Full wwPDB EM Validation Report ⓘ

Feb 21, 2023 – 01:22 am GMT

PDB ID	:	7A5H
EMDB ID	:	EMD-11643
Title	:	Structure of the split human mitoribosomal large subunit with rescue factors mtRF-R and MTRES1
Authors	:	Desai, N.; Yang, H.; Chandrasekaran, V.; Kazi, R.; Minczuk, M.; Ramakrishnan, V.
Deposited on	:	2020-08-21
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

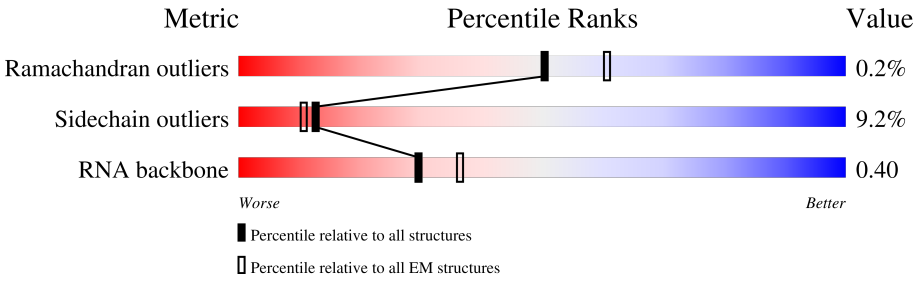
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.30 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	D	305	6% 70% 7% 23%
2	E	348	9% 82% 5% 13%
3	F	311	6% 72% 8% 20%
4	H	267	12% 32% 64%
5	I	261	39% 56% 5% 39%
6	J	192	63% 67% 6% 27%
7	K	178	7% 95%
8	L	145	8% 72% 8% 21%

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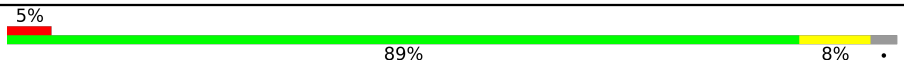
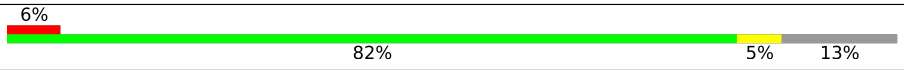
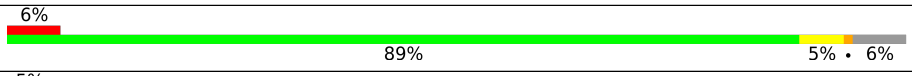
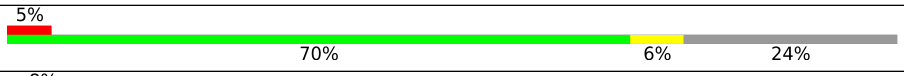
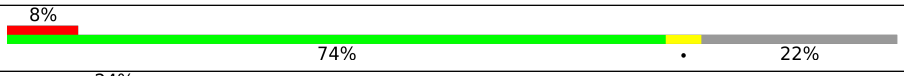
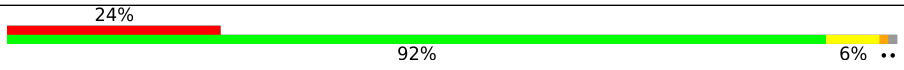
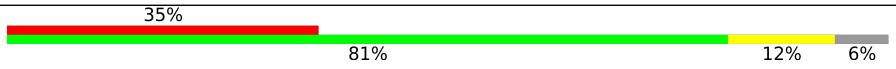
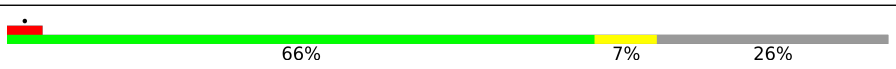
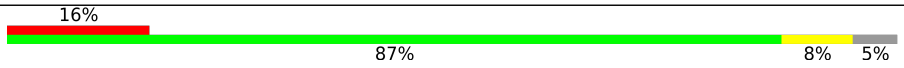
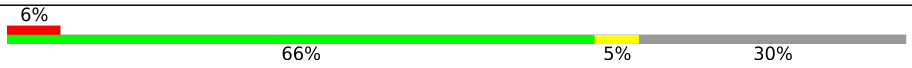
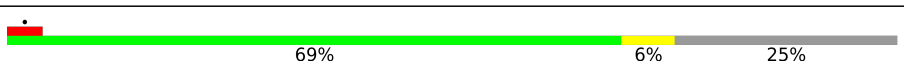
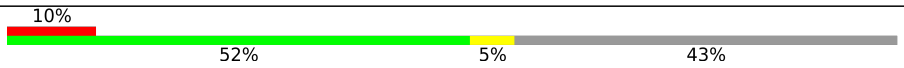
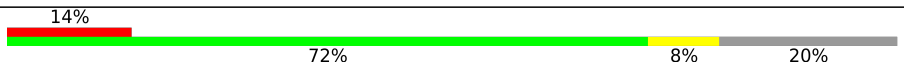
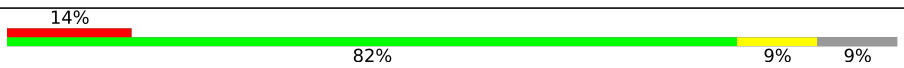
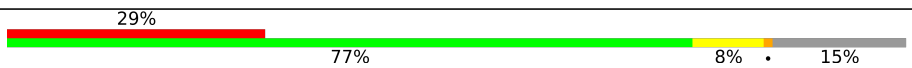
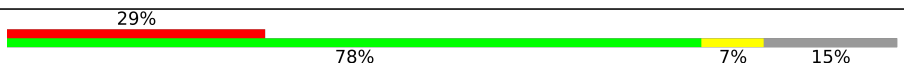
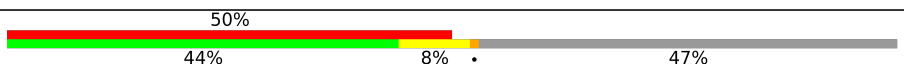
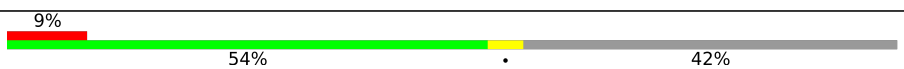
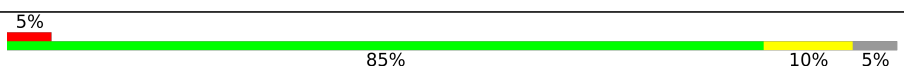
Mol	Chain	Length	Quality of chain
9	M	296	
10	N	251	
11	O	175	
12	P	179	
13	Q	292	
14	R	149	
15	S	205	
16	T	212	
17	U	153	
18	V	216	
19	W	148	
20	X	256	
21	Y	250	
22	Z	161	
23	0	188	
24	1	65	
25	2	92	
26	3	188	
27	5	423	
28	6	380	
29	7	338	
30	8	206	
31	9	137	
32	a	142	
33	b	155	

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Mol	Chain	Length	Quality of chain
34	c	332	13% 78% 5% 17%
35	d	306	30% 65% 31%
36	e	279	77% 71% 6% 22%
37	f	194	48% 53% 7% 40%
38	g	166	9% 73% 22%
39	h	158	24% 56% 7% 37%
40	i	128	70% 5% 24%
41	j	123	12% 68% 31%
42	k	112	42% 66% 5% 29%
43	l	138	16% 83%
44	m	128	33% 34% 65%
45	o	102	80% 9% 11%
46	p	206	18% 57% 38%
47	q	222	20% 52% 5% 42%
48	r	196	8% 68% 6% 26%
49	s	439	10% 76% 8% 16%
50	t	28	100% 100%
51	u	234	24% 44% 53%
52	v	70	83% 87% 11%
53	w	156	49% 42% 8% 49%
54	A	1559	56% 31% 7% 7%
55	B	73	37% 40% 36% 23%
56	24	73	92% 45% 48% 7%
57	Y2	29	97% 97%
58	C	166	46% 60% 8% 31%

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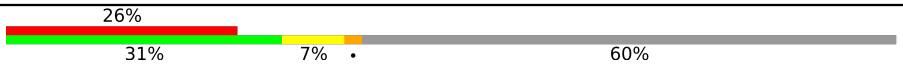
Mol	Chain	Length	Quality of chain
59	G	240	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 102610 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 39S ribosomal protein L2, mitochondrial.

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

- Molecule 2 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	304	2396	1539	416	430	11	0	0

- Molecule 3 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 4 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 5 is a protein called 39S ribosomal protein L10, mitochondrial.

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

- Molecule 6 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 7 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 8 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 9 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 10 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 11 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 12 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	141	Total	C	N	O	S	0	0
			1148	719	221	203	5		

- Molecule 13 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	217	Total	C	N	O	S	0	0
			1805	1159	317	320	9		

- Molecule 14 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 17 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	152	Total	C	N	O	S	0	0
			1218	772	233	210	3		

- Molecule 18 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	202	Total	C	N	O	S	0	0
			1624	1032	291	293	8		

- Molecule 19 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	109	Total	C	N	O	S	0	0
			859	552	162	142	3		

- Molecule 20 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	243	Total	C	N	O	S	0	0
			2035	1317	351	362	5		

- Molecule 21 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 24 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 25 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	45	Total	C	N	O	S	0	0
			367	227	81	58	1		

- Molecule 26 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 27 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	387	Total	C	N	O	S	0	0
			3156	2039	548	558	11		

- Molecule 28 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	324	Total	C	N	O	S	0	0
			2640	1694	470	468	8		

- Molecule 29 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	287	Total	C	N	O	S	0	0
			2334	1495	397	425	17		

- Molecule 30 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	110	Total	C	N	O	S	0	0
			890	567	155	166	2		

- Molecule 31 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	117	Total	C	N	O	S	0	0
			947	614	163	168	2		

- Molecule 32 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 33 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	211	Total	C	N	O	S	0	0
			1741	1123	299	309	10		

- Molecule 36 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	116	Total	C	N	O	S	0	0
			915	585	152	175	3		

- Molecule 38 is a protein called 39S ribosomal protein L49, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 41 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
41	j	85	Total	C	N	O	S	0	0
			684	423	133	126	2		

- Molecule 42 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	80	Total	C	N	O	S	0	0
			627	392	116	114	5		

- Molecule 43 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 45 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	91	Total	C	N	O	S	0	0
			771	487	156	125	3		

- Molecule 46 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 47 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

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

- Molecule 48 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 49 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 50 is a protein called Unknown protein/protein extension.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	t	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 51 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	111	Total	C	N	O	S	0	0
			927	595	155	167	10		

- Molecule 52 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	v	69	Total	C	N	O	0	0
			588	372	116	100		

- Molecule 53 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	79	Total	C	N	O	S	0	0
			638	410	95	128	5		

- Molecule 54 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	A	1457	Total	C	N	O	P	0	0
			30945	13883	5590	10015	1457		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 55 is a RNA chain called mt-tRNAVal.

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

- Molecule 56 is a RNA chain called mt-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	24	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		

- Molecule 57 is a protein called nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	Y2	29	Total	C	N	O	0	0
			157	96	32	29		

- Molecule 58 is a protein called Probable peptide chain release factor C12orf65, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	C	114	Total	C	N	O	S	1	0
			928	578	177	171	2		

- Molecule 59 is a protein called Mitochondrial transcription rescue factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	G	96	Total	C	N	O	S	0	0
			809	523	142	143	1		

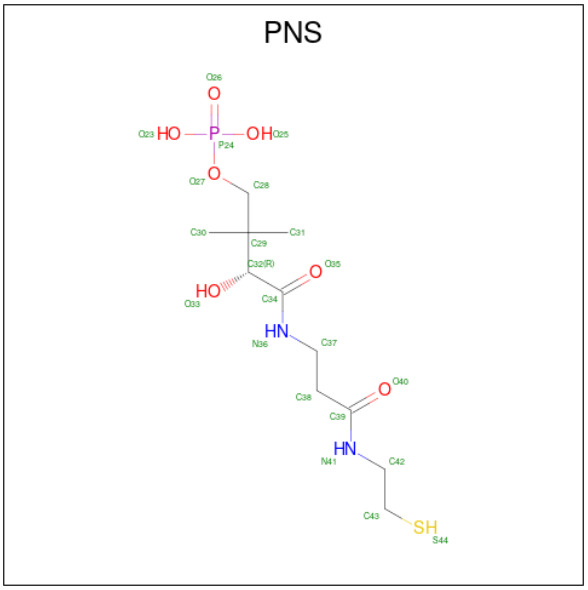
- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	D	1	Total	Mg	0
			1	1	
60	W	1	Total	Mg	0
			1	1	
60	g	1	Total	Mg	0
			1	1	
60	A	89	Total	Mg	0
			89	89	

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
61	0	1	Total Zn 1 1	0
61	r	1	Total Zn 1 1	0

- Molecule 62 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



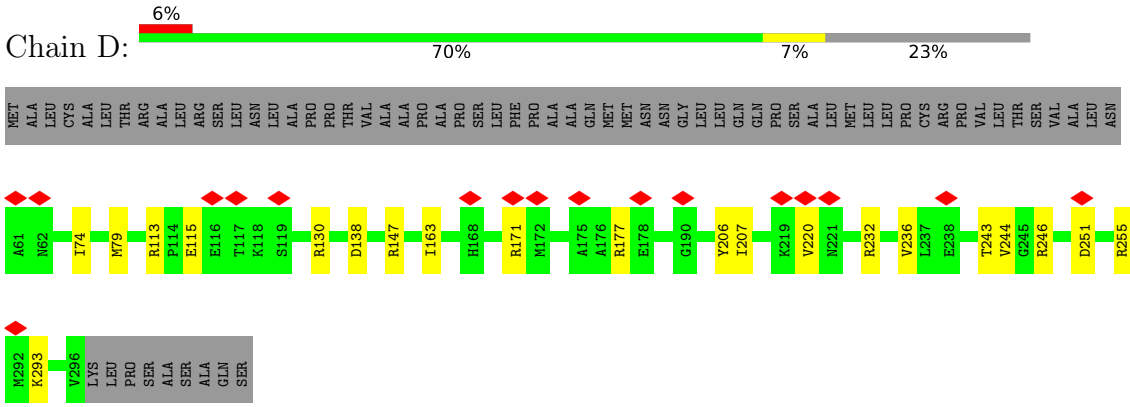
Mol	Chain	Residues	Atoms	AltConf
62	v	1	Total C N O P S 21 11 2 6 1 1	0

3 Residue-property plots (i)

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

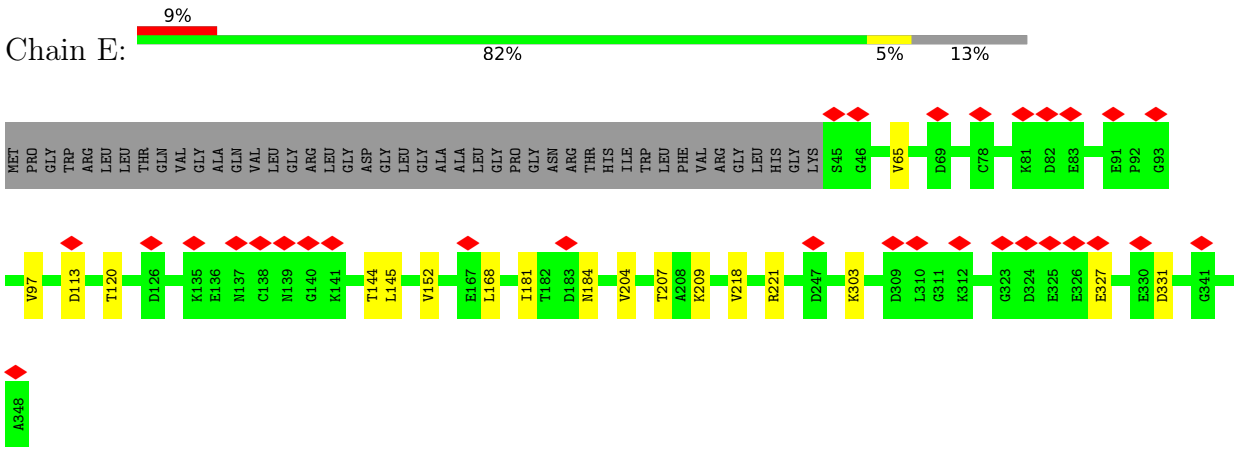
• Molecule 1: 39S ribosomal protein L2, mitochondrial

Chain D:



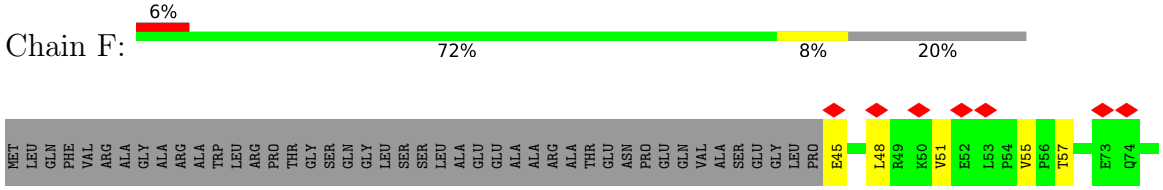
• Molecule 2: 39S ribosomal protein L3, mitochondrial

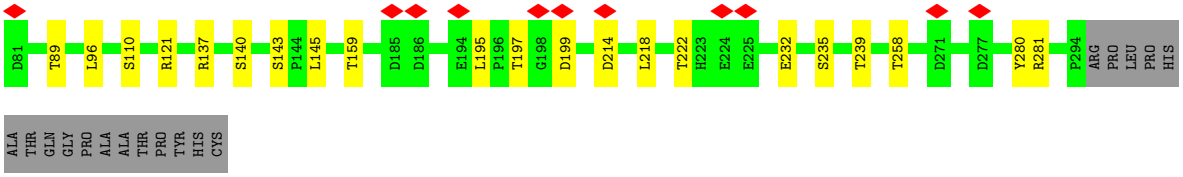
Chain E:



• Molecule 3: 39S ribosomal protein L4, mitochondrial

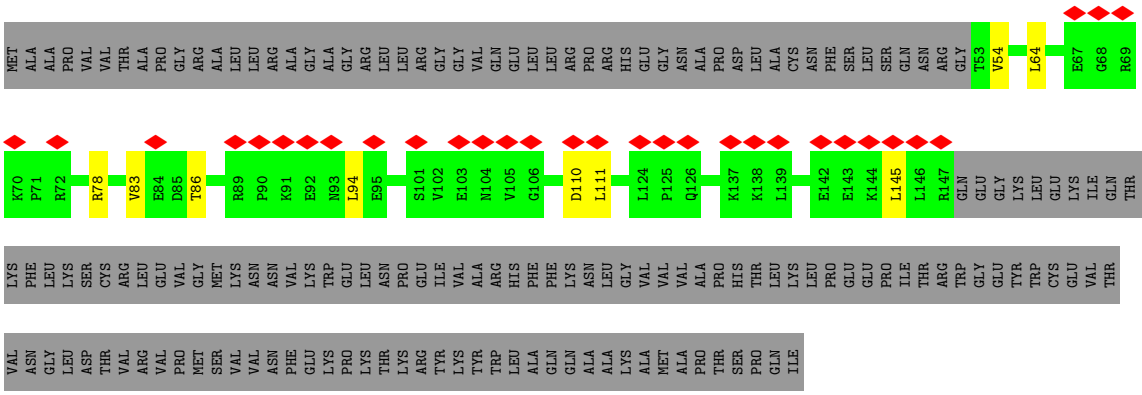
Chain F:





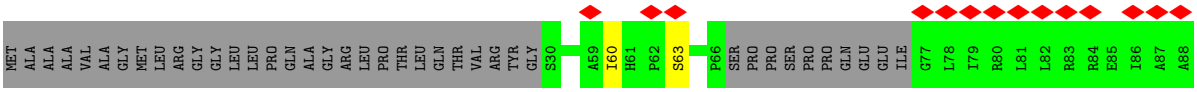
• Molecule 4: 39S ribosomal protein L9, mitochondrial

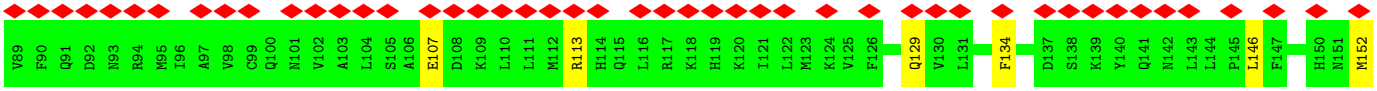
Chain H:

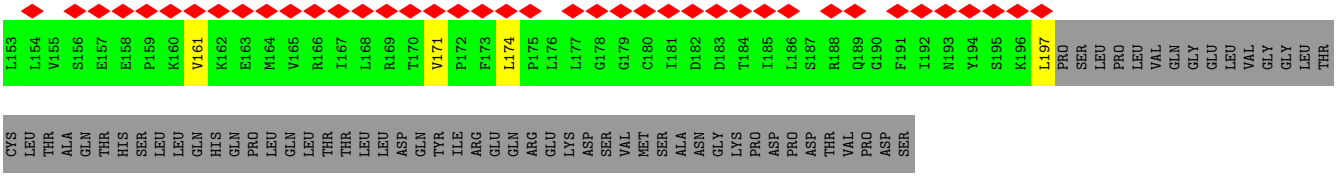


• Molecule 5: 39S ribosomal protein L10, mitochondrial

Chain I:

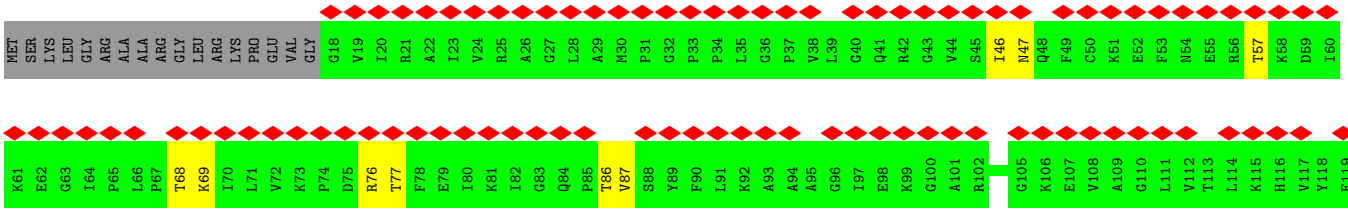


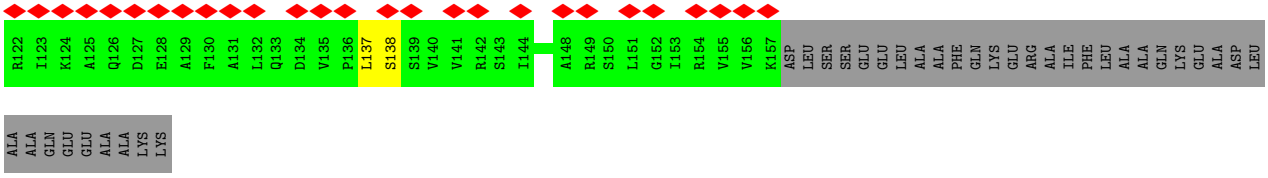




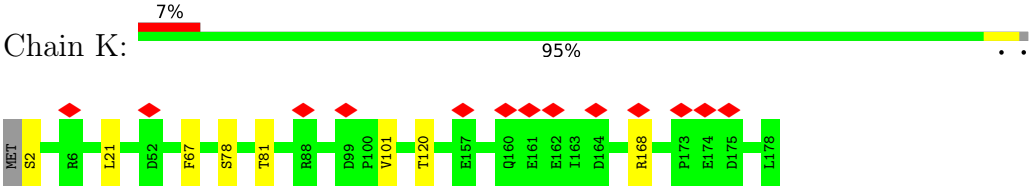
• Molecule 6: 39S ribosomal protein L11, mitochondrial

