5190
23	0.8361	0.5970
33	0.8170	0.5820
43	0.8404	0.5810
53	0.7141	0.5220
63	0.6671	0.4880
73	0.6230	0.4920
83	0.4027	0.3890
93	0.7024	0.5200
94	0.3775	0.3530
99	0.0194	0.1600
A3	0.8326	0.5430
A5	0.0142	0.2530
A6	0.7719	0.5010
B3	0.6071	0.3700
B6	0.6875	0.5130
C6	0.6270	0.5160
D3	0.7451	0.5560
D6	0.5819	0.4980
E3	0.7510	0.5480
E6	0.6106	0.5070
F3	0.7669	0.5480
F6	0.5471	0.4640
G6	0.5518	0.4720
H3	0.6016	0.5130
H6	0.5947	0.4820
I3	0.4187	0.4190
I6	0.6516	0.5120
J3	0.2849	0.3340
J6	0.5742	0.5070
K3	0.7785	0.5550
K6	0.6556	0.5010
L3	0.6924	0.5410

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
L6	0.6222	0.4990
M3	0.7445	0.5440
M6	0.4663	0.4300
N3	0.7237	0.5400
N6	0.6566	0.5060
O3	0.7625	0.5470
O6	0.4682	0.4300
P3	0.7146	0.5290
P6	0.6583	0.5130
Q3	0.6802	0.5320
Q6	0.7060	0.5300
R3	0.7726	0.5640
R6	0.4035	0.4110
S3	0.7561	0.5530
S6	0.5416	0.4580
T3	0.7438	0.5520
T6	0.6173	0.5010
U3	0.7714	0.5490
U6	0.4818	0.4330
V3	0.5951	0.4870
V6	0.2469	0.3250
W3	0.7814	0.5700
W6	0.6257	0.4970
X	0.1409	0.2370
X3	0.6849	0.5110
X6	0.4688	0.4200
Y2	0.2276	0.3150
Y3	0.7509	0.5450
Y6	0.4447	0.4310
Z3	0.7729	0.5590
Z6	0.5474	0.4690
a3	0.7308	0.5420
a6	0.3742	0.3940
b3	0.7671	0.5480
b6	0.4686	0.4250
c3	0.6860	0.5180
c6	0.5050	0.4700
d3	0.6132	0.4830
d6	0.6667	0.5380
e3	0.3362	0.3660
e6	0.2902	0.3500
f3	0.5210	0.4630

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g3	0.7313	0.5340
h3	0.5789	0.4620
i3	0.8050	0.5700
i4	0.5510	0.4430
j3	0.6868	0.5330
k3	0.3994	0.3730
l3	0.6311	0.4940
m3	0.5751	0.4800
o3	0.7916	0.5650
p3	0.6096	0.4900
q3	0.5882	0.4970
r3	0.7522	0.5380
s3	0.7259	0.5370
t3	0.2857	0.3230