Chain J:

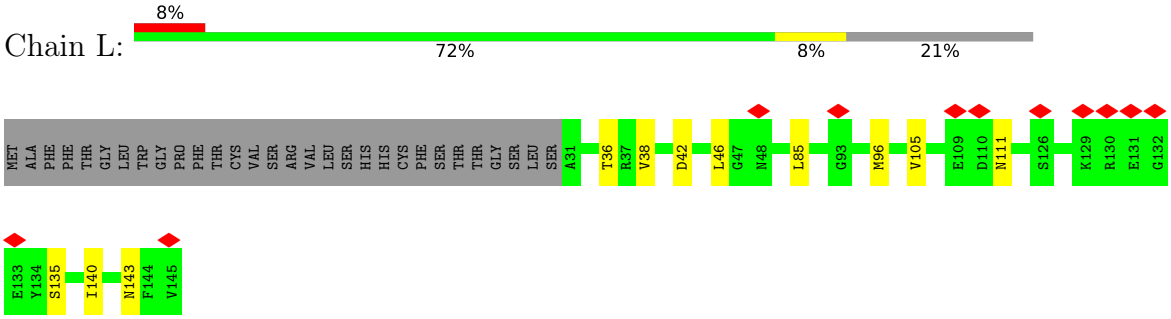




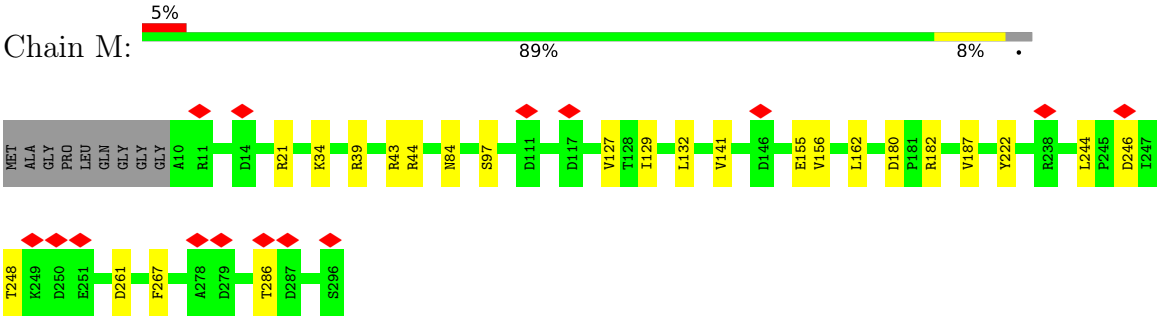
• Molecule 7: 39S ribosomal protein L13, mitochondrial



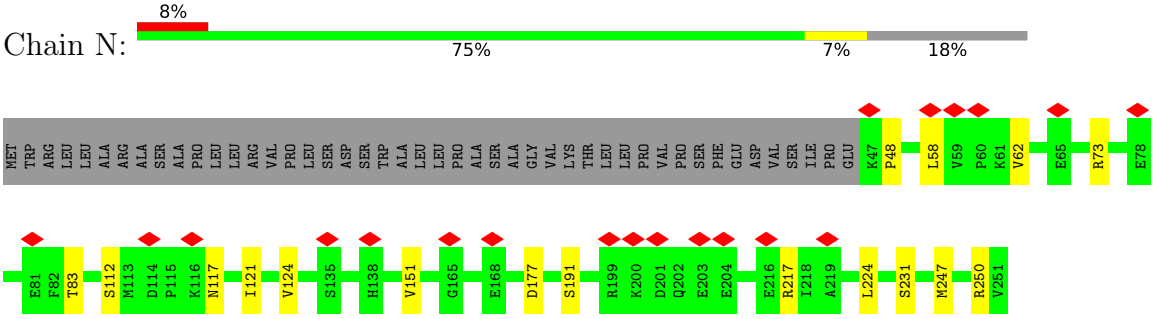
• Molecule 8: 39S ribosomal protein L14, mitochondrial



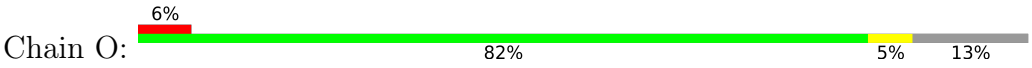
• Molecule 9: 39S ribosomal protein L15, mitochondrial

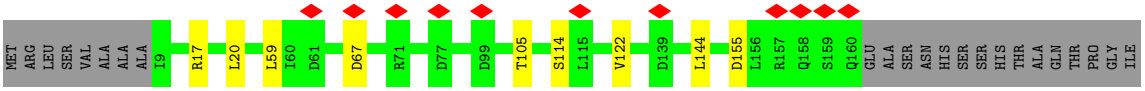


• Molecule 10: 39S ribosomal protein L16, mitochondrial

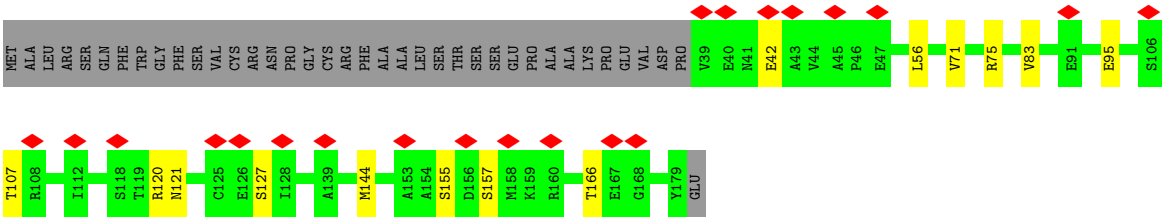


• Molecule 11: 39S ribosomal protein L17, mitochondrial

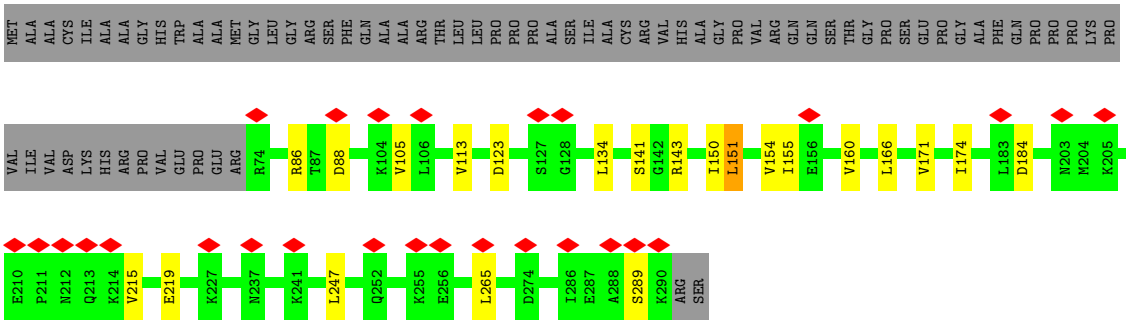




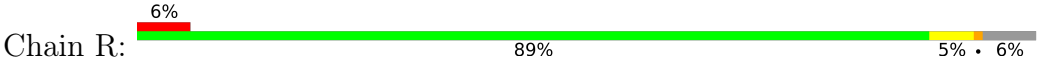
• Molecule 12: Mitochondrial ribosomal protein L18, isoform CRA_b

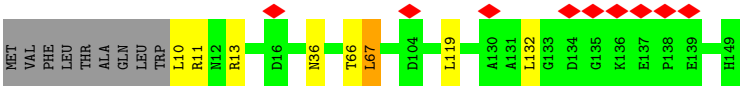


• Molecule 13: 39S ribosomal protein L19, mitochondrial

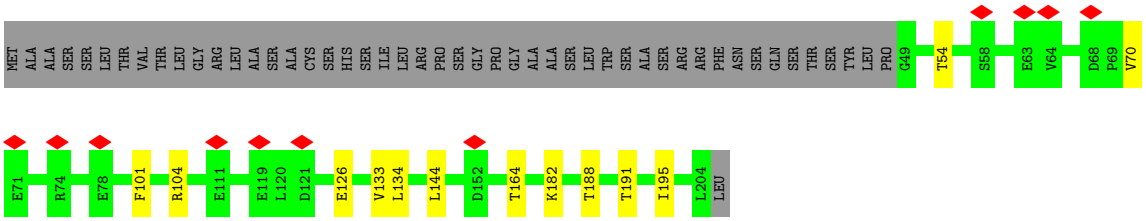


• Molecule 14: 39S ribosomal protein L20, mitochondrial



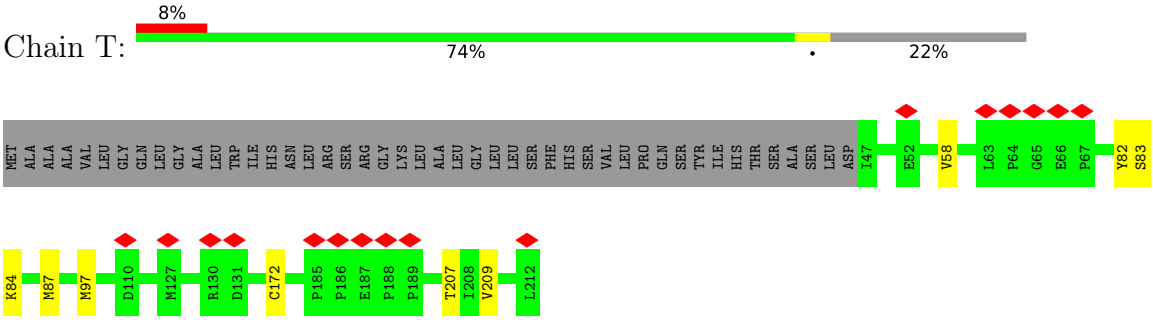


• Molecule 15: 39S ribosomal protein L21, mitochondrial



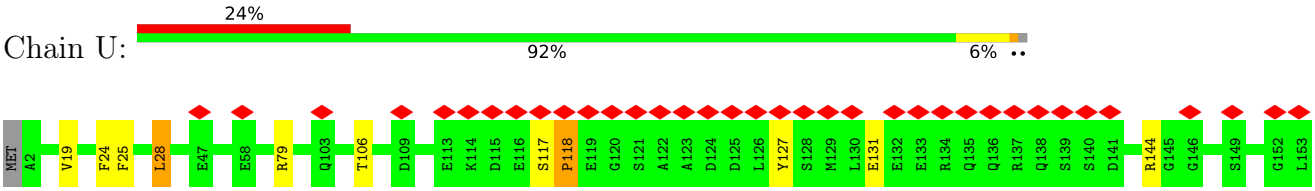
• Molecule 16: 39S ribosomal protein L22, mitochondrial

Chain T:



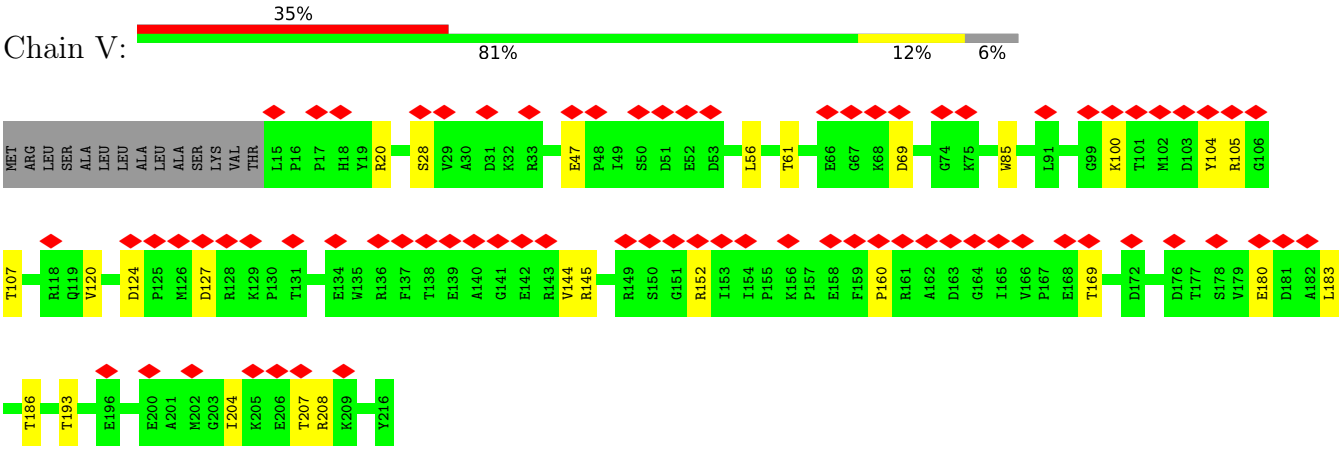
• Molecule 17: 39S ribosomal protein L23, mitochondrial

Chain U:



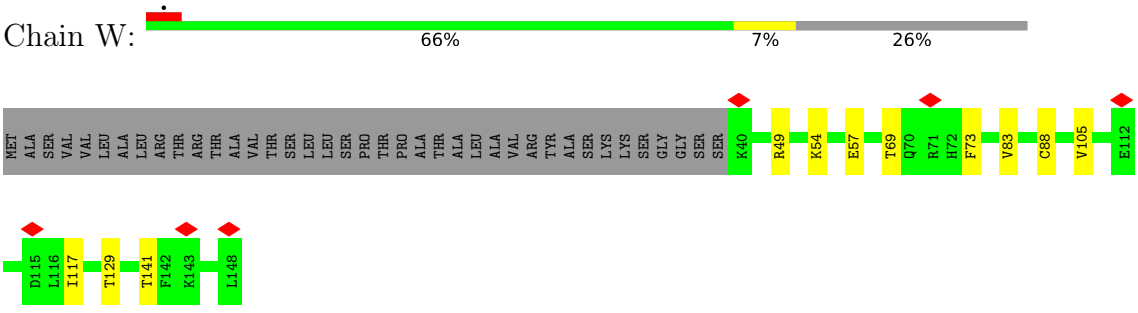
• Molecule 18: 39S ribosomal protein L24, mitochondrial

Chain V:



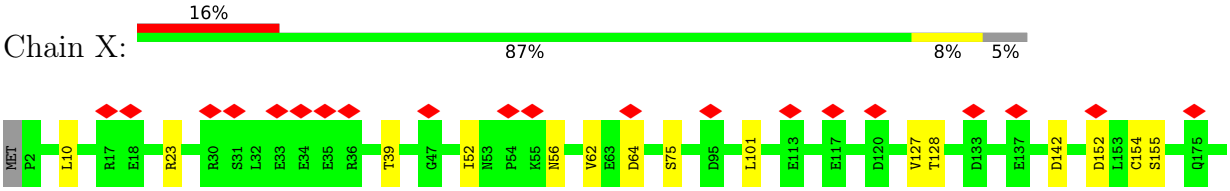
• Molecule 19: 39S ribosomal protein L27, mitochondrial

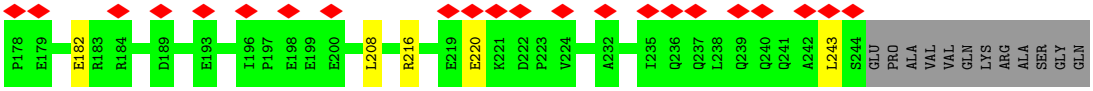
Chain W:



• Molecule 20: 39S ribosomal protein L28, mitochondrial

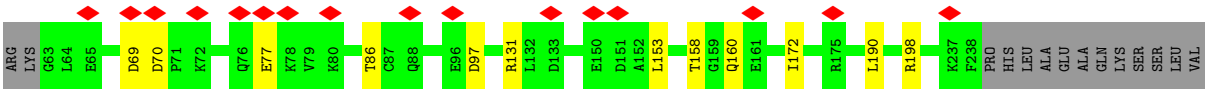
Chain X:





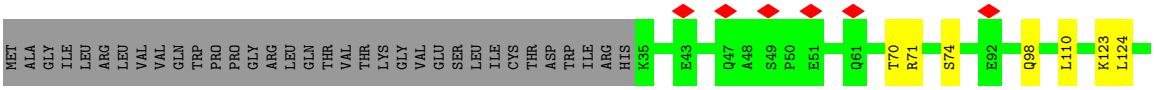
• Molecule 21: 39S ribosomal protein L47, mitochondrial

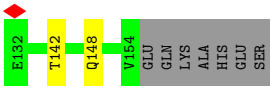
Chain Y:



• Molecule 22: 39S ribosomal protein L30, mitochondrial

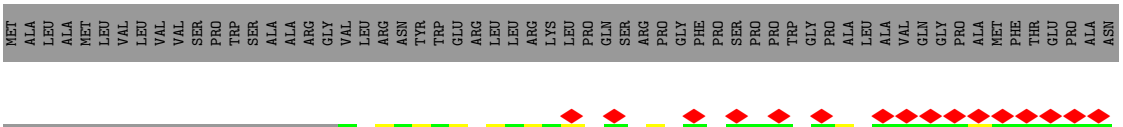
Chain Z:

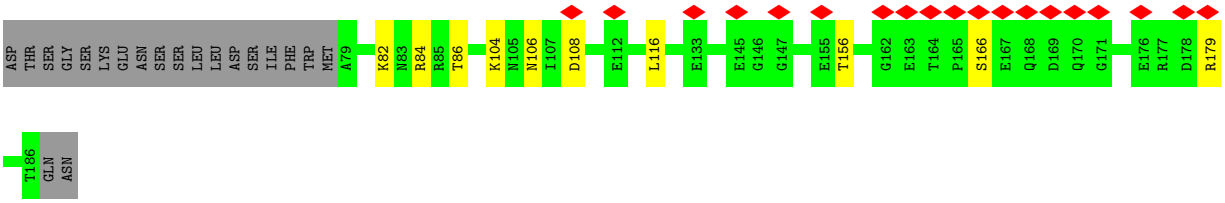




• Molecule 23: 39S ribosomal protein L32, mitochondrial

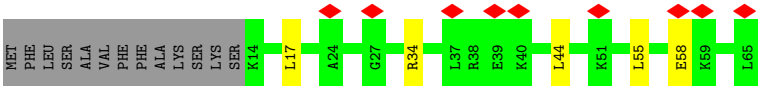
Chain 0:





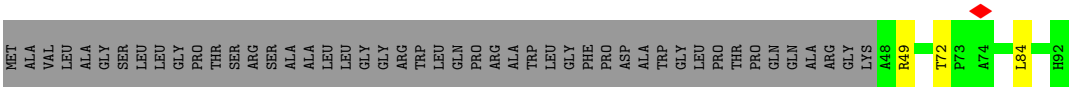
• Molecule 24: 39S ribosomal protein L33, mitochondrial

Chain 1:



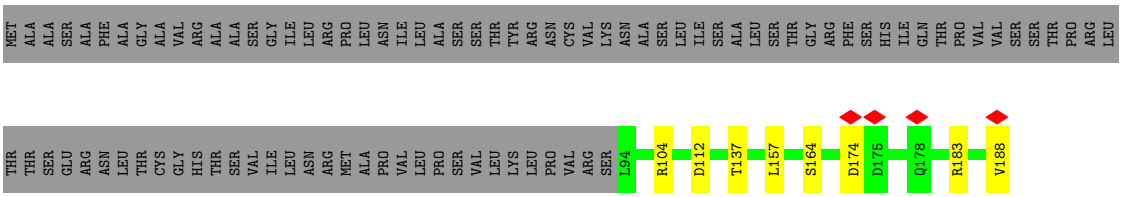
• Molecule 25: 39S ribosomal protein L34, mitochondrial

Chain 2:



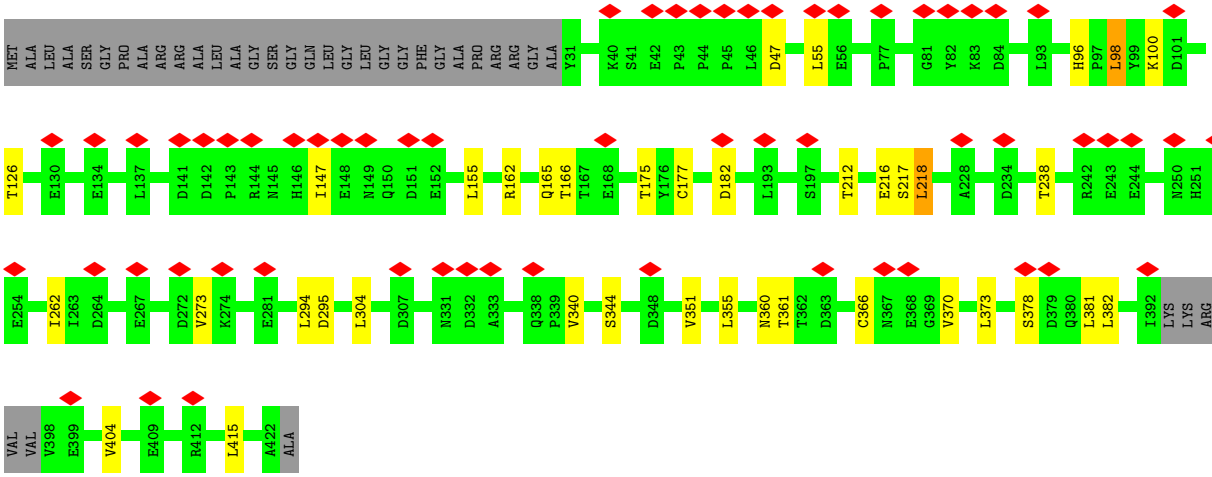
• Molecule 26: 39S ribosomal protein L35, mitochondrial

Chain 3:



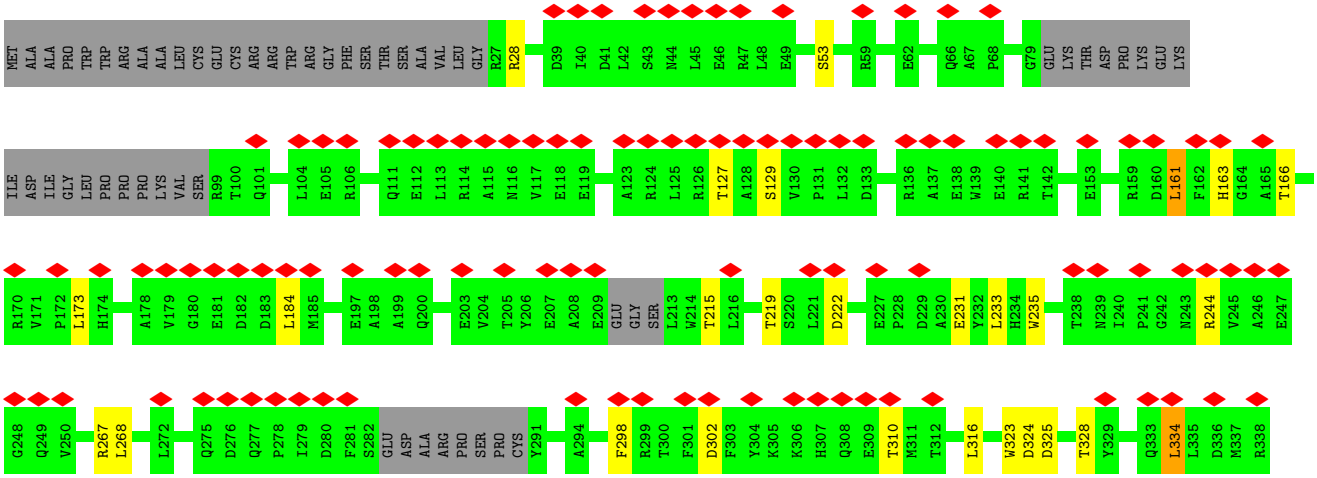
• Molecule 27: 39S ribosomal protein L37, mitochondrial

Chain 5:



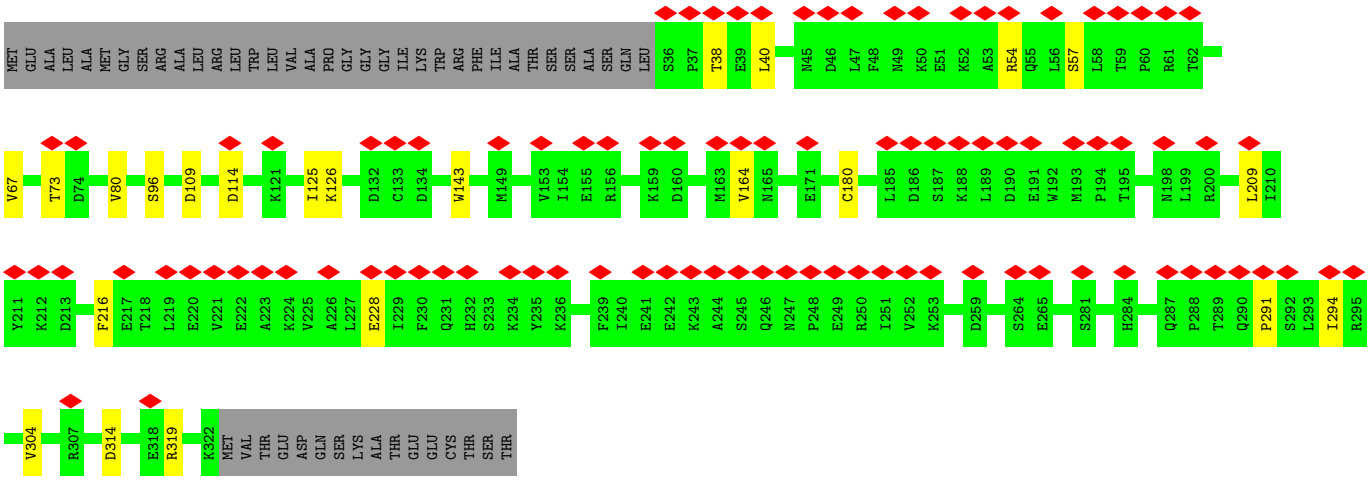
• Molecule 28: 39S ribosomal protein L38, mitochondrial

Chain 6:



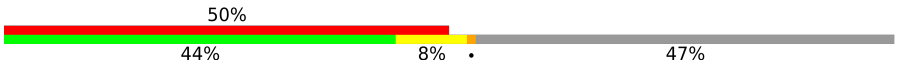
• Molecule 29: 39S ribosomal protein L39, mitochondrial

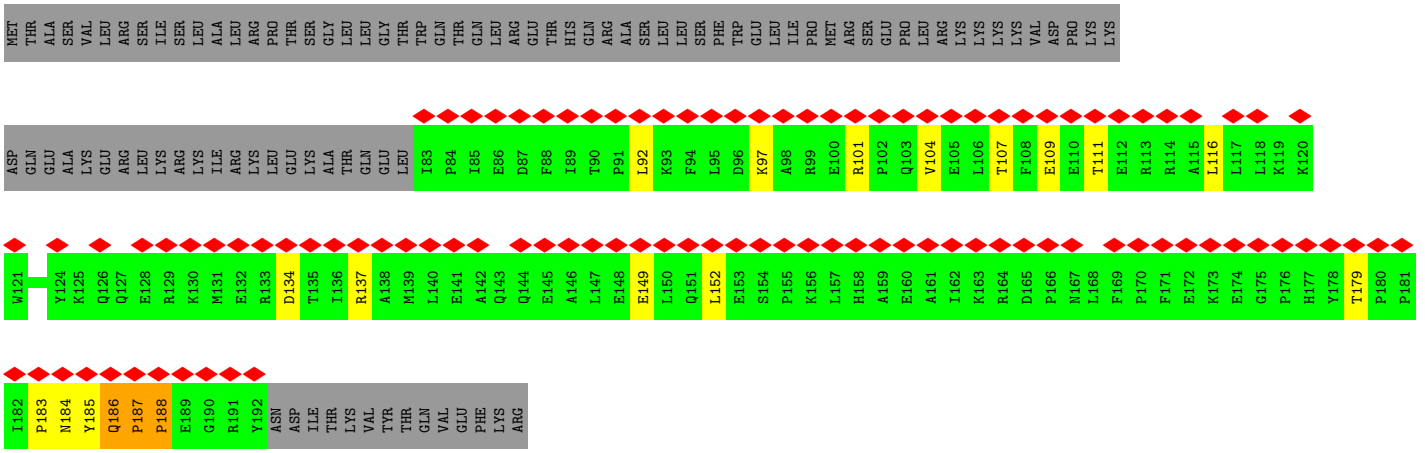
Chain 7:



• Molecule 30: 39S ribosomal protein L40, mitochondrial

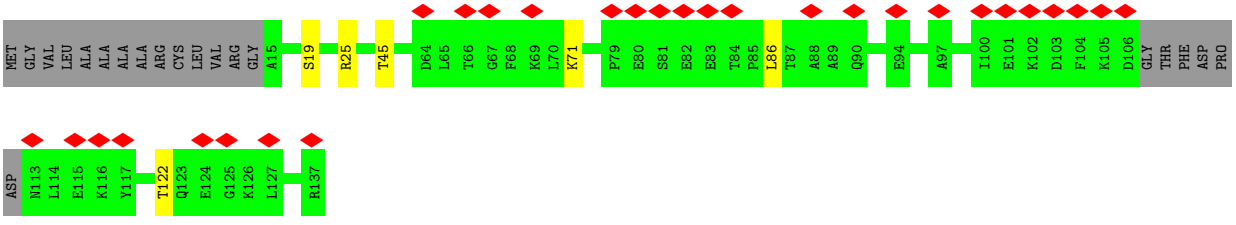
Chain 8:





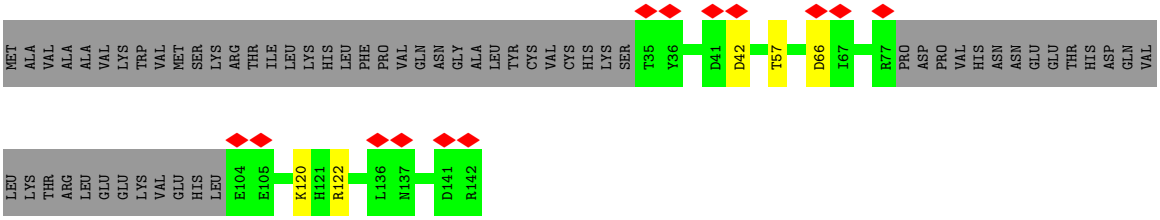
• Molecule 31: 39S ribosomal protein L41, mitochondrial

Chain 9:



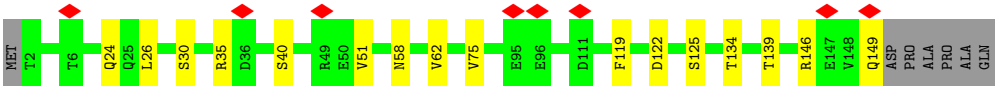
• Molecule 32: 39S ribosomal protein L42, mitochondrial

Chain a:



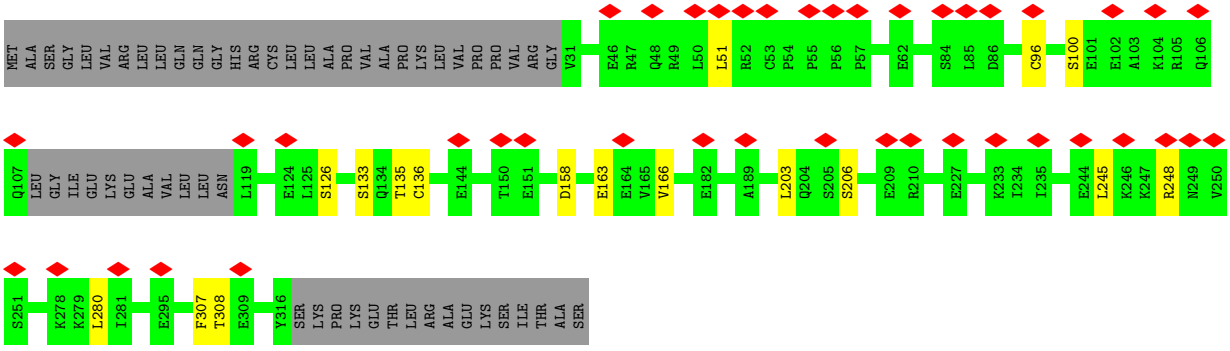
• Molecule 33: 39S ribosomal protein L43, mitochondrial

Chain b:



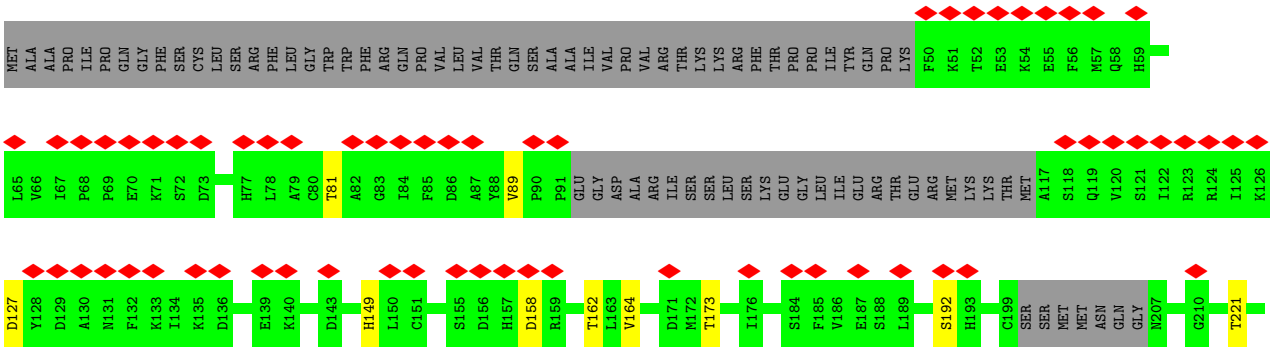
• Molecule 34: 39S ribosomal protein L44, mitochondrial

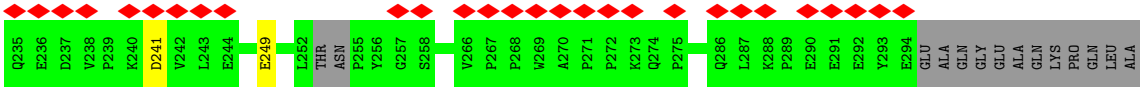
Chain c:



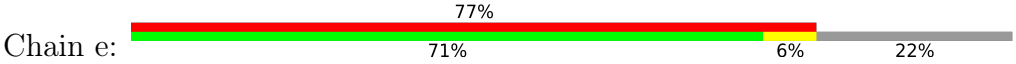
• Molecule 35: 39S ribosomal protein L45, mitochondrial

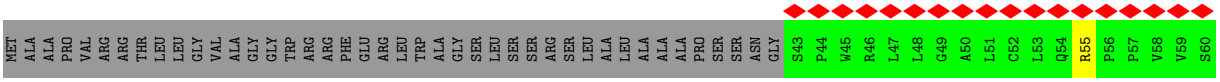
Chain d:

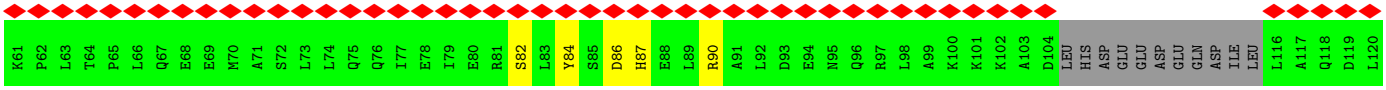


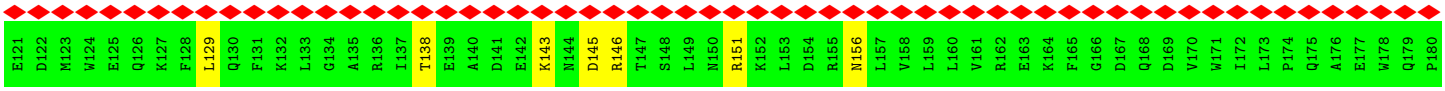


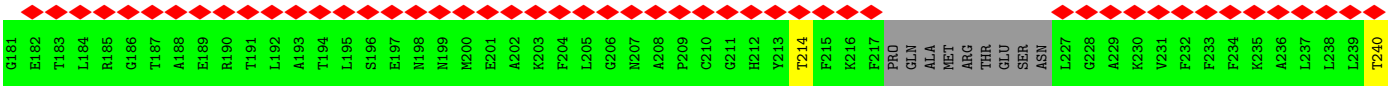
• Molecule 36: 39S ribosomal protein L46, mitochondrial

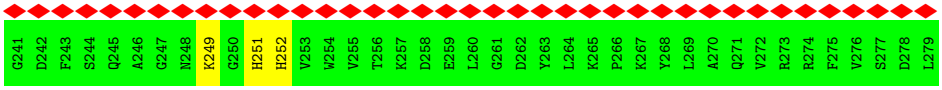




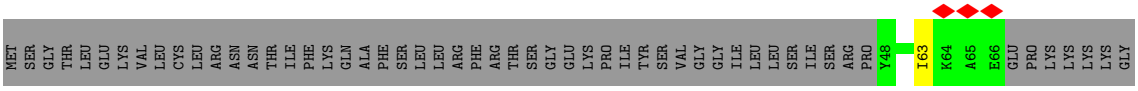


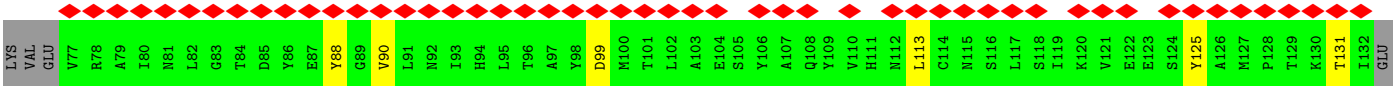


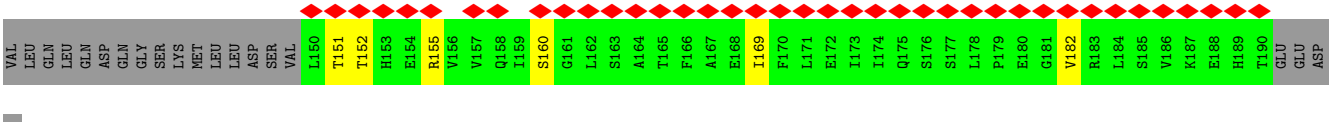




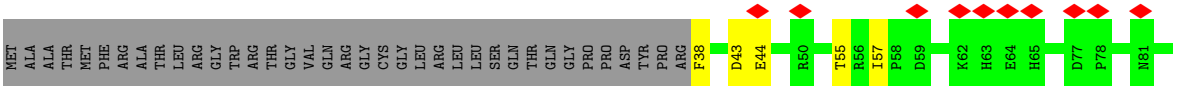
• Molecule 37: 39S ribosomal protein L48, mitochondrial

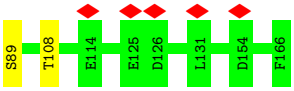






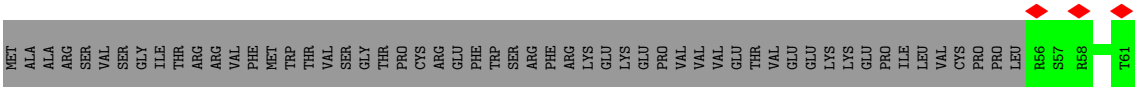
• Molecule 38: 39S ribosomal protein L49, mitochondrial

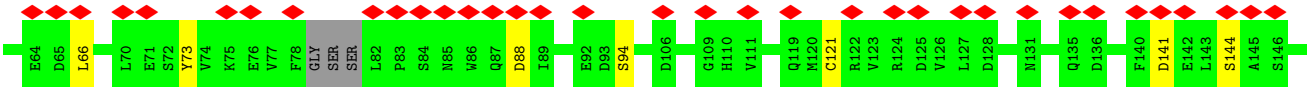


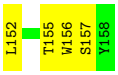


• Molecule 39: 39S ribosomal protein L50, mitochondrial

Chain h:

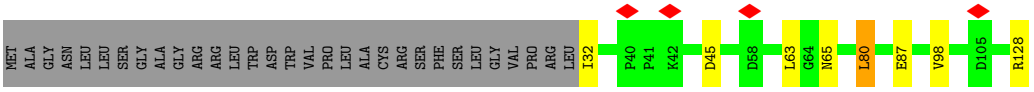






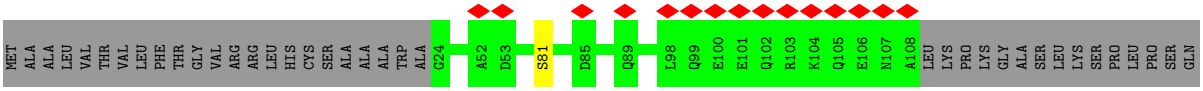
• Molecule 40: 39S ribosomal protein L51, mitochondrial

Chain i:



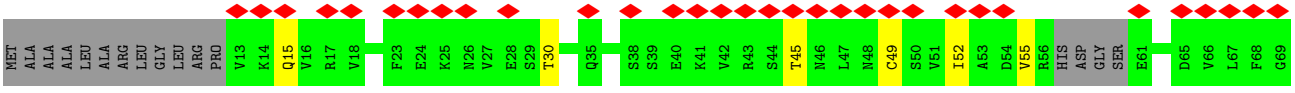
• Molecule 41: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA

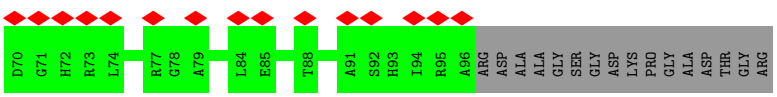
Chain j:



• Molecule 42: 39S ribosomal protein L53, mitochondrial

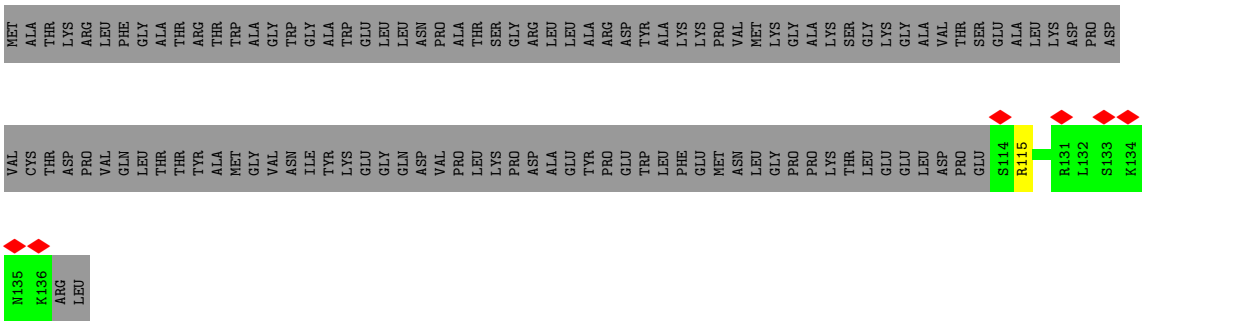
Chain k:





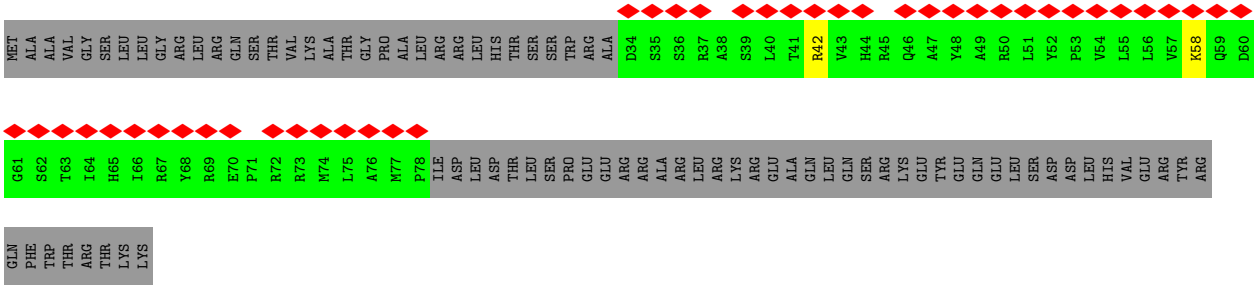
• Molecule 43: 39S ribosomal protein L54, mitochondrial

Chain l:



• Molecule 44: 39S ribosomal protein L55, mitochondrial

Chain m:

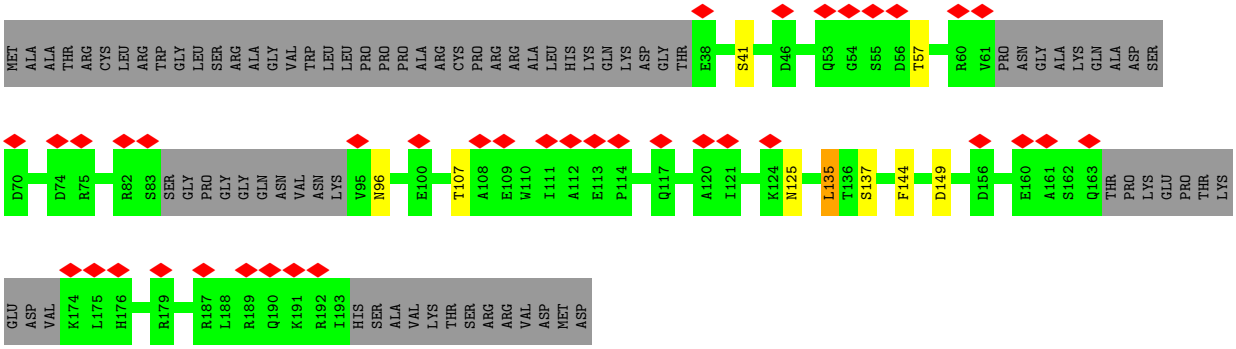


• Molecule 45: Ribosomal protein 63, mitochondrial

Chain o:

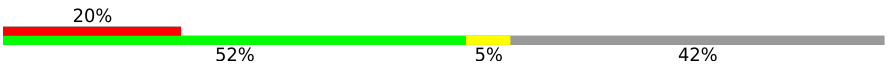
• Molecule 46: Peptidyl-tRNA hydrolase ICT1, mitochondrial

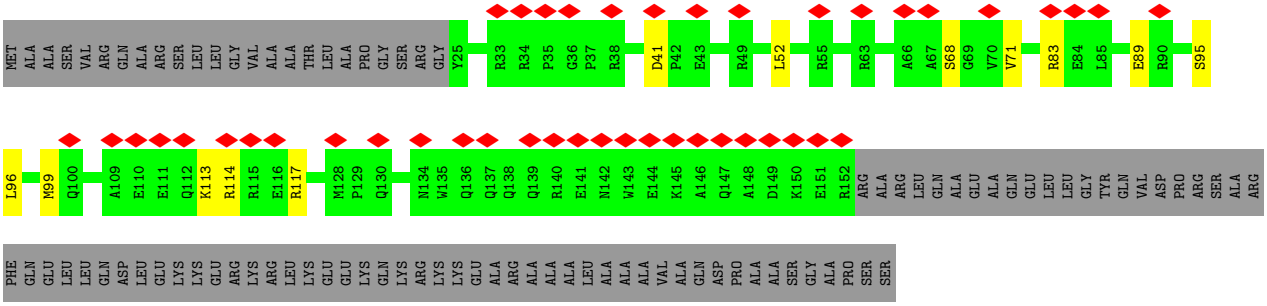
Chain p:



• Molecule 47: Growth arrest and DNA damage-inducible proteins-interacting protein 1

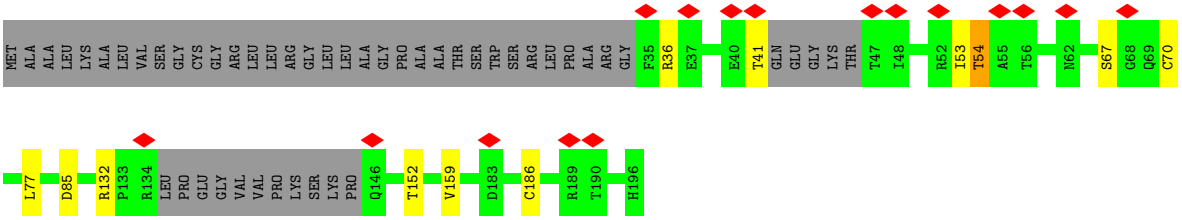
Chain q:





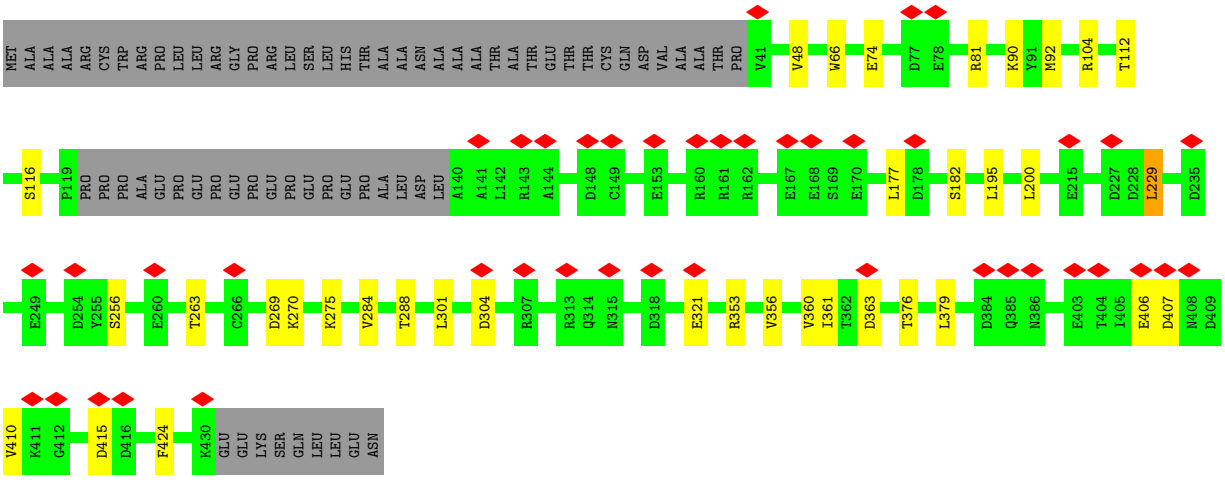
• Molecule 48: 39S ribosomal protein S18a, mitochondrial

Chain r:



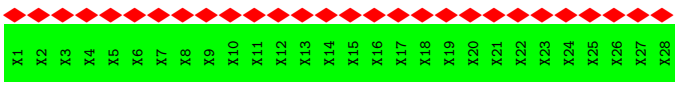
• Molecule 49: 39S ribosomal protein S30, mitochondrial

Chain s:



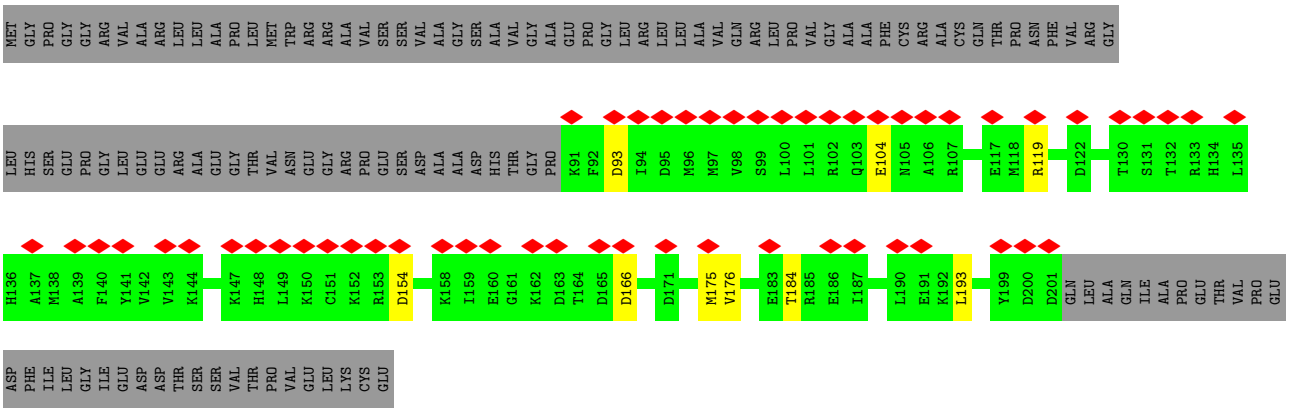
• Molecule 50: Unknown protein/protein extension

Chain t:



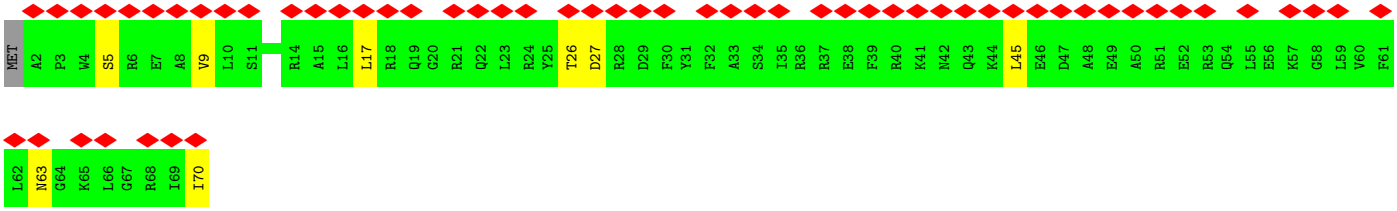
• Molecule 51: Mitochondrial assembly of ribosomal large subunit protein 1

Chain u:



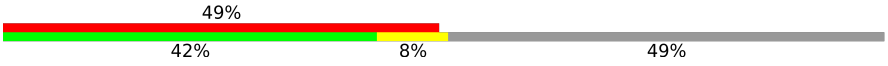
• Molecule 52: MIEF1 upstream open reading frame protein

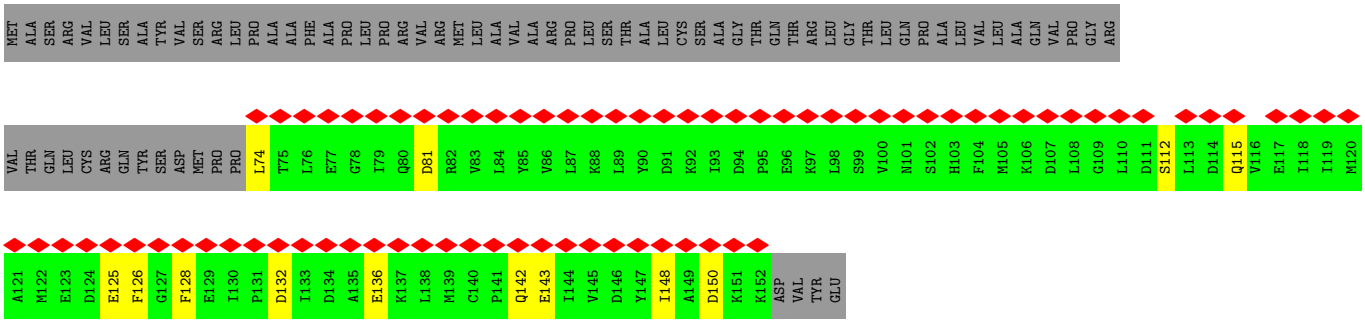
Chain v:



• Molecule 53: Acyl carrier protein, mitochondrial

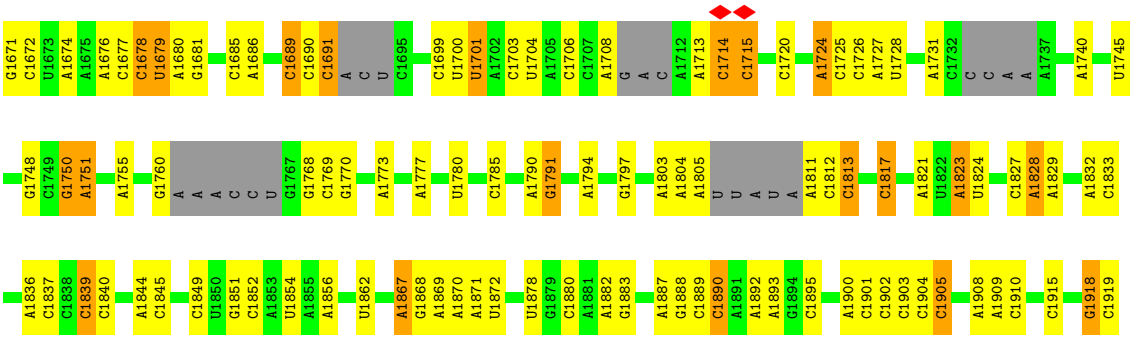
Chain w:

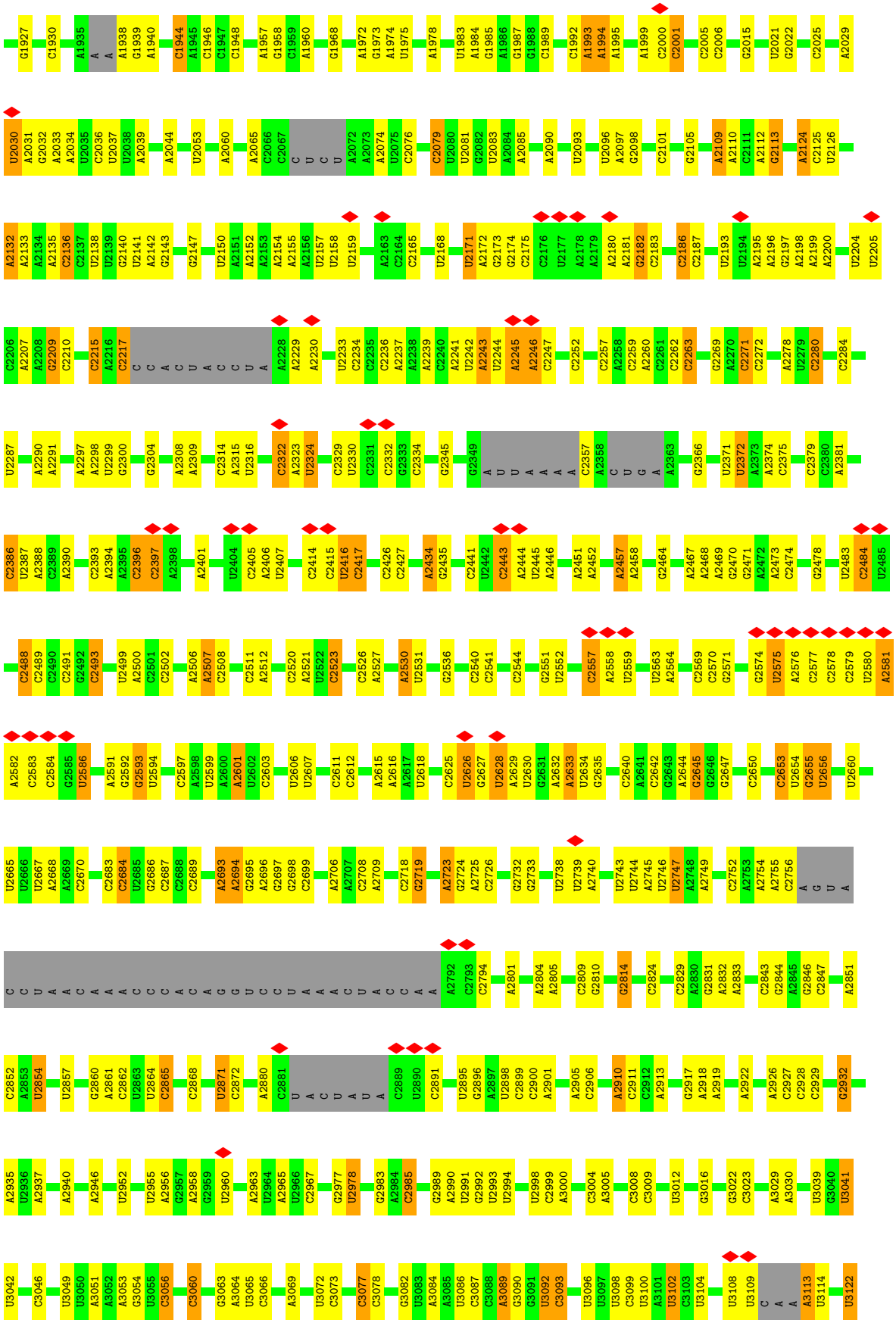


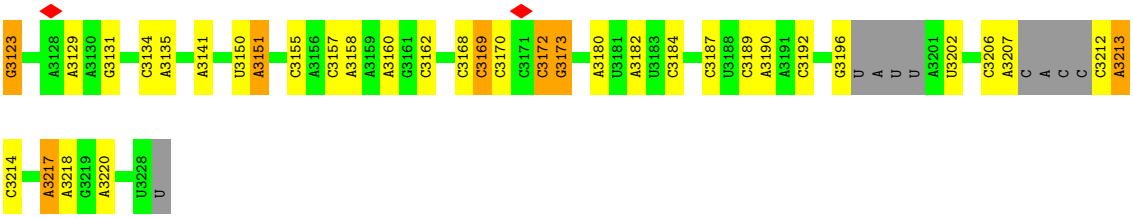


• Molecule 54: 16S rRNA

Chain A:

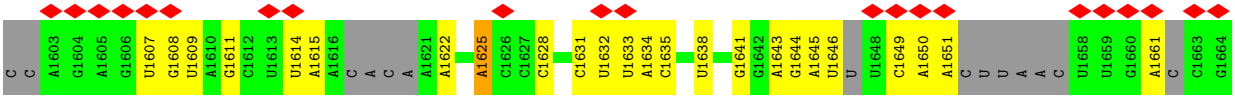


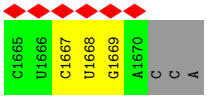




• Molecule 55: mt-tRNAVal

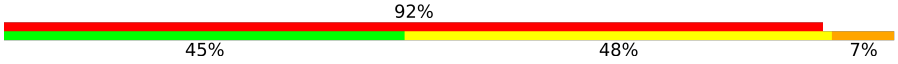
Chain B:

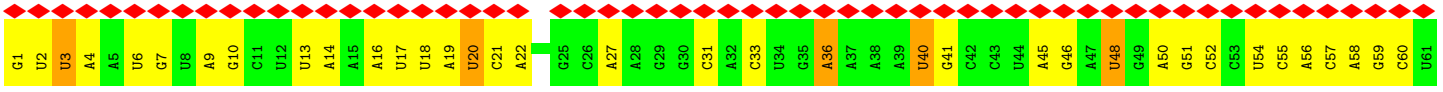


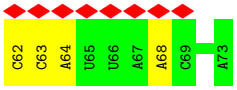


• Molecule 56: mt-tRNA

Chain 24:

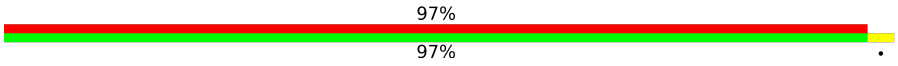


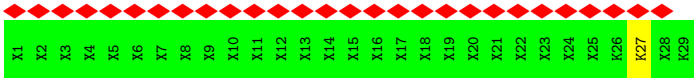




• Molecule 57: nascent chain

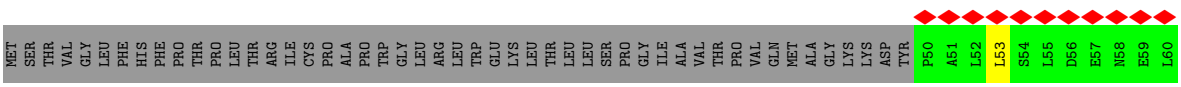
Chain Y2:

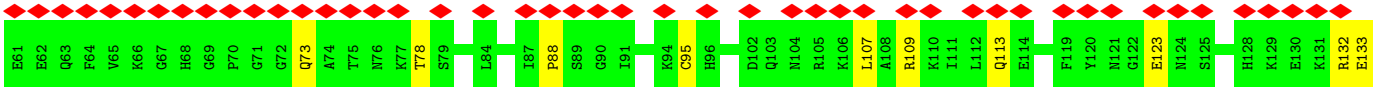


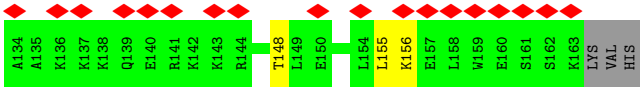


• Molecule 58: Probable peptide chain release factor C12orf65, mitochondrial

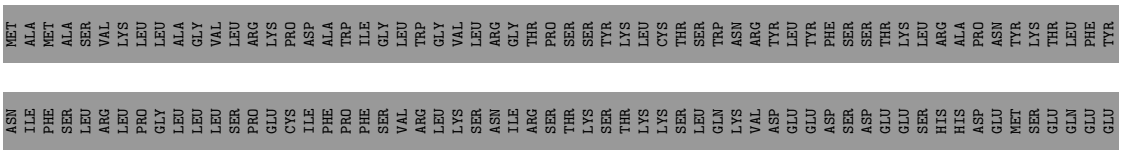
Chain C:

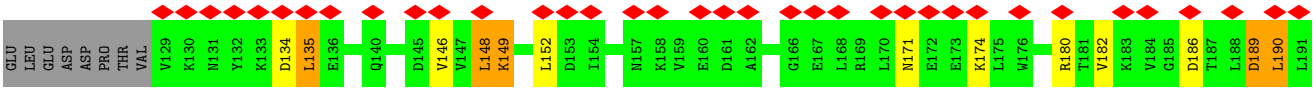


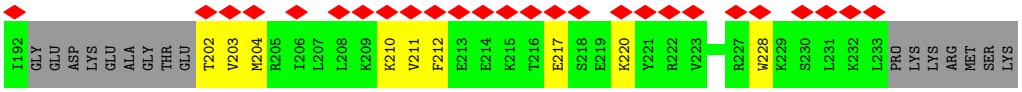




• Molecule 59: Mitochondrial transcription rescue factor 1







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48245	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 ($e^-/Å^2$)	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	0.675	Depositor
Minimum map value	-0.378	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.11	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: ZN, PNS, MEQ, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	D	0.68	0/1879	0.70	1/2527 (0.0%)
2	E	0.72	0/2465	0.67	0/3344
3	F	0.74	0/2071	0.65	0/2817
4	H	0.60	0/798	0.69	0/1073
5	I	0.47	0/1308	0.70	2/1761 (0.1%)
6	J	0.40	0/1077	0.67	0/1452
7	K	0.72	0/1495	0.63	0/2029
8	L	0.65	0/904	0.72	1/1218 (0.1%)
9	M	0.72	0/2359	0.67	0/3185
10	N	0.66	0/1697	0.65	0/2281
11	O	0.65	0/1269	0.70	1/1708 (0.1%)
12	P	0.61	0/1173	0.62	0/1588
13	Q	0.62	0/1846	0.65	2/2487 (0.1%)
14	R	0.78	0/1174	0.66	1/1572 (0.1%)
15	S	0.72	0/1276	0.69	0/1729
16	T	0.76	1/1402 (0.1%)	0.64	0/1886
17	U	0.66	0/1247	0.71	2/1689 (0.1%)
18	V	0.59	0/1666	0.63	1/2260 (0.0%)
19	W	0.81	0/881	0.64	0/1188
20	X	0.62	0/2090	0.63	0/2825
21	Y	0.67	0/1552	0.62	0/2079
22	Z	0.66	0/1003	0.64	0/1354
23	0	0.69	0/895	0.64	0/1201
24	1	0.64	0/438	0.72	1/583 (0.2%)
25	2	0.80	0/373	0.72	2/496 (0.4%)
26	3	0.82	0/852	0.62	0/1136
27	5	0.62	0/3250	0.68	4/4429 (0.1%)
28	6	0.60	1/2726 (0.0%)	0.65	3/3715 (0.1%)
29	7	0.57	0/2391	0.63	0/3234
30	8	0.39	0/909	0.78	6/1227 (0.5%)
31	9	0.66	0/972	0.61	0/1306
32	a	0.65	0/709	0.60	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	b	0.69	0/1202	0.67	0/1626
34	c	0.60	0/2264	0.61	0/3059
35	d	0.50	0/1790	0.59	0/2423
36	e	0.39	0/1797	0.68	0/2422
37	f	0.48	0/931	0.64	0/1259
38	g	0.71	0/1102	0.68	0/1503
39	h	0.49	0/847	0.64	1/1150 (0.1%)
40	i	0.80	0/849	0.71	1/1135 (0.1%)
41	j	0.55	0/698	0.55	0/940
42	k	0.45	0/635	0.60	0/855
43	l	0.49	0/226	0.47	0/299
44	m	0.36	0/379	0.81	0/510
45	o	0.73	0/792	0.67	0/1064
46	p	0.47	0/1071	0.59	1/1433 (0.1%)
47	q	0.51	0/1107	0.56	0/1498
48	r	0.68	0/1238	0.62	0/1676
49	s	0.66	1/3114 (0.0%)	0.66	1/4225 (0.0%)
51	u	0.53	0/949	0.66	0/1281
52	v	0.46	0/597	0.68	1/796 (0.1%)
53	w	0.35	0/647	0.63	0/871
54	A	1.61	68/34613 (0.2%)	1.37	459/53854 (0.9%)
55	B	0.72	0/1328	1.33	11/2056 (0.5%)
56	24	0.66	0/1731	1.30	13/2693 (0.5%)
57	Y2	0.53	0/25	0.67	0/27
58	C	0.48	0/929	0.69	1/1235 (0.1%)
59	G	0.53	0/818	0.93	4/1090 (0.4%)
All	All	1.05	71/107826 (0.1%)	0.99	520/153322 (0.3%)

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	D	0	1
15	S	0	1
18	V	0	1
27	5	0	2
30	8	0	3
48	r	0	2
49	s	0	1
57	Y2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
59	G	0	2
All	All	0	14

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A	1828	A	N9-C4	-11.55	1.30	1.37
16	T	58	VAL	C-N	-8.32	1.15	1.34
28	6	28	ARG	C-N	-6.89	1.18	1.34
54	A	1790	A	N7-C5	-6.78	1.35	1.39
54	A	1908	A	N9-C4	-6.61	1.33	1.37
54	A	2152	A	N9-C4	-6.59	1.33	1.37
54	A	1828	A	N3-C4	-6.51	1.30	1.34
54	A	1983	U	C2-N3	-6.37	1.33	1.37
54	A	1984	A	N9-C4	-6.37	1.34	1.37
54	A	1851	G	N7-C5	-6.33	1.35	1.39
54	A	2298	A	N9-C4	-6.23	1.34	1.37
54	A	1900	A	N9-C4	-6.22	1.34	1.37
54	A	2668	A	N7-C5	-6.00	1.35	1.39
54	A	1751	A	N9-C8	-5.96	1.32	1.37
54	A	2470	G	C5-C4	-5.94	1.34	1.38
54	A	2645	G	N7-C5	-5.93	1.35	1.39
54	A	2693	A	C5-C4	-5.93	1.34	1.38
54	A	3029	A	C5-C4	-5.84	1.34	1.38
54	A	1918	G	N1-C2	-5.81	1.33	1.37
54	A	1960	A	N7-C5	-5.79	1.35	1.39
54	A	2308	A	N7-C5	-5.76	1.35	1.39
54	A	2132	A	C5-C4	-5.70	1.34	1.38
54	A	1994	A	N9-C4	-5.67	1.34	1.37
49	s	301	LEU	C-N	-5.63	1.21	1.34
54	A	2616	A	N9-C4	-5.56	1.34	1.37
54	A	2304	G	C5-C4	-5.56	1.34	1.38
54	A	3064	A	N9-C4	-5.52	1.34	1.37
54	A	1905	C	N3-C4	-5.50	1.30	1.33
54	A	2615	A	N9-C4	-5.49	1.34	1.37
54	A	2001	C	N3-C4	-5.46	1.30	1.33
54	A	2932	G	C5-C4	-5.40	1.34	1.38
54	A	2132	A	N7-C5	-5.38	1.36	1.39
54	A	2593	G	C5-C4	-5.36	1.34	1.38
54	A	1867	A	N3-C4	-5.33	1.31	1.34
54	A	2694	A	N7-C5	-5.29	1.36	1.39
54	A	1918	G	C2-N3	-5.27	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A	2633	A	N7-C5	-5.27	1.36	1.39
54	A	1862	U	C2-N3	-5.27	1.34	1.37
54	A	2693	A	N3-C4	-5.27	1.31	1.34
54	A	2143	G	C2-N3	-5.26	1.28	1.32
54	A	3213	A	N7-C5	-5.26	1.36	1.39
54	A	2998	U	C2-N3	-5.25	1.34	1.37
54	A	2467	A	N9-C4	-5.25	1.34	1.37
54	A	2591	A	N9-C4	-5.24	1.34	1.37
54	A	1755	A	N7-C5	-5.22	1.36	1.39
54	A	3066	C	N3-C4	-5.21	1.30	1.33
54	A	2723	A	N9-C4	-5.18	1.34	1.37
54	A	1904	C	N3-C4	-5.16	1.30	1.33
54	A	1731	A	N7-C5	-5.16	1.36	1.39
54	A	1845	C	N3-C4	-5.16	1.30	1.33
54	A	3173	G	N7-C5	-5.15	1.36	1.39
54	A	1750	G	N7-C5	-5.15	1.36	1.39
54	A	2468	A	N7-C5	-5.15	1.36	1.39
54	A	2946	A	N7-C5	-5.15	1.36	1.39
54	A	2983	G	C5-C4	-5.15	1.34	1.38
54	A	2090	A	N9-C4	-5.11	1.34	1.37
54	A	2719	G	C8-N7	-5.08	1.27	1.30
54	A	1978	A	N9-C4	-5.07	1.34	1.37
54	A	2133	A	N7-C5	-5.06	1.36	1.39
54	A	2278	A	N9-C4	-5.06	1.34	1.37
54	A	2569	C	N3-C4	-5.05	1.30	1.33
54	A	2155	A	N9-C4	-5.04	1.34	1.37
54	A	1740	A	N9-C4	-5.03	1.34	1.37
54	A	2138	U	C2-N3	-5.03	1.34	1.37
54	A	2805	A	N9-C4	-5.03	1.34	1.37
54	A	2507	A	N7-C5	-5.02	1.36	1.39
54	A	3064	A	C5-C4	-5.02	1.35	1.38
54	A	1867	A	N7-C5	-5.01	1.36	1.39
54	A	2726	C	C2-O2	-5.01	1.20	1.24
54	A	2809	C	N3-C4	-5.01	1.30	1.33
54	A	1828	A	N7-C5	-5.01	1.36	1.39

All (520) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A	2523	C	N1-C2-O2	15.27	128.06	118.90
54	A	2523	C	C2-N1-C1'	12.60	132.66	118.80
54	A	2653	C	C6-N1-C2	-12.11	115.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A	2626	U	C2-N1-C1'	11.72	131.76	117.70
54	A	2322	C	N1-C2-O2	11.37	125.72	118.90
54	A	3060	C	C6-N1-C2	-11.15	115.84	120.30
55	B	1649	C	N1-C2-O2	11.11	125.56	118.90
54	A	1828	A	C2-N3-C4	-10.93	105.14	110.60
54	A	1714	C	N1-C2-O2	10.75	125.35	118.90
54	A	2523	C	N3-C2-O2	-10.68	114.42	121.90
54	A	3173	G	N7-C8-N9	10.24	118.22	113.10
54	A	3169	C	N1-C2-O2	10.15	124.99	118.90
54	A	2005	C	C6-N1-C2	-10.14	116.24	120.30
54	A	3173	G	C8-N9-C4	-10.05	102.38	106.40
54	A	2322	C	C6-N1-C2	-10.03	116.29	120.30
54	A	2626	U	N1-C2-O2	9.92	129.75	122.80
54	A	2484	C	C2-N1-C1'	9.91	129.70	118.80
54	A	2079	C	C2-N1-C1'	9.89	129.68	118.80
55	B	1649	C	C2-N1-C1'	9.62	129.38	118.80
54	A	1828	A	N3-C4-C5	9.59	133.51	126.80
54	A	2523	C	C6-N1-C1'	-9.54	109.35	120.80
54	A	2484	C	N1-C2-O2	9.38	124.53	118.90
54	A	2898	U	C2-N1-C1'	9.30	128.86	117.70
54	A	2626	U	N3-C2-O2	-9.28	115.70	122.20
54	A	2322	C	C5-C6-N1	9.26	125.63	121.00
54	A	2329	C	N1-C2-O2	9.22	124.43	118.90
54	A	1828	A	N3-C4-N9	-9.16	120.08	127.40
54	A	2386	C	N1-C2-O2	9.06	124.33	118.90
54	A	2113	G	O5'-P-OP2	-9.01	97.59	105.70
54	A	3060	C	C5-C6-N1	9.00	125.50	121.00
54	A	2493	C	C2-N1-C1'	8.99	128.69	118.80
54	A	3169	C	N3-C2-O2	-8.89	115.68	121.90
54	A	2493	C	N1-C2-O2	8.82	124.19	118.90
54	A	3212	C	C6-N1-C2	-8.80	116.78	120.30
54	A	2322	C	N3-C2-O2	-8.72	115.80	121.90
54	A	2357	C	N1-C2-O2	8.70	124.12	118.90
54	A	1714	C	N3-C2-O2	-8.66	115.84	121.90
54	A	2204	U	N3-C2-O2	-8.64	116.15	122.20
54	A	1714	C	C2-N1-C1'	8.64	128.30	118.80
54	A	2898	U	N3-C2-O2	-8.60	116.18	122.20
54	A	2079	C	N3-C2-O2	-8.59	115.89	121.90
54	A	3187	C	C6-N1-C2	-8.57	116.87	120.30
54	A	2205	U	C2-N1-C1'	8.56	127.97	117.70
54	A	2625	C	C5-C6-N1	8.54	125.27	121.00
54	A	3173	G	C6-C5-N7	-8.53	125.28	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	B	1649	C	N3-C2-O2	-8.49	115.96	121.90
54	A	2205	U	N1-C2-O2	8.48	128.74	122.80
54	A	3173	G	C5-N7-C8	-8.46	100.07	104.30
54	A	2653	C	C5-C6-N1	8.43	125.22	121.00
54	A	3170	C	N1-C2-O2	8.37	123.92	118.90
54	A	2079	C	N1-C2-O2	8.37	123.92	118.90
54	A	2329	C	N3-C2-O2	-8.37	116.04	121.90
54	A	3169	C	C2-N1-C1'	8.35	127.98	118.80
54	A	1989	C	C6-N1-C2	-8.35	116.96	120.30
54	A	2357	C	N3-C2-O2	-8.33	116.07	121.90
54	A	1993	A	C2-N3-C4	8.26	114.73	110.60
54	A	1689	C	C2-N1-C1'	8.25	127.87	118.80
54	A	3122	U	N1-C2-O2	8.24	128.57	122.80
54	A	2569	C	N1-C2-O2	8.23	123.84	118.90
54	A	2158	U	N1-C2-O2	8.21	128.55	122.80
54	A	3134	C	C2-N1-C1'	8.20	127.82	118.80
54	A	2005	C	C5-C6-N1	8.12	125.06	121.00
54	A	1839	C	C6-N1-C2	-8.01	117.10	120.30
54	A	2569	C	N3-C2-O2	-7.98	116.31	121.90
54	A	3122	U	N3-C2-O2	-7.94	116.64	122.20
54	A	2474	C	C6-N1-C2	-7.89	117.14	120.30
54	A	2396	C	N1-C2-O2	7.89	123.63	118.90
54	A	3134	C	N1-C2-O2	7.85	123.61	118.90
54	A	3170	C	C2-N1-C1'	7.85	127.43	118.80
54	A	2599	U	N1-C2-O2	7.84	128.29	122.80
54	A	2656	U	N3-C2-O2	-7.82	116.73	122.20
54	A	2626	U	C6-N1-C1'	-7.79	110.30	121.20
54	A	2684	C	N1-C2-O2	7.78	123.57	118.90
54	A	3173	G	C4-C5-N7	7.78	113.91	110.80
54	A	3212	C	C2-N1-C1'	7.78	127.35	118.80
54	A	2205	U	N3-C2-O2	-7.74	116.78	122.20
54	A	2739	U	N1-C2-O2	7.71	128.20	122.80
54	A	3173	G	C2-N3-C4	-7.71	108.04	111.90
54	A	1785	C	C6-N1-C2	-7.70	117.22	120.30
54	A	1689	C	N1-C2-O2	7.69	123.51	118.90
54	A	2322	C	C2-N1-C1'	7.68	127.25	118.80
54	A	2158	U	N3-C2-O2	-7.68	116.83	122.20
54	A	3212	C	N1-C2-O2	7.67	123.50	118.90
54	A	2417	C	N1-C2-O2	7.61	123.47	118.90
54	A	2101	C	C6-N1-C2	-7.60	117.26	120.30
54	A	2204	U	N1-C2-O2	7.60	128.12	122.80
54	A	1823	A	P-O3'-C3'	7.59	128.81	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A	2372	U	N3-C2-O2	-7.58	116.89	122.20
54	A	2158	U	C2-N1-C1'	7.56	126.77	117.70
54	A	3134	C	C5-C6-N1	7.56	124.78	121.00
54	A	2684	C	N3-C2-O2	-7.53	116.63	121.90
54	A	2379	C	C2-N1-C1'	7.52	127.07	118.80
54	A	2625	C	C6-N1-C2	-7.52	117.29	120.30
54	A	2484	C	C6-N1-C1'	-7.50	111.80	120.80
54	A	2386	C	N3-C2-O2	-7.50	116.65	121.90
54	A	3122	U	C2-N1-C1'	7.49	126.69	117.70
54	A	3092	U	C6-N1-C2	-7.46	116.52	121.00
54	A	1691	C	C5-C6-N1	7.43	124.71	121.00
54	A	2484	C	C5-C6-N1	7.42	124.71	121.00
54	A	2493	C	N3-C2-O2	-7.42	116.71	121.90
54	A	2898	U	N1-C2-O2	7.39	127.97	122.80
49	s	229	LEU	CA-CB-CG	7.37	132.26	115.30
54	A	2599	U	N3-C2-O2	-7.37	117.04	122.20
54	A	2895	U	N3-C2-O2	-7.37	117.04	122.20
54	A	2215	C	N1-C2-O2	7.34	123.30	118.90
54	A	1689	C	N3-C2-O2	-7.30	116.79	121.90
54	A	2215	C	C6-N1-C2	-7.30	117.38	120.30
54	A	1672	C	N1-C2-O2	7.27	123.26	118.90
54	A	2243	A	P-O3'-C3'	7.23	128.38	119.70
55	B	1649	C	C6-N1-C2	-7.22	117.41	120.30
54	A	3065	U	N1-C2-O2	7.21	127.85	122.80
54	A	2136	C	C5-C6-N1	7.21	124.60	121.00
54	A	1839	C	C5-C6-N1	7.19	124.59	121.00
54	A	2507	A	O5'-P-OP1	-7.14	99.27	105.70
54	A	3217	A	OP1-P-O3'	7.10	120.83	105.20
54	A	1902	C	N3-C4-C5	7.09	124.74	121.90
54	A	3170	C	N3-C2-O2	-7.09	116.94	121.90
54	A	2215	C	C5-C6-N1	7.07	124.53	121.00
54	A	3087	C	C6-N1-C2	-7.06	117.48	120.30
17	U	118	PRO	N-CA-CB	7.05	111.75	103.30
54	A	2493	C	C6-N1-C1'	-7.04	112.35	120.80
54	A	1880	C	C6-N1-C2	-7.02	117.49	120.30
54	A	2079	C	C6-N1-C1'	-7.00	112.41	120.80
54	A	2443	C	N1-C2-O2	6.98	123.09	118.90
54	A	2263	C	N1-C2-O2	6.97	123.08	118.90
54	A	2109	A	O4'-C1'-N9	6.96	113.77	108.20
54	A	2445	U	N3-C2-O2	-6.95	117.33	122.20
54	A	3065	U	N3-C2-O2	-6.93	117.35	122.20
54	A	1813	C	C6-N1-C2	-6.92	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A	2457	A	P-O3'-C3'	6.92	128.01	119.70
54	A	2271	C	N1-C2-O2	6.89	123.03	118.90
54	A	1904	C	C6-N1-C2	-6.88	117.55	120.30
54	A	3212	C	C5-C6-N1	6.86	124.43	121.00
56	24	48	U	N3-C2-O2	-6.83	117.42	122.20
54	A	3102	U	N1-C2-O2	6.80	127.56	122.80
55	B	1668	U	C5-C6-N1	6.79	126.09	122.70
54	A	2574	G	C8-N9-C4	-6.79	103.69	106.40
54	A	2280	C	N1-C2-O2	6.77	122.96	118.90
54	A	3187	C	C2-N1-C1'	6.75	126.23	118.80
54	A	3123	G	O4'-C1'-N9	6.74	113.59	108.20
54	A	3172	C	N1-C2-O2	6.74	122.94	118.90
54	A	2445	U	N1-C2-O2	6.74	127.52	122.80
54	A	2960	U	N1-C2-O2	6.73	127.51	122.80
54	A	1724	A	C2-N3-C4	6.72	113.96	110.60
54	A	2372	U	C2-N1-C1'	6.71	125.75	117.70
54	A	2396	C	C5-C6-N1	6.71	124.36	121.00
54	A	3093	C	C6-N1-C2	-6.71	117.62	120.30
54	A	2386	C	C2-N1-C1'	6.70	126.17	118.80
54	A	1785	C	C5-C6-N1	6.69	124.35	121.00
55	B	1649	C	C5-C6-N1	6.69	124.34	121.00
54	A	3214	C	C6-N1-C2	-6.68	117.63	120.30
54	A	2416	U	C2-N1-C1'	6.67	125.70	117.70
54	A	2898	U	C6-N1-C1'	-6.67	111.87	121.20
54	A	2329	C	C6-N1-C2	-6.65	117.64	120.30
56	24	48	U	N1-C2-O2	6.64	127.45	122.80
54	A	2739	U	N3-C2-O2	-6.64	117.55	122.20
30	8	183	PRO	N-CA-CB	6.62	111.25	103.30
54	A	2252	C	C5-C6-N1	6.61	124.31	121.00
54	A	2397	C	C6-N1-C2	-6.61	117.66	120.30
54	A	2372	U	N1-C2-O2	6.61	127.42	122.80
54	A	3093	C	N1-C2-O2	6.58	122.85	118.90
54	A	2379	C	C6-N1-C1'	-6.55	112.94	120.80
54	A	2441	C	C6-N1-C2	-6.55	117.68	120.30
25	2	84	LEU	CA-CB-CG	6.53	130.31	115.30
54	A	2814	G	C2-N3-C4	6.51	115.16	111.90
54	A	2575	U	C6-N1-C2	-6.50	117.10	121.00
54	A	1890	C	C6-N1-C2	-6.50	117.70	120.30
54	A	2136	C	C6-N1-C2	-6.49	117.70	120.30
54	A	3073	C	C6-N1-C2	-6.49	117.70	120.30
54	A	3212	C	N3-C2-O2	-6.49	117.36	121.90
55	B	1649	C	C6-N1-C1'	-6.49	113.01	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	B	1635	C	N1-C2-O2	6.48	122.79	118.90
54	A	1958	G	O4'-C1'-N9	6.47	113.38	108.20
54	A	2865	C	N1-C2-O2	6.47	122.78	118.90
54	A	2699	C	C6-N1-C2	-6.47	117.71	120.30
54	A	1993	A	C8-N9-C4	-6.46	103.22	105.80
8	L	96	MET	C-N-CA	6.45	137.83	121.70
54	A	1715	C	C2-N1-C1'	6.45	125.89	118.80
54	A	2871	U	C5-C6-N1	6.44	125.92	122.70
54	A	2626	U	C5-C6-N1	6.43	125.91	122.70
17	U	28	LEU	CA-CB-CG	6.43	130.08	115.30
54	A	1691	C	C6-N1-C2	-6.42	117.73	120.30
54	A	2960	U	N3-C2-O2	-6.42	117.71	122.20
54	A	2967	C	N1-C2-O2	6.41	122.74	118.90
59	G	190	LEU	CA-CB-CG	6.41	130.03	115.30
54	A	2653	C	N3-C2-O2	-6.38	117.43	121.90
54	A	1919	C	N1-C2-O2	6.38	122.73	118.90
54	A	2182	G	P-O3'-C3'	6.38	127.36	119.70
54	A	2135	A	C2-N3-C4	6.38	113.79	110.60
54	A	2417	C	N3-C2-O2	-6.37	117.44	121.90
59	G	152	LEU	CA-CB-CG	6.37	129.95	115.30
54	A	2687	C	C6-N1-C2	-6.37	117.75	120.30
27	5	218	LEU	CA-CB-CG	6.35	129.90	115.30
54	A	2093	U	N3-C2-O2	-6.34	117.76	122.20
54	A	2499	U	N1-C2-O2	6.34	127.24	122.80
52	v	45	LEU	CA-CB-CG	6.34	129.88	115.30
54	A	3187	C	C5-C6-N1	6.34	124.17	121.00
54	A	2998	U	N3-C2-O2	-6.33	117.77	122.20
59	G	135	LEU	CA-CB-CG	6.32	129.84	115.30
54	A	2030	U	OP2-P-O3'	6.32	119.10	105.20
54	A	1845	C	C6-N1-C2	-6.32	117.77	120.30
54	A	2824	C	N1-C2-O2	6.31	122.69	118.90
54	A	1726	C	C5-C6-N1	6.30	124.15	121.00
54	A	2684	C	C2-N1-C1'	6.30	125.73	118.80
54	A	2397	C	C5-C6-N1	6.27	124.14	121.00
54	A	2656	U	N1-C2-O2	6.27	127.19	122.80
54	A	3192	C	N1-C2-O2	6.27	122.66	118.90
54	A	2940	A	O5'-P-OP1	-6.27	100.06	105.70
59	G	189	ASP	C-N-CA	6.26	137.36	121.70
54	A	1714	C	C6-N1-C1'	-6.26	113.29	120.80
54	A	1993	A	N1-C6-N6	-6.24	114.85	118.60
54	A	3102	U	N3-C2-O2	-6.24	117.83	122.20
54	A	2030	U	P-O3'-C3'	6.23	127.18	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A	2243	A	OP2-P-O3'	6.23	118.91	105.20
54	A	2865	C	N3-C2-O2	-6.21	117.55	121.90
54	A	2927	C	C6-N1-C2	-6.21	117.81	120.30
54	A	2416	U	C5-C6-N1	6.21	125.80	122.70
54	A	2854	U	N1-C2-O2	6.20	127.14	122.80
54	A	2665	U	C5-C6-N1	6.20	125.80	122.70
54	A	2523	C	C5-C6-N1	6.20	124.10	121.00
54	A	2499	U	N3-C2-O2	-6.20	117.86	122.20
54	A	2140	G	C8-N9-C4	-6.18	103.93	106.40
54	A	2246	A	C8-N9-C4	6.18	108.27	105.80
54	A	2271	C	C5-C6-N1	6.17	124.09	121.00
54	A	2489	C	C6-N1-C2	-6.17	117.83	120.30
54	A	2124	A	C8-N9-C4	-6.16	103.33	105.80
54	A	1946	C	C6-N1-C2	-6.14	117.84	120.30
54	A	2324	U	N1-C2-O2	6.14	127.10	122.80
54	A	2259	C	N1-C2-O2	6.13	122.58	118.90
54	A	2215	C	C2-N1-C1'	6.13	125.55	118.80
54	A	3060	C	C2-N1-C1'	6.13	125.55	118.80
54	A	2530	A	P-O3'-C3'	6.13	127.05	119.70
54	A	2474	C	C5-C6-N1	6.12	124.06	121.00
54	A	2599	U	C2-N1-C1'	6.11	125.03	117.70
54	A	2234	C	C5-C6-N1	6.11	124.05	121.00
27	5	98	LEU	CA-CB-CG	6.10	129.34	115.30
54	A	2175	C	N1-C2-O2	6.10	122.56	118.90
54	A	3066	C	N1-C2-O2	6.09	122.56	118.90
5	I	174	LEU	CA-CB-CG	6.08	129.28	115.30
54	A	2112	A	OP2-P-O3'	6.07	118.56	105.20
56	24	6	U	N1-C2-O2	6.07	127.05	122.80
54	A	2846	G	N1-C6-O6	-6.06	116.26	119.90
54	A	2895	U	N1-C2-O2	6.05	127.04	122.80
54	A	2739	U	C2-N1-C1'	6.04	124.95	117.70
54	A	3023	C	C5-C6-N1	6.04	124.02	121.00
54	A	1823	A	OP2-P-O3'	6.04	118.48	105.20
54	A	2079	C	C6-N1-C2	-6.03	117.89	120.30
54	A	2263	C	C5-C6-N1	6.02	124.01	121.00
54	A	3173	G	N1-C2-N2	-6.00	110.80	116.20
54	A	1751	A	N7-C8-N9	5.99	116.80	113.80
54	A	1679	U	O4'-C1'-N1	5.99	112.99	108.20
54	A	1701	U	N3-C2-O2	-5.99	118.01	122.20
54	A	3170	C	C6-N1-C1'	-5.99	113.62	120.80
54	A	3023	C	C6-N1-C2	-5.98	117.91	120.30
56	24	3	U	C2-N1-C1'	5.98	124.88	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A	3212	C	O4'-C1'-N1	5.96	112.97	108.20
54	A	2280	C	N3-C2-O2	-5.96	117.73	121.90
54	A	2843	C	N1-C2-O2	5.96	122.47	118.90
54	A	1726	C	C6-N1-C2	-5.96	117.92	120.30
54	A	2862	C	C6-N1-C2	-5.95	117.92	120.30
54	A	2489	C	N1-C2-O2	5.95	122.47	118.90
54	A	2843	C	C6-N1-C2	-5.95	117.92	120.30
54	A	2280	C	C6-N1-C2	-5.93	117.93	120.30
54	A	2271	C	C6-N1-C2	-5.93	117.93	120.30
54	A	2314	C	C6-N1-C2	-5.90	117.94	120.30
54	A	2689	C	C5-C6-N1	5.89	123.95	121.00
54	A	3073	C	N1-C2-O2	5.89	122.43	118.90
54	A	1837	C	C6-N1-C2	-5.88	117.95	120.30
54	A	2900	C	C6-N1-C2	-5.88	117.95	120.30
54	A	1671	G	O4'-C1'-N9	5.87	112.90	108.20
54	A	2670	C	C6-N1-C2	-5.87	117.95	120.30
14	R	67	LEU	CA-CB-CG	5.87	128.79	115.30
54	A	1725	C	N1-C2-O2	5.86	122.42	118.90
54	A	3073	C	N3-C2-O2	-5.86	117.80	121.90
54	A	2794	C	C6-N1-C2	-5.85	117.96	120.30
54	A	2171	U	N3-C2-O2	-5.85	118.11	122.20
54	A	2136	C	N1-C2-O2	5.85	122.41	118.90
54	A	3169	C	C6-N1-C1'	-5.83	113.80	120.80
54	A	2650	C	N1-C2-O2	5.83	122.39	118.90
54	A	2136	C	C2-N1-C1'	5.82	125.21	118.80
54	A	2150	U	N3-C2-O2	-5.82	118.13	122.20
54	A	2689	C	C6-N1-C2	-5.82	117.97	120.30
54	A	1701	U	N1-C2-O2	5.81	126.87	122.80
54	A	2843	C	N3-C2-O2	-5.80	117.84	121.90
11	O	144	LEU	CA-CB-CG	5.79	128.60	115.30
54	A	2523	C	C6-N1-C2	-5.79	117.99	120.30
27	5	382	LEU	CA-CB-CG	5.78	128.59	115.30
54	A	2165	C	C6-N1-C2	-5.78	117.99	120.30
56	24	20	U	C5-C6-N1	5.77	125.58	122.70
54	A	3134	C	C6-N1-C2	-5.76	117.99	120.30
54	A	1720	C	C6-N1-C2	-5.75	118.00	120.30
54	A	1993	A	N3-C4-C5	-5.74	122.78	126.80
54	A	2484	C	N3-C2-O2	-5.74	117.89	121.90
54	A	1833	C	C5-C6-N1	5.73	123.87	121.00
54	A	2394	A	O4'-C1'-N9	-5.73	103.61	108.20
54	A	3093	C	N3-C2-O2	-5.72	117.89	121.90
54	A	1993	A	C4-N9-C1'	5.72	136.59	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A	2217	C	C5-C6-N1	5.72	123.86	121.00
54	A	3134	C	C6-N1-C1'	-5.72	113.94	120.80
54	A	2386	C	C6-N1-C2	-5.71	118.01	120.30
54	A	1689	C	C6-N1-C1'	-5.71	113.95	120.80
54	A	2507	A	P-O3'-C3'	5.71	126.56	119.70
54	A	2738	U	C5-C6-N1	5.71	125.55	122.70
54	A	1902	C	N3-C2-O2	-5.70	117.91	121.90
54	A	2723	A	O5'-P-OP1	-5.69	100.58	105.70
54	A	3123	G	C4-N9-C1'	-5.68	119.12	126.50
54	A	2186	C	C6-N1-C2	-5.67	118.03	120.30
54	A	2488	C	C6-N1-C2	-5.66	118.04	120.30
54	A	2960	U	C2-N1-C1'	5.65	124.48	117.70
54	A	1948	C	C6-N1-C2	-5.65	118.04	120.30
54	A	3173	G	N1-C2-N3	5.65	127.29	123.90
54	A	2434	A	N7-C8-N9	5.64	116.62	113.80
54	A	3113	A	P-O3'-C3'	5.64	126.47	119.70
54	A	2747	U	N3-C2-O2	-5.64	118.25	122.20
54	A	2597	C	C6-N1-C2	-5.63	118.05	120.30
54	A	1902	C	N1-C2-O2	5.63	122.28	118.90
5	I	146	LEU	CA-CB-CG	5.62	128.24	115.30
54	A	1975	U	N3-C2-O2	-5.62	118.26	122.20
55	B	1635	C	N3-C2-O2	-5.62	117.96	121.90
56	24	3	U	N1-C2-O2	5.62	126.73	122.80
54	A	3046	C	C6-N1-C2	-5.62	118.05	120.30
55	B	1638	U	C5-C6-N1	5.61	125.51	122.70
54	A	2396	C	C2-N1-C1'	5.61	124.97	118.80
54	A	2205	U	C5-C6-N1	5.60	125.50	122.70
54	A	2324	U	C2-N1-C1'	5.60	124.42	117.70
54	A	3089	A	N9-C4-C5	-5.60	103.56	105.80
1	D	138	ASP	CB-CG-OD1	5.60	123.34	118.30
30	8	152	LEU	CA-CB-CG	5.59	128.17	115.30
54	A	2076	C	N1-C2-O2	5.59	122.25	118.90
56	24	6	U	N3-C2-O2	-5.58	118.29	122.20
56	24	33	C	C5-C6-N1	5.58	123.79	121.00
54	A	2824	C	N3-C2-O2	-5.58	117.99	121.90
54	A	2491	C	C6-N1-C2	-5.58	118.07	120.30
54	A	2868	C	C6-N1-C2	-5.58	118.07	120.30
54	A	2443	C	C2-N1-C1'	5.58	124.93	118.80
54	A	2006	C	C5-C6-N1	5.57	123.79	121.00
54	A	2245	A	P-O3'-C3'	5.57	126.39	119.70
54	A	1833	C	C6-N1-C2	-5.57	118.07	120.30
54	A	1930	C	C6-N1-C2	-5.57	118.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A	1720	C	N3-C2-O2	-5.56	118.01	121.90
54	A	2101	C	C5-C6-N1	5.56	123.78	121.00
40	i	80	LEU	CA-CB-CG	5.56	128.08	115.30
54	A	2541	C	C5-C6-N1	5.55	123.78	121.00
54	A	2857	U	N3-C2-O2	-5.55	118.32	122.20
54	A	1868	G	N3-C4-C5	-5.55	125.83	128.60
54	A	2457	A	OP2-P-O3'	5.54	117.40	105.20
54	A	2684	C	C6-N1-C2	-5.54	118.08	120.30
54	A	3041	U	OP1-P-O3'	5.54	117.39	105.20
54	A	2999	C	C5-C6-N1	5.54	123.77	121.00
54	A	3009	C	C5-C6-N1	5.53	123.77	121.00
54	A	2900	C	N1-C2-O2	5.53	122.22	118.90
54	A	2937	A	N1-C2-N3	-5.52	126.54	129.30
56	24	36	A	C4-C5-N7	5.52	113.46	110.70
54	A	1889	C	C6-N1-C2	-5.51	118.10	120.30
54	A	3151	A	N1-C6-N6	-5.51	115.30	118.60
54	A	1957	A	C4-C5-C6	-5.49	114.25	117.00
39	h	66	LEU	CA-CB-CG	5.49	127.92	115.30
54	A	2929	C	C6-N1-C2	-5.48	118.11	120.30
54	A	2252	C	N1-C2-O2	5.48	122.19	118.90
54	A	2150	U	N1-C2-O2	5.47	126.63	122.80
54	A	2186	C	N1-C2-O2	5.47	122.19	118.90
54	A	2366	G	N1-C6-O6	-5.46	116.63	119.90
54	A	2245	A	N9-C1'-C2'	5.45	121.09	114.00
54	A	2445	U	C2-N1-C1'	5.45	124.24	117.70
54	A	2687	C	C5-C6-N1	5.45	123.72	121.00
54	A	2165	C	C2-N1-C1'	5.43	124.78	118.80
54	A	3134	C	O4'-C1'-N1	5.43	112.55	108.20
54	A	2655	G	O4'-C1'-N9	-5.43	103.86	108.20
54	A	2112	A	P-O3'-C3'	5.43	126.21	119.70
54	A	2557	C	C2-N1-C1'	5.43	124.77	118.80
54	A	3104	U	N3-C2-O2	-5.43	118.40	122.20
54	A	2693	A	N7-C8-N9	-5.42	111.09	113.80
54	A	2611	C	N1-C2-O2	5.41	122.15	118.90
58	C	107	LEU	CA-CB-CG	5.41	127.74	115.30
54	A	1840	C	C5-C6-N1	5.41	123.70	121.00
54	A	2158	U	C5-C6-N1	5.40	125.40	122.70
54	A	2747	U	N1-C2-O2	5.39	126.58	122.80
54	A	1908	A	N1-C6-N6	-5.38	115.37	118.60
54	A	2719	G	C4-C5-N7	5.38	112.95	110.80
27	5	355	LEU	CA-CB-CG	5.38	127.68	115.30
54	A	2271	C	N3-C2-O2	-5.38	118.13	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A	2196	A	O4'-C1'-N9	5.38	112.50	108.20
54	A	2416	U	N1-C2-O2	5.38	126.56	122.80
54	A	2491	C	C5-C6-N1	5.37	123.69	121.00
54	A	3122	U	C6-N1-C1'	-5.37	113.68	121.20
54	A	2489	C	N3-C2-O2	-5.37	118.14	121.90
54	A	1745	U	C5-C6-N1	5.36	125.38	122.70
54	A	2483	U	C5-C6-N1	5.36	125.38	122.70
30	8	187	PRO	N-CA-CB	5.34	109.71	103.30
54	A	2081	U	C5-C6-N1	5.34	125.37	122.70
54	A	2667	U	N3-C2-O2	-5.34	118.46	122.20
54	A	2079	C	O4'-C1'-N1	5.33	112.47	108.20
54	A	1706	C	N1-C2-O2	5.33	122.09	118.90
54	A	1724	A	N3-C4-N9	5.33	131.66	127.40
54	A	3082	G	N1-C6-O6	-5.33	116.70	119.90
54	A	1813	C	C5-C6-N1	5.32	123.66	121.00
30	8	97	LYS	CA-CB-CG	5.32	125.10	113.40
54	A	2898	U	O4'-C1'-N1	5.31	112.45	108.20
54	A	2484	C	O4'-C1'-N1	5.31	112.44	108.20
54	A	1689	C	C6-N1-C2	-5.30	118.18	120.30
28	6	334	LEU	CA-CB-CG	5.29	127.47	115.30
54	A	1930	C	C5-C6-N1	5.29	123.65	121.00
54	A	2215	C	N3-C2-O2	-5.29	118.20	121.90
46	p	135	LEU	CB-CG-CD1	-5.29	102.02	111.00
54	A	3092	U	C5-C6-N1	5.28	125.34	122.70
13	Q	166	LEU	CA-CB-CG	5.28	127.44	115.30
54	A	2900	C	C2-N1-C1'	5.28	124.60	118.80
54	A	2865	C	C2-N1-C1'	5.27	124.60	118.80
54	A	1993	A	C5-C6-N1	5.27	120.34	117.70
54	A	2375	C	C5-C6-N1	5.27	123.63	121.00
18	V	160	PRO	N-CA-CB	5.27	109.62	103.30
54	A	3087	C	C5-C6-N1	5.27	123.63	121.00
54	A	1672	C	N3-C2-O2	-5.26	118.21	121.90
54	A	2006	C	C6-N1-C2	-5.26	118.19	120.30
54	A	2473	A	C4-N9-C1'	5.26	135.76	126.30
54	A	3172	C	N3-C2-O2	-5.26	118.22	121.90
54	A	2236	C	N1-C2-O2	5.25	122.05	118.90
54	A	3029	A	N1-C6-N6	-5.25	115.45	118.60
13	Q	151	LEU	CA-CB-CG	5.25	127.38	115.30
54	A	3134	C	N3-C2-O2	-5.25	118.22	121.90
54	A	2895	U	C2-N1-C1'	5.25	124.00	117.70
28	6	302	ASP	CB-CG-OD1	5.25	123.02	118.30
28	6	161	LEU	CA-CB-CG	5.24	127.35	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A	1790	A	C8-N9-C4	-5.23	103.71	105.80
54	A	1731	A	N9-C4-C5	-5.23	103.71	105.80
54	A	1817	C	N3-C2-O2	-5.23	118.24	121.90
54	A	2871	U	C6-N1-C2	-5.23	117.86	121.00
54	A	1840	C	C6-N1-C2	-5.23	118.21	120.30
55	B	1625	A	C2-N3-C4	5.23	113.21	110.60
30	8	188	PRO	N-CA-CB	5.22	109.57	103.30
54	A	2900	C	C5-C6-N1	5.22	123.61	121.00
54	A	1958	G	C8-N9-C4	-5.22	104.31	106.40
54	A	3092	U	N3-C2-O2	-5.22	118.55	122.20
54	A	3187	C	N3-C2-O2	-5.22	118.25	121.90
54	A	2699	C	C5-C6-N1	5.22	123.61	121.00
54	A	3039	U	C5-C6-N1	5.22	125.31	122.70
54	A	2601	A	C4-C5-N7	5.21	113.31	110.70
54	A	2857	U	N1-C2-O2	5.21	126.44	122.80
54	A	1915	C	C5-C6-N1	5.21	123.60	121.00
54	A	2259	C	N3-C2-O2	-5.21	118.26	121.90
54	A	2581	A	C8-N9-C4	-5.20	103.72	105.80
54	A	3169	C	C6-N1-C2	-5.20	118.22	120.30
54	A	2746	U	N3-C2-O2	-5.20	118.56	122.20
54	A	1944	C	N1-C2-O2	5.20	122.02	118.90
54	A	2441	C	C5-C6-N1	5.20	123.60	121.00
54	A	3089	A	O4'-C1'-N9	5.20	112.36	108.20
54	A	2653	C	N1-C2-O2	5.19	122.02	118.90
54	A	2252	C	C2-N3-C4	5.19	122.50	119.90
54	A	2929	C	N3-C2-O2	-5.19	118.27	121.90
30	8	185	TYR	C-N-CA	5.18	134.66	121.70
54	A	1678	C	C6-N1-C2	-5.18	118.23	120.30
54	A	2209	G	C5-C6-O6	-5.18	125.49	128.60
54	A	2272	C	N1-C2-O2	5.18	122.01	118.90
54	A	3078	C	N3-C2-O2	-5.18	118.27	121.90
54	A	3172	C	C2-N1-C1'	5.18	124.50	118.80
54	A	2829	C	C6-N1-C2	-5.18	118.23	120.30
54	A	2186	C	P-O3'-C3'	5.17	125.91	119.70
54	A	3213	A	C5-N7-C8	-5.17	101.31	103.90
54	A	2205	U	C6-N1-C1'	-5.17	113.97	121.20
54	A	3056	C	C6-N1-C2	-5.15	118.24	120.30
54	A	2234	C	C6-N1-C2	-5.15	118.24	120.30
54	A	2334	C	C6-N1-C2	-5.15	118.24	120.30
54	A	2978	U	N3-C4-O4	-5.15	115.80	119.40
54	A	3213	A	C4-C5-N7	5.15	113.28	110.70
54	A	3041	U	P-O3'-C3'	5.15	125.88	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	24	33	C	C2-N1-C1'	5.14	124.46	118.80
54	A	2726	C	C6-N1-C2	-5.14	118.24	120.30
54	A	1908	A	C4-C5-C6	-5.14	114.43	117.00
54	A	1706	C	N3-C2-O2	-5.14	118.31	121.90
54	A	1904	C	C5-C6-N1	5.14	123.57	121.00
54	A	2441	C	N1-C2-O2	5.13	121.98	118.90
54	A	2601	A	C5-C6-N6	-5.13	119.60	123.70
54	A	2612	C	N1-C2-O2	5.13	121.98	118.90
54	A	2586	U	N3-C2-O2	-5.13	118.61	122.20
54	A	3077	C	C5-C6-N1	5.13	123.56	121.00
54	A	2628	U	O5'-P-OP2	-5.13	101.09	105.70
54	A	3092	U	P-O3'-C3'	5.12	125.85	119.70
54	A	2985	C	N1-C2-O2	5.12	121.97	118.90
54	A	2507	A	C2'-C3'-O3'	5.12	121.89	113.70
54	A	2205	U	C6-N1-C2	-5.12	117.93	121.00
56	24	40	U	N1-C2-O2	5.11	126.38	122.80
54	A	2025	C	C6-N1-C2	-5.11	118.25	120.30
54	A	1791	G	O5'-P-OP2	-5.11	101.11	105.70
54	A	1910	C	C6-N1-C2	-5.10	118.26	120.30
54	A	2626	U	C6-N1-C2	-5.10	117.94	121.00
54	A	2557	C	O4'-C1'-N1	5.10	112.28	108.20
54	A	1958	G	N9-C4-C5	5.09	107.44	105.40
54	A	3123	G	OP2-P-O3'	5.09	116.40	105.20
54	A	1845	C	N3-C2-O2	-5.09	118.34	121.90
54	A	1833	C	C2-N3-C4	5.09	122.44	119.90
54	A	3184	C	N1-C2-O2	5.08	121.95	118.90
54	A	3184	C	C6-N1-C2	-5.08	118.27	120.30
54	A	3184	C	N3-C2-O2	-5.08	118.34	121.90
56	24	36	A	N9-C4-C5	-5.08	103.77	105.80
54	A	1715	C	C6-N1-C1'	-5.08	114.71	120.80
54	A	3008	C	N1-C2-O2	5.08	121.95	118.90
54	A	2357	C	C6-N1-C2	-5.07	118.27	120.30
54	A	1817	C	N1-C2-O2	5.07	121.94	118.90
54	A	2574	G	N7-C8-N9	5.06	115.63	113.10
54	A	2229	A	P-O3'-C3'	5.06	125.77	119.70
24	1	17	LEU	CA-CB-CG	5.06	126.93	115.30
54	A	1944	C	N3-C2-O2	-5.05	118.36	121.90
54	A	1828	A	C5-N7-C8	-5.05	101.38	103.90
54	A	2245	A	OP1-P-O3'	5.05	116.30	105.20
54	A	3004	C	C6-N1-C2	-5.05	118.28	120.30
54	A	3009	C	C6-N1-C2	-5.04	118.28	120.30
54	A	2581	A	N7-C8-N9	5.04	116.32	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A	3039	U	C6-N1-C2	-5.03	117.98	121.00
54	A	1938	A	O4'-C1'-N9	5.03	112.22	108.20
54	A	2489	C	C5-C6-N1	5.03	123.51	121.00
54	A	3192	C	N3-C2-O2	-5.02	118.39	121.90
54	A	1895	C	C6-N1-C2	-5.02	118.29	120.30
25	2	84	LEU	CB-CG-CD2	-5.02	102.47	111.00
56	24	33	C	N1-C2-O2	5.02	121.91	118.90
54	A	2872	C	N1-C2-O2	5.02	121.91	118.90
54	A	2910	A	P-O3'-C3'	5.02	125.72	119.70
54	A	2186	C	N3-C2-O2	-5.01	118.39	121.90
54	A	1745	U	C2-N1-C1'	5.01	123.71	117.70
54	A	2899	C	C6-N1-C2	-5.00	118.30	120.30
54	A	3008	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	5	216	GLU	Peptide
27	5	217	SER	Peptide
30	8	179	THR	Peptide
30	8	184	ASN	Peptide
30	8	186	GLN	Peptide
1	D	206	TYR	Peptide
59	G	148	LEU	Peptide
59	G	211	VAL	Peptide
15	S	101	PHE	Peptide
18	V	100	LYS	Peptide
57	Y2	27	LYS	Peptide
48	r	54	THR	Peptide
48	r	67	SER	Peptide
49	s	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
1	D	234/305 (77%)	219 (94%)	14 (6%)	1 (0%)	34 66
2	E	302/348 (87%)	284 (94%)	18 (6%)	0	100 100
3	F	248/311 (80%)	240 (97%)	8 (3%)	0	100 100
4	H	93/267 (35%)	86 (92%)	7 (8%)	0	100 100
5	I	154/261 (59%)	135 (88%)	19 (12%)	0	100 100
6	J	138/192 (72%)	127 (92%)	11 (8%)	0	100 100
7	K	175/178 (98%)	165 (94%)	10 (6%)	0	100 100
8	L	113/145 (78%)	102 (90%)	11 (10%)	0	100 100
9	M	285/296 (96%)	267 (94%)	18 (6%)	0	100 100
10	N	203/251 (81%)	193 (95%)	9 (4%)	1 (0%)	29 61
11	O	150/175 (86%)	144 (96%)	6 (4%)	0	100 100
12	P	139/179 (78%)	129 (93%)	10 (7%)	0	100 100
13	Q	215/292 (74%)	202 (94%)	13 (6%)	0	100 100
14	R	138/149 (93%)	136 (99%)	2 (1%)	0	100 100
15	S	154/205 (75%)	148 (96%)	6 (4%)	0	100 100
16	T	164/212 (77%)	156 (95%)	8 (5%)	0	100 100
17	U	148/153 (97%)	132 (89%)	14 (10%)	2 (1%)	11 38
18	V	200/216 (93%)	187 (94%)	13 (6%)	0	100 100
19	W	107/148 (72%)	104 (97%)	3 (3%)	0	100 100
20	X	241/256 (94%)	231 (96%)	10 (4%)	0	100 100
21	Y	174/250 (70%)	170 (98%)	4 (2%)	0	100 100
22	Z	118/161 (73%)	113 (96%)	5 (4%)	0	100 100
23	0	106/188 (56%)	104 (98%)	2 (2%)	0	100 100
24	1	50/65 (77%)	48 (96%)	2 (4%)	0	100 100
25	2	43/92 (47%)	42 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	3	93/188 (50%)	88 (95%)	5 (5%)	0	100	100
27	5	383/423 (90%)	361 (94%)	22 (6%)	0	100	100
28	6	316/380 (83%)	293 (93%)	23 (7%)	0	100	100
29	7	285/338 (84%)	267 (94%)	17 (6%)	1 (0%)	34	66
30	8	108/206 (52%)	86 (80%)	19 (18%)	3 (3%)	5	25
31	9	113/137 (82%)	106 (94%)	7 (6%)	0	100	100
32	a	78/142 (55%)	74 (95%)	4 (5%)	0	100	100
33	b	146/155 (94%)	133 (91%)	13 (9%)	0	100	100
34	c	271/332 (82%)	263 (97%)	8 (3%)	0	100	100
35	d	203/306 (66%)	189 (93%)	14 (7%)	0	100	100
36	e	211/279 (76%)	189 (90%)	22 (10%)	0	100	100
37	f	110/194 (57%)	95 (86%)	15 (14%)	0	100	100
38	g	127/166 (76%)	119 (94%)	8 (6%)	0	100	100
39	h	96/158 (61%)	92 (96%)	4 (4%)	0	100	100
40	i	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
41	j	83/123 (68%)	79 (95%)	4 (5%)	0	100	100
42	k	76/112 (68%)	68 (90%)	8 (10%)	0	100	100
43	l	21/138 (15%)	19 (90%)	2 (10%)	0	100	100
44	m	43/128 (34%)	34 (79%)	9 (21%)	0	100	100
45	o	89/102 (87%)	86 (97%)	3 (3%)	0	100	100
46	p	119/206 (58%)	115 (97%)	4 (3%)	0	100	100
47	q	126/222 (57%)	121 (96%)	5 (4%)	0	100	100
48	r	140/196 (71%)	133 (95%)	7 (5%)	0	100	100
49	s	366/439 (83%)	347 (95%)	19 (5%)	0	100	100
51	u	109/234 (47%)	99 (91%)	10 (9%)	0	100	100
52	v	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
53	w	77/156 (49%)	66 (86%)	11 (14%)	0	100	100
57	Y2	2/29 (7%)	0	2 (100%)	0	100	100
58	C	112/166 (68%)	96 (86%)	15 (13%)	1 (1%)	17	48
59	G	92/240 (38%)	60 (65%)	28 (30%)	4 (4%)	2	16
All	All	8249/11388 (72%)	7695 (93%)	541 (7%)	13 (0%)	50	77

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	207	ILE
17	U	118	PRO
30	8	186	GLN
30	8	187	PRO
30	8	188	PRO
59	G	149	LYS
17	U	117	SER
59	G	190	LEU
10	N	48	PRO
59	G	171	ASN
59	G	189	ASP
29	7	291	PRO
58	C	88	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	190/245 (78%)	172 (90%)	18 (10%)	8 29
2	E	259/290 (89%)	241 (93%)	18 (7%)	15 44
3	F	217/262 (83%)	191 (88%)	26 (12%)	5 20
4	H	86/228 (38%)	77 (90%)	9 (10%)	7 25
5	I	145/232 (62%)	135 (93%)	10 (7%)	15 44
6	J	113/150 (75%)	102 (90%)	11 (10%)	8 29
7	K	155/156 (99%)	147 (95%)	8 (5%)	23 54
8	L	98/124 (79%)	88 (90%)	10 (10%)	7 27
9	M	245/249 (98%)	221 (90%)	24 (10%)	8 29
10	N	172/211 (82%)	156 (91%)	16 (9%)	9 30
11	O	133/150 (89%)	125 (94%)	8 (6%)	19 49
12	P	123/154 (80%)	109 (89%)	14 (11%)	5 22
13	Q	199/256 (78%)	177 (89%)	22 (11%)	6 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	R	118/126 (94%)	110 (93%)	8 (7%)	16 44
15	S	141/180 (78%)	129 (92%)	12 (8%)	10 35
16	T	146/182 (80%)	138 (94%)	8 (6%)	21 52
17	U	124/135 (92%)	115 (93%)	9 (7%)	14 41
18	V	172/191 (90%)	148 (86%)	24 (14%)	3 16
19	W	89/119 (75%)	78 (88%)	11 (12%)	4 19
20	X	219/229 (96%)	199 (91%)	20 (9%)	9 31
21	Y	159/223 (71%)	147 (92%)	12 (8%)	13 39
22	Z	111/147 (76%)	102 (92%)	9 (8%)	11 36
23	0	97/164 (59%)	87 (90%)	10 (10%)	7 26
24	1	49/60 (82%)	45 (92%)	4 (8%)	11 36
25	2	39/72 (54%)	37 (95%)	2 (5%)	24 54
26	3	88/166 (53%)	80 (91%)	8 (9%)	9 31
27	5	348/368 (95%)	313 (90%)	35 (10%)	7 27
28	6	265/332 (80%)	236 (89%)	29 (11%)	6 24
29	7	263/303 (87%)	241 (92%)	22 (8%)	11 35
30	8	91/190 (48%)	81 (89%)	10 (11%)	6 24
31	9	99/112 (88%)	93 (94%)	6 (6%)	18 48
32	a	78/133 (59%)	73 (94%)	5 (6%)	17 46
33	b	130/135 (96%)	114 (88%)	16 (12%)	4 20
34	c	241/288 (84%)	224 (93%)	17 (7%)	14 42
35	d	193/274 (70%)	181 (94%)	12 (6%)	18 47
36	e	188/236 (80%)	170 (90%)	18 (10%)	8 29
37	f	101/173 (58%)	88 (87%)	13 (13%)	4 18
38	g	119/148 (80%)	112 (94%)	7 (6%)	19 49
39	h	95/148 (64%)	85 (90%)	10 (10%)	7 25
40	i	86/110 (78%)	78 (91%)	8 (9%)	9 30
41	j	68/97 (70%)	67 (98%)	1 (2%)	65 81
42	k	71/90 (79%)	65 (92%)	6 (8%)	10 35
43	l	23/116 (20%)	22 (96%)	1 (4%)	29 59
44	m	40/113 (35%)	38 (95%)	2 (5%)	24 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
45	o	78/87 (90%)	69 (88%)	9 (12%)	5 22
46	p	117/181 (65%)	108 (92%)	9 (8%)	13 38
47	q	110/178 (62%)	98 (89%)	12 (11%)	6 24
48	r	133/169 (79%)	122 (92%)	11 (8%)	11 36
49	s	326/381 (86%)	292 (90%)	34 (10%)	7 25
51	u	105/200 (52%)	96 (91%)	9 (9%)	10 35
52	v	59/60 (98%)	52 (88%)	7 (12%)	5 21
53	w	73/136 (54%)	60 (82%)	13 (18%)	2 8
57	Y2	3/3 (100%)	3 (100%)	0	100 100
58	C	102/146 (70%)	90 (88%)	12 (12%)	5 21
59	G	90/221 (41%)	73 (81%)	17 (19%)	1 6
All	All	7382/9829 (75%)	6700 (91%)	682 (9%)	13 31

All (682) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	74	ILE
1	D	79	MET
1	D	113	ARG
1	D	115	GLU
1	D	130	ARG
1	D	147	ARG
1	D	163	ILE
1	D	171	ARG
1	D	177	ARG
1	D	220	VAL
1	D	232	ARG
1	D	236	VAL
1	D	243	THR
1	D	244	VAL
1	D	246	ARG
1	D	251	ASP
1	D	255	ARG
1	D	293	LYS
2	E	65	VAL
2	E	97	VAL
2	E	113	ASP
2	E	120	THR

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Mol	Chain	Res	Type
2	E	144	THR
2	E	145	LEU
2	E	152	VAL
2	E	168	LEU
2	E	181	ILE
2	E	184	ASN
2	E	204	VAL
2	E	207	THR
2	E	209	LYS
2	E	218	VAL
2	E	221	ARG
2	E	303	LYS
2	E	327	GLU
2	E	331	ASP
3	F	45	GLU
3	F	48	LEU
3	F	51	VAL
3	F	55	VAL
3	F	57	THR
3	F	89	THR
3	F	96	LEU
3	F	110	SER
3	F	121	ARG
3	F	137	ARG
3	F	140	SER
3	F	143	SER
3	F	145	LEU
3	F	159	THR
3	F	195	LEU
3	F	197	THR
3	F	199	ASP
3	F	214	ASP
3	F	218	LEU
3	F	222	THR
3	F	232	GLU
3	F	235	SER
3	F	239	THR
3	F	258	THR
3	F	280	TYR
3	F	281	ARG
4	H	54	VAL
4	H	64	LEU

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Mol	Chain	Res	Type
4	H	78	ARG
4	H	83	VAL
4	H	86	THR
4	H	94	LEU
4	H	110	ASP
4	H	111	LEU
4	H	145	LEU
5	I	60	ILE
5	I	63	SER
5	I	107	GLU
5	I	113	ARG
5	I	129	GLN
5	I	134	PHE
5	I	152	MET
5	I	161	VAL
5	I	171	VAL
5	I	197	LEU
6	J	46	ILE
6	J	47	ASN
6	J	57	THR
6	J	68	THR
6	J	69	LYS
6	J	76	ARG
6	J	77	THR
6	J	86	THR
6	J	87	VAL
6	J	137	LEU
6	J	138	SER
7	K	2	SER
7	K	21	LEU
7	K	67	PHE
7	K	78	SER
7	K	81	THR
7	K	101	VAL
7	K	120	THR
7	K	168	ARG
8	L	36	THR
8	L	38	VAL
8	L	42	ASP
8	L	46	LEU
8	L	85	LEU
8	L	105	VAL

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Mol	Chain	Res	Type
8	L	111	ASN
8	L	135	SER
8	L	140	ILE
8	L	143	ASN
9	M	21	ARG
9	M	34	LYS
9	M	39	ARG
9	M	43	ARG
9	M	44	ARG
9	M	84	ASN
9	M	97	SER
9	M	127	VAL
9	M	129	ILE
9	M	132	LEU
9	M	141	VAL
9	M	155	GLU
9	M	156	VAL
9	M	162	LEU
9	M	180	ASP
9	M	182	ARG
9	M	187	VAL
9	M	222	TYR
9	M	244	LEU
9	M	246	ASP
9	M	248	THR
9	M	261	ASP
9	M	267	PHE
9	M	286	THR
10	N	58	LEU
10	N	62	VAL
10	N	73	ARG
10	N	83	THR
10	N	112	SER
10	N	117	ASN
10	N	121	ILE
10	N	124	VAL
10	N	151	VAL
10	N	177	ASP
10	N	191	SER
10	N	217	ARG
10	N	224	LEU
10	N	231	SER

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Mol	Chain	Res	Type
10	N	247	MET
10	N	250	ARG
11	O	17	ARG
11	O	20	LEU
11	O	59	LEU
11	O	67	ASP
11	O	105	THR
11	O	114	SER
11	O	122	VAL
11	O	155	ASP
12	P	42	GLU
12	P	56	LEU
12	P	71	VAL
12	P	75	ARG
12	P	83	VAL
12	P	95	GLU
12	P	107	THR
12	P	120	ARG
12	P	121	ASN
12	P	127	SER
12	P	144	MET
12	P	155	SER
12	P	157	SER
12	P	166	THR
13	Q	86	ARG
13	Q	88	ASP
13	Q	105	VAL
13	Q	113	VAL
13	Q	123	ASP
13	Q	134	LEU
13	Q	141	SER
13	Q	143	ARG
13	Q	150	ILE
13	Q	151	LEU
13	Q	154	VAL
13	Q	155	ILE
13	Q	160	VAL
13	Q	171	VAL
13	Q	174	ILE
13	Q	184	ASP
13	Q	209	GLN
13	Q	215	VAL

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Mol	Chain	Res	Type
13	Q	219	GLU
13	Q	247	LEU
13	Q	265	LEU
13	Q	289	SER
14	R	10	LEU
14	R	11	ARG
14	R	13	ARG
14	R	36	ASN
14	R	66	THR
14	R	67	LEU
14	R	119	LEU
14	R	132	LEU
15	S	54	THR
15	S	70	VAL
15	S	104	ARG
15	S	126	GLU
15	S	133	VAL
15	S	134	LEU
15	S	144	LEU
15	S	164	THR
15	S	182	LYS
15	S	188	THR
15	S	191	THR
15	S	195	ILE
16	T	82	TYR
16	T	83	SER
16	T	84	LYS
16	T	87	MET
16	T	97	MET
16	T	172	CYS
16	T	207	THR
16	T	209	VAL
17	U	19	VAL
17	U	24	PHE
17	U	25	PHE
17	U	28	LEU
17	U	79	ARG
17	U	106	THR
17	U	127	TYR
17	U	131	GLU
17	U	144	ARG
18	V	20	ARG

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Mol	Chain	Res	Type
18	V	28	SER
18	V	47	GLU
18	V	56	LEU
18	V	61	THR
18	V	69	ASP
18	V	85	TRP
18	V	104	TYR
18	V	105	ARG
18	V	107	THR
18	V	120	VAL
18	V	124	ASP
18	V	127	ASP
18	V	144	VAL
18	V	145	ARG
18	V	152	ARG
18	V	169	THR
18	V	180	GLU
18	V	183	LEU
18	V	186	THR
18	V	193	THR
18	V	204	ILE
18	V	207	THR
18	V	208	ARG
19	W	49	ARG
19	W	54	LYS
19	W	57	GLU
19	W	69	THR
19	W	73	PHE
19	W	83	VAL
19	W	88	CYS
19	W	105	VAL
19	W	117	ILE
19	W	129	THR
19	W	141	THR
20	X	10	LEU
20	X	23	ARG
20	X	39	THR
20	X	52	ILE
20	X	56	ASN
20	X	62	VAL
20	X	64	ASP
20	X	75	SER

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Mol	Chain	Res	Type
20	X	101	LEU
20	X	127	VAL
20	X	128	THR
20	X	142	ASP
20	X	152	ASP
20	X	154	CYS
20	X	155	SER
20	X	182	GLU
20	X	208	LEU
20	X	216	ARG
20	X	220	GLU
20	X	243	LEU
21	Y	69	ASP
21	Y	70	ASP
21	Y	77	GLU
21	Y	86	THR
21	Y	97	ASP
21	Y	131	ARG
21	Y	153	LEU
21	Y	158	THR
21	Y	160	GLN
21	Y	172	ILE
21	Y	190	LEU
21	Y	198	ARG
22	Z	70	THR
22	Z	71	ARG
22	Z	74	SER
22	Z	98	GLN
22	Z	110	LEU
22	Z	123	LYS
22	Z	124	LEU
22	Z	142	THR
22	Z	148	GLN
23	0	82	LYS
23	0	84	ARG
23	0	86	THR
23	0	104	LYS
23	0	106	ASN
23	0	108	ASP
23	0	116	LEU
23	0	156	THR
23	0	166	SER

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Mol	Chain	Res	Type
23	0	179	ARG
24	1	34	ARG
24	1	44	LEU
24	1	55	LEU
24	1	58	GLU
25	2	49	ARG
25	2	72	THR
26	3	104	ARG
26	3	112	ASP
26	3	137	THR
26	3	157	LEU
26	3	164	SER
26	3	174	ASP
26	3	183	ARG
26	3	188	VAL
27	5	47	ASP
27	5	55	LEU
27	5	96	HIS
27	5	98	LEU
27	5	100	LYS
27	5	126	THR
27	5	147	ILE
27	5	155	LEU
27	5	162	ARG
27	5	165	GLN
27	5	166	THR
27	5	175	THR
27	5	177	CYS
27	5	182	ASP
27	5	212	THR
27	5	218	LEU
27	5	238	THR
27	5	253	LEU
27	5	262	ILE
27	5	273	VAL
27	5	294	LEU
27	5	295	ASP
27	5	304	LEU
27	5	340	VAL
27	5	344	SER
27	5	351	VAL
27	5	360	ASN

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Mol	Chain	Res	Type
27	5	361	THR
27	5	366	CYS
27	5	370	VAL
27	5	373	LEU
27	5	378	SER
27	5	381	LEU
27	5	404	VAL
27	5	415	LEU
28	6	53	SER
28	6	127	THR
28	6	129	SER
28	6	161	LEU
28	6	163	HIS
28	6	166	THR
28	6	173	LEU
28	6	184	LEU
28	6	215	THR
28	6	219	THR
28	6	222	ASP
28	6	231	GLU
28	6	233	LEU
28	6	235	TRP
28	6	244	ARG
28	6	267	ARG
28	6	268	LEU
28	6	298	PHE
28	6	310	THR
28	6	316	LEU
28	6	323	TRP
28	6	324	ASP
28	6	325	ASP
28	6	328	THR
28	6	334	LEU
28	6	341	VAL
28	6	364	ARG
28	6	371	ASP
28	6	376	THR
29	7	38	THR
29	7	40	LEU
29	7	54	ARG
29	7	57	SER
29	7	67	VAL

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Mol	Chain	Res	Type
29	7	73	THR
29	7	80	VAL
29	7	96	SER
29	7	109	ASP
29	7	114	ASP
29	7	125	ILE
29	7	126	LYS
29	7	143	TRP
29	7	164	VAL
29	7	180	CYS
29	7	209	LEU
29	7	216	PHE
29	7	228	GLU
29	7	294	ILE
29	7	304	VAL
29	7	314	ASP
29	7	319	ARG
30	8	92	LEU
30	8	101	ARG
30	8	104	VAL
30	8	107	THR
30	8	109	GLU
30	8	111	THR
30	8	116	LEU
30	8	134	ASP
30	8	137	ARG
30	8	149	GLU
31	9	19	SER
31	9	25	ARG
31	9	45	THR
31	9	71	LYS
31	9	86	LEU
31	9	122	THR
32	a	42	ASP
32	a	57	THR
32	a	66	ASP
32	a	120	LYS
32	a	122	ARG
33	b	24	GLN
33	b	26	LEU
33	b	30	SER
33	b	35	ARG

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Mol	Chain	Res	Type
33	b	40	SER
33	b	51	VAL
33	b	58	ASN
33	b	62	VAL
33	b	75	VAL
33	b	119	PHE
33	b	122	ASP
33	b	125	SER
33	b	134	THR
33	b	139	THR
33	b	146	ARG
33	b	149	GLN
34	c	51	LEU
34	c	96	CYS
34	c	100	SER
34	c	126	SER
34	c	133	SER
34	c	135	THR
34	c	136	CYS
34	c	158	ASP
34	c	163	GLU
34	c	166	VAL
34	c	203	LEU
34	c	206	SER
34	c	245	LEU
34	c	248	ARG
34	c	280	LEU
34	c	307	PHE
34	c	308	THR
35	d	81	THR
35	d	89	VAL
35	d	127	ASP
35	d	149	HIS
35	d	158	ASP
35	d	162	THR
35	d	164	VAL
35	d	173	THR
35	d	192	SER
35	d	221	THR
35	d	241	ASP
35	d	249	GLU
36	e	55	ARG

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Mol	Chain	Res	Type
36	e	82	SER
36	e	84	TYR
36	e	86	ASP
36	e	87	HIS
36	e	90	ARG
36	e	129	LEU
36	e	138	THR
36	e	143	LYS
36	e	145	ASP
36	e	146	ARG
36	e	151	ARG
36	e	156	ASN
36	e	214	THR
36	e	240	THR
36	e	249	LYS
36	e	251	HIS
36	e	252	HIS
37	f	63	ILE
37	f	88	TYR
37	f	90	VAL
37	f	99	ASP
37	f	113	LEU
37	f	125	TYR
37	f	131	THR
37	f	151	THR
37	f	152	THR
37	f	155	ARG
37	f	160	SER
37	f	169	ILE
37	f	182	VAL
38	g	38	PHE
38	g	43	ASP
38	g	44	GLU
38	g	55	THR
38	g	57	ILE
38	g	89	SER
38	g	108	THR
39	h	73	TYR
39	h	88	ASP
39	h	94	SER
39	h	121	CYS
39	h	141	ASP

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Mol	Chain	Res	Type
39	h	144	SER
39	h	152	LEU
39	h	155	THR
39	h	156	TRP
39	h	157	SER
40	i	32	ILE
40	i	45	ASP
40	i	63	LEU
40	i	65	ASN
40	i	80	LEU
40	i	87	GLU
40	i	98	VAL
40	i	128	ARG
41	j	81	SER
42	k	15	GLN
42	k	30	THR
42	k	45	THR
42	k	49	CYS
42	k	52	ILE
42	k	55	VAL
43	l	115	ARG
44	m	42	ARG
44	m	58	LYS
45	o	28	SER
45	o	29	LEU
45	o	37	ARG
45	o	46	HIS
45	o	59	GLU
45	o	65	VAL
45	o	82	PHE
45	o	90	ASP
45	o	93	ASP
46	p	41	SER
46	p	57	THR
46	p	96	ASN
46	p	107	THR
46	p	125	ASN
46	p	135	LEU
46	p	137	SER
46	p	144	PHE
46	p	149	ASP
47	q	41	ASP

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Mol	Chain	Res	Type
47	q	52	LEU
47	q	68	SER
47	q	71	VAL
47	q	83	ARG
47	q	89	GLU
47	q	95	SER
47	q	96	LEU
47	q	99	MET
47	q	113	LYS
47	q	114	ARG
47	q	117	ARG
48	r	36	ARG
48	r	41	THR
48	r	53	ILE
48	r	54	THR
48	r	70	CYS
48	r	77	LEU
48	r	85	ASP
48	r	132	ARG
48	r	152	THR
48	r	159	VAL
48	r	186	CYS
49	s	48	VAL
49	s	66	TRP
49	s	74	GLU
49	s	81	ARG
49	s	90	LYS
49	s	92	MET
49	s	104	ARG
49	s	112	THR
49	s	116	SER
49	s	177	LEU
49	s	182	SER
49	s	195	LEU
49	s	200	LEU
49	s	229	LEU
49	s	256	SER
49	s	263	THR
49	s	269	ASP
49	s	275	LYS
49	s	284	VAL
49	s	288	THR

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Mol	Chain	Res	Type
49	s	304	ASP
49	s	321	GLU
49	s	353	ARG
49	s	356	VAL
49	s	360	VAL
49	s	361	ILE
49	s	363	ASP
49	s	376	THR
49	s	379	LEU
49	s	406	GLU
49	s	407	ASP
49	s	410	VAL
49	s	415	ASP
49	s	424	PHE
51	u	93	ASP
51	u	104	GLU
51	u	119	ARG
51	u	154	ASP
51	u	166	ASP
51	u	175	MET
51	u	176	VAL
51	u	184	THR
51	u	193	LEU
52	v	5	SER
52	v	9	VAL
52	v	17	LEU
52	v	26	THR
52	v	27	ASP
52	v	63	ASN
52	v	70	ILE
53	w	74	LEU
53	w	81	ASP
53	w	112	SER
53	w	115	GLN
53	w	125	GLU
53	w	126	PHE
53	w	128	PHE
53	w	132	ASP
53	w	136	GLU
53	w	142	GLN
53	w	143	GLU
53	w	148	ILE

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Mol	Chain	Res	Type
53	w	150	ASP
58	C	53	LEU
58	C	78	THR
58	C	95	CYS
58	C	109[A]	ARG
58	C	109[B]	ARG
58	C	113	GLN
58	C	123	GLU
58	C	132	ARG
58	C	133	GLU
58	C	148	THR
58	C	155	LEU
58	C	156	LYS
59	G	134	ASP
59	G	135	LEU
59	G	146	VAL
59	G	148	LEU
59	G	149	LYS
59	G	174	LYS
59	G	180	ARG
59	G	182	VAL
59	G	186	ASP
59	G	202	THR
59	G	203	VAL
59	G	204	MET
59	G	210	LYS
59	G	212	PHE
59	G	217	GLU
59	G	220	LYS
59	G	228	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	235	GLN
2	E	57	ASN
2	E	139	ASN
2	E	231	HIS
3	F	58	HIS
3	F	184	GLN
4	H	104	ASN
4	H	126	GLN

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Mol	Chain	Res	Type
5	I	61	HIS
5	I	101	ASN
7	K	80	HIS
7	K	89	GLN
8	L	43	ASN
8	L	80	GLN
8	L	143	ASN
9	M	114	GLN
11	O	69	ASN
11	O	147	GLN
11	O	150	GLN
12	P	50	ASN
12	P	87	GLN
12	P	97	GLN
13	Q	93	GLN
13	Q	158	GLN
13	Q	172	GLN
13	Q	175	GLN
13	Q	252	GLN
14	R	22	GLN
14	R	30	HIS
14	R	79	HIS
14	R	89	ASN
15	S	140	ASN
16	T	62	GLN
16	T	132	HIS
17	U	4	ASN
17	U	55	ASN
17	U	82	HIS
18	V	92	ASN
20	X	241	GLN
21	Y	147	GLN
21	Y	160	GLN
21	Y	195	ASN
21	Y	225	ASN
22	Z	107	ASN
27	5	96	HIS
27	5	165	GLN
28	6	149	GLN
28	6	320	GLN
28	6	359	HIS
29	7	45	ASN

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Mol	Chain	Res	Type
29	7	55	GLN
29	7	69	HIS
29	7	94	HIS
29	7	247	ASN
29	7	287	GLN
30	8	143	GLN
30	8	177	HIS
32	a	44	ASN
33	b	27	GLN
33	b	129	GLN
34	c	42	GLN
34	c	128	GLN
34	c	155	ASN
34	c	172	ASN
35	d	149	HIS
35	d	217	HIS
36	e	54	GLN
36	e	95	ASN
36	e	198	ASN
36	e	207	ASN
36	e	248	ASN
36	e	251	HIS
36	e	252	HIS
37	f	81	ASN
37	f	153	HIS
39	h	119	GLN
40	i	65	ASN
46	p	163	GLN
47	q	138	GLN
47	q	142	ASN
48	r	112	HIS
48	r	184	ASN
51	u	156	HIS
53	w	142	GLN
58	C	63	GLN
58	C	128	HIS
58	C	139	GLN
59	G	131	ASN
59	G	171	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	A	1443/1559 (92%)	420 (29%)	22 (1%)
55	B	51/73 (69%)	23 (45%)	1 (1%)
56	24	73/73 (100%)	37 (50%)	1 (1%)
All	All	1567/1705 (91%)	480 (30%)	24 (1%)

All (480) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
54	A	1674	A
54	A	1676	A
54	A	1677	C
54	A	1678	C
54	A	1679	U
54	A	1680	A
54	A	1681	G
54	A	1685	C
54	A	1686	A
54	A	1689	C
54	A	1690	C
54	A	1691	C
54	A	1699	C
54	A	1700	U
54	A	1701	U
54	A	1703	C
54	A	1704	U
54	A	1708	A
54	A	1713	A
54	A	1714	C
54	A	1715	C
54	A	1724	A
54	A	1727	A
54	A	1728	U
54	A	1748	G
54	A	1750	G
54	A	1751	A
54	A	1760	G
54	A	1768	G
54	A	1769	C
54	A	1770	G
54	A	1773	A
54	A	1777	A
54	A	1780	U
54	A	1791	G

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Mol	Chain	Res	Type
54	A	1794	A
54	A	1797	G
54	A	1803	A
54	A	1804	A
54	A	1805	A
54	A	1812	C
54	A	1813	C
54	A	1817	C
54	A	1821	A
54	A	1823	A
54	A	1824	U
54	A	1827	C
54	A	1828	A
54	A	1829	A
54	A	1832	A
54	A	1836	A
54	A	1839	C
54	A	1844	A
54	A	1849	C
54	A	1852	C
54	A	1854	U
54	A	1856	A
54	A	1867	A
54	A	1869	A
54	A	1870	A
54	A	1872	U
54	A	1878	U
54	A	1882	A
54	A	1883	G
54	A	1887	A
54	A	1888	G
54	A	1890	C
54	A	1892	A
54	A	1893	A
54	A	1901	C
54	A	1903	C
54	A	1905	C
54	A	1909	A
54	A	1918	G
54	A	1927	G
54	A	1939	G
54	A	1940	A

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Mol	Chain	Res	Type
54	A	1944	C
54	A	1968	G
54	A	1972	A
54	A	1973	G
54	A	1974	A
54	A	1985	G
54	A	1987	G
54	A	1992	C
54	A	1993	A
54	A	1994	A
54	A	1995	A
54	A	1999	A
54	A	2000	C
54	A	2001	C
54	A	2015	G
54	A	2021	U
54	A	2022	G
54	A	2029	A
54	A	2030	U
54	A	2031	A
54	A	2032	G
54	A	2033	A
54	A	2034	A
54	A	2036	C
54	A	2037	U
54	A	2039	A
54	A	2044	A
54	A	2053	U
54	A	2060	A
54	A	2065	A
54	A	2074	A
54	A	2079	C
54	A	2083	U
54	A	2085	A
54	A	2096	U
54	A	2097	A
54	A	2098	G
54	A	2105	G
54	A	2109	A
54	A	2110	A
54	A	2113	G
54	A	2124	A

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Mol	Chain	Res	Type
54	A	2125	C
54	A	2126	U
54	A	2132	A
54	A	2136	C
54	A	2141	U
54	A	2142	A
54	A	2147	G
54	A	2154	A
54	A	2157	U
54	A	2159	U
54	A	2168	U
54	A	2171	U
54	A	2172	A
54	A	2173	G
54	A	2174	G
54	A	2180	A
54	A	2181	A
54	A	2182	G
54	A	2183	C
54	A	2187	C
54	A	2193	U
54	A	2195	A
54	A	2197	G
54	A	2198	A
54	A	2199	A
54	A	2200	A
54	A	2207	A
54	A	2209	G
54	A	2210	C
54	A	2215	C
54	A	2217	C
54	A	2230	A
54	A	2233	U
54	A	2237	A
54	A	2239	A
54	A	2241	A
54	A	2242	U
54	A	2243	A
54	A	2244	U
54	A	2245	A
54	A	2246	A
54	A	2247	C

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Mol	Chain	Res	Type
54	A	2257	C
54	A	2260	A
54	A	2262	C
54	A	2263	C
54	A	2269	G
54	A	2271	C
54	A	2280	C
54	A	2284	C
54	A	2287	U
54	A	2290	A
54	A	2291	A
54	A	2297	A
54	A	2299	U
54	A	2300	G
54	A	2309	A
54	A	2315	A
54	A	2316	U
54	A	2322	C
54	A	2323	A
54	A	2324	U
54	A	2330	U
54	A	2332	C
54	A	2345	G
54	A	2371	U
54	A	2372	U
54	A	2374	A
54	A	2381	A
54	A	2386	C
54	A	2387	U
54	A	2388	A
54	A	2390	A
54	A	2393	C
54	A	2396	C
54	A	2397	C
54	A	2401	A
54	A	2405	C
54	A	2406	A
54	A	2407	U
54	A	2414	C
54	A	2415	C
54	A	2416	U
54	A	2417	C

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Mol	Chain	Res	Type
54	A	2426	C
54	A	2427	C
54	A	2434	A
54	A	2435	G
54	A	2443	C
54	A	2444	A
54	A	2446	A
54	A	2451	A
54	A	2452	A
54	A	2458	A
54	A	2464	G
54	A	2469	A
54	A	2471	G
54	A	2478	G
54	A	2484	C
54	A	2488	C
54	A	2493	C
54	A	2500	A
54	A	2502	C
54	A	2506	A
54	A	2507	A
54	A	2508	C
54	A	2511	C
54	A	2512	A
54	A	2520	C
54	A	2521	A
54	A	2523	C
54	A	2526	C
54	A	2527	A
54	A	2530	A
54	A	2531	U
54	A	2536	G
54	A	2540	C
54	A	2544	C
54	A	2551	G
54	A	2552	U
54	A	2557	C
54	A	2558	A
54	A	2559	U
54	A	2563	U
54	A	2564	A
54	A	2570	C

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Mol	Chain	Res	Type
54	A	2571	G
54	A	2575	U
54	A	2576	A
54	A	2577	C
54	A	2578	C
54	A	2579	C
54	A	2580	U
54	A	2581	A
54	A	2582	A
54	A	2583	C
54	A	2584	C
54	A	2586	U
54	A	2592	G
54	A	2593	G
54	A	2594	U
54	A	2601	A
54	A	2603	C
54	A	2607	U
54	A	2618	U
54	A	2626	U
54	A	2627	G
54	A	2628	U
54	A	2629	A
54	A	2630	U
54	A	2632	A
54	A	2633	A
54	A	2634	U
54	A	2635	G
54	A	2640	C
54	A	2642	C
54	A	2644	A
54	A	2645	G
54	A	2647	G
54	A	2654	U
54	A	2655	G
54	A	2656	U
54	A	2660	U
54	A	2683	C
54	A	2684	C
54	A	2686	G
54	A	2693	A
54	A	2694	A

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Mol	Chain	Res	Type
54	A	2695	G
54	A	2696	A
54	A	2697	G
54	A	2698	G
54	A	2706	A
54	A	2708	C
54	A	2709	A
54	A	2718	C
54	A	2719	G
54	A	2723	A
54	A	2724	G
54	A	2725	A
54	A	2732	G
54	A	2733	G
54	A	2740	A
54	A	2743	U
54	A	2744	U
54	A	2745	A
54	A	2747	U
54	A	2749	A
54	A	2752	C
54	A	2754	A
54	A	2755	A
54	A	2756	C
54	A	2801	A
54	A	2804	A
54	A	2810	G
54	A	2814	G
54	A	2831	G
54	A	2832	A
54	A	2833	A
54	A	2844	G
54	A	2847	C
54	A	2851	A
54	A	2852	C
54	A	2854	U
54	A	2860	G
54	A	2861	A
54	A	2864	U
54	A	2865	C
54	A	2871	U
54	A	2880	A

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Mol	Chain	Res	Type
54	A	2891	C
54	A	2896	G
54	A	2901	A
54	A	2906	C
54	A	2910	A
54	A	2911	C
54	A	2913	A
54	A	2917	G
54	A	2918	A
54	A	2919	A
54	A	2922	A
54	A	2926	A
54	A	2928	C
54	A	2932	G
54	A	2935	A
54	A	2952	U
54	A	2955	U
54	A	2956	A
54	A	2958	A
54	A	2963	A
54	A	2965	A
54	A	2977	G
54	A	2978	U
54	A	2985	C
54	A	2989	G
54	A	2990	A
54	A	2991	U
54	A	2992	G
54	A	2993	U
54	A	2994	U
54	A	3000	A
54	A	3005	A
54	A	3012	U
54	A	3016	G
54	A	3022	G
54	A	3030	A
54	A	3041	U
54	A	3042	U
54	A	3049	U
54	A	3051	A
54	A	3053	A
54	A	3054	G

Continued on next page...

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Mol	Chain	Res	Type
54	A	3056	C
54	A	3060	C
54	A	3063	G
54	A	3069	A
54	A	3072	U
54	A	3077	C
54	A	3084	A
54	A	3086	U
54	A	3089	A
54	A	3090	G
54	A	3092	U
54	A	3093	C
54	A	3096	U
54	A	3098	U
54	A	3099	C
54	A	3100	U
54	A	3102	U
54	A	3108	U
54	A	3109	U
54	A	3114	U
54	A	3122	U
54	A	3123	G
54	A	3129	A
54	A	3131	G
54	A	3135	A
54	A	3141	A
54	A	3150	U
54	A	3151	A
54	A	3155	C
54	A	3157	C
54	A	3158	A
54	A	3160	A
54	A	3162	C
54	A	3168	C
54	A	3169	C
54	A	3172	C
54	A	3173	G
54	A	3180	A
54	A	3182	A
54	A	3189	C
54	A	3190	A
54	A	3196	G

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Mol	Chain	Res	Type
54	A	3202	U
54	A	3206	C
54	A	3207	A
54	A	3213	A
54	A	3217	A
54	A	3218	A
54	A	3220	A
55	B	1607	U
55	B	1608	G
55	B	1609	U
55	B	1611	G
55	B	1614	U
55	B	1615	A
55	B	1622	A
55	B	1625	A
55	B	1628	C
55	B	1631	C
55	B	1632	U
55	B	1633	U
55	B	1634	A
55	B	1641	G
55	B	1643	A
55	B	1644	G
55	B	1645	A
55	B	1646	U
55	B	1650	A
55	B	1651	A
55	B	1661	A
55	B	1667	C
55	B	1669	G
56	24	2	U
56	24	3	U
56	24	4	A
56	24	7	G
56	24	9	A
56	24	10	G
56	24	13	U
56	24	14	A
56	24	16	A
56	24	17	U
56	24	18	U
56	24	19	A

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Mol	Chain	Res	Type
56	24	20	U
56	24	21	C
56	24	22	A
56	24	27	A
56	24	31	C
56	24	36	A
56	24	40	U
56	24	41	G
56	24	45	A
56	24	46	G
56	24	48	U
56	24	50	A
56	24	51	G
56	24	52	C
56	24	54	U
56	24	55	C
56	24	56	A
56	24	57	C
56	24	58	A
56	24	59	G
56	24	60	C
56	24	62	C
56	24	63	C
56	24	64	A
56	24	68	A

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	A	1703	C
54	A	1811	A
54	A	1823	A
54	A	1871	A
54	A	2021	U
54	A	2030	U
54	A	2125	C
54	A	2182	G
54	A	2186	C
54	A	2243	A
54	A	2245	A
54	A	2457	A
54	A	2507	A

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Mol	Chain	Res	Type
54	A	2530	A
54	A	2606	U
54	A	2653	C
54	A	2905	A
54	A	2910	A
54	A	2989	G
54	A	3041	U
54	A	3092	U
54	A	3113	A
55	B	1607	U
56	24	1	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
58	MEQ	C	73	58	8,9,10	0.96	1 (12%)	5,10,12	0.73	0

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
58	MEQ	C	73	58	-	4/8/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	C	73	MEQ	CE-NE2	-2.01	1.42	1.45

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	C	73	MEQ	C-CA-CB-CG
58	C	73	MEQ	CG-CD-NE2-CE
58	C	73	MEQ	OE1-CD-NE2-CE
58	C	73	MEQ	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 95 ligands modelled in this entry, 94 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	$\#\|Z\| > 2$
62	PNS	v	101	53	13,20,21	2.43	4 (30%)	18,26,29	1.88	5 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PNS	v	101	53	-	9/24/26/27	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	v	101	PNS	C39-N41	5.39	1.45	1.33
62	v	101	PNS	C34-N36	5.37	1.45	1.33
62	v	101	PNS	O40-C39	-2.80	1.17	1.23
62	v	101	PNS	O35-C34	-2.16	1.19	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	v	101	PNS	C37-N36-C34	-4.06	115.34	122.59
62	v	101	PNS	C38-C39-N41	3.57	122.42	116.42
62	v	101	PNS	C31-C29-C32	3.26	114.47	108.82
62	v	101	PNS	C32-C34-N36	2.30	121.16	116.58
62	v	101	PNS	O40-C39-C38	-2.08	118.21	122.02

There are no chirality outliers.

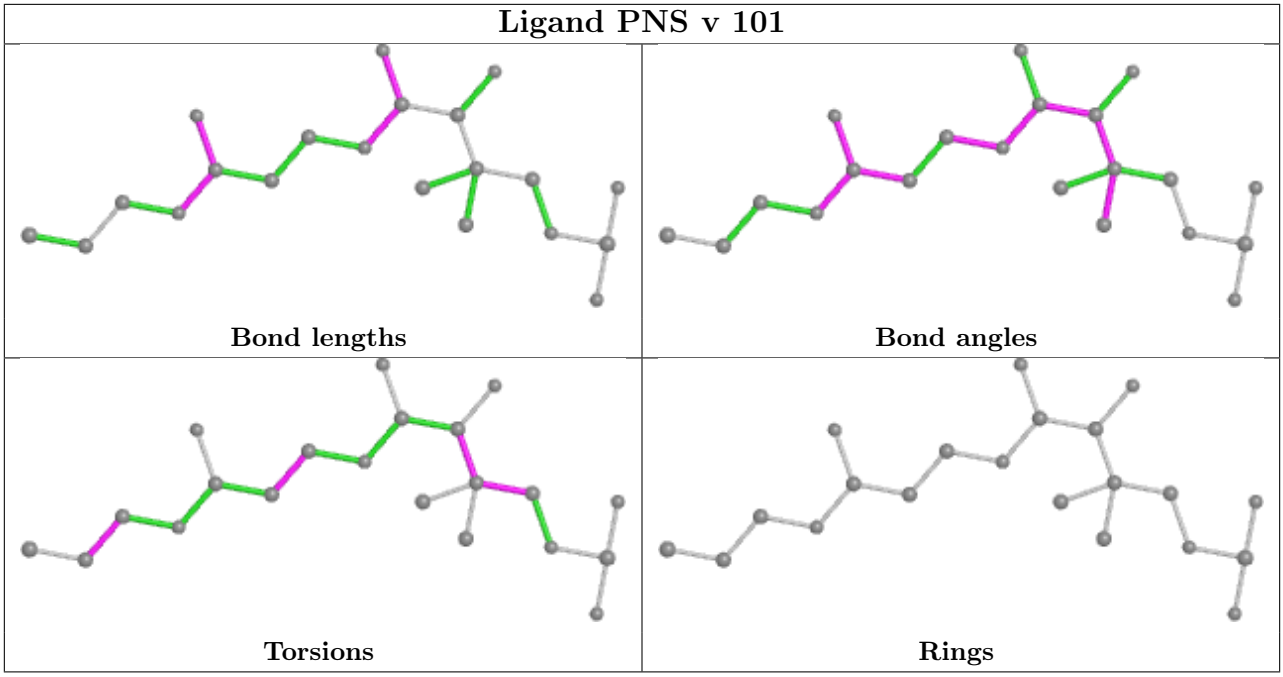
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	v	101	PNS	C28-C29-C32-O33
62	v	101	PNS	C28-C29-C32-C34
62	v	101	PNS	C30-C29-C32-O33
62	v	101	PNS	C30-C29-C32-C34
62	v	101	PNS	C31-C29-C32-O33
62	v	101	PNS	C31-C29-C32-C34
62	v	101	PNS	N41-C42-C43-S44
62	v	101	PNS	N36-C37-C38-C39
62	v	101	PNS	O27-C28-C29-C30

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.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	U	1
28	6	1
16	T	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	124:ASP	C	125:ASP	N	3.71
1	6	28:ARG	C	29:THR	N	1.18
1	T	58:VAL	C	59:TYR	N	1.14

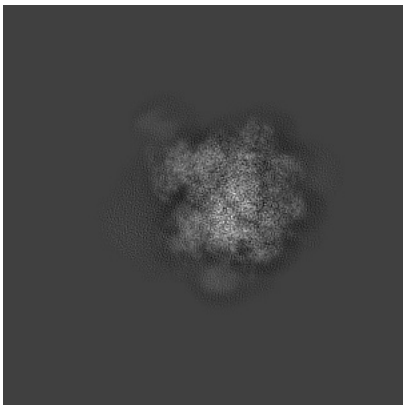
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11643. These allow visual inspection of the internal detail of the map and identification of artifacts.

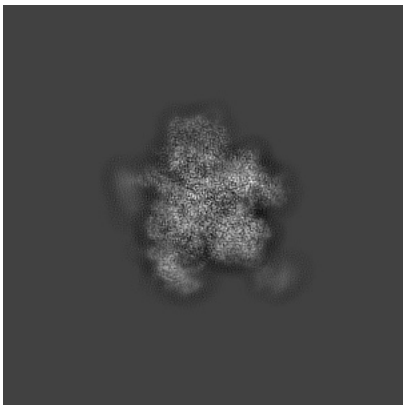
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

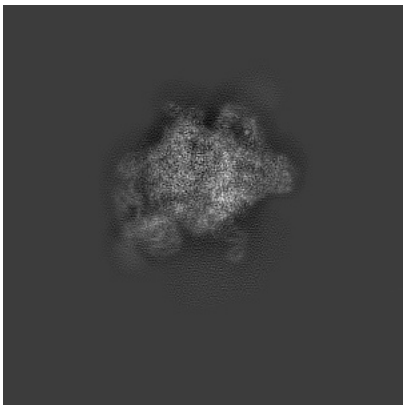
6.1.1 Primary map



X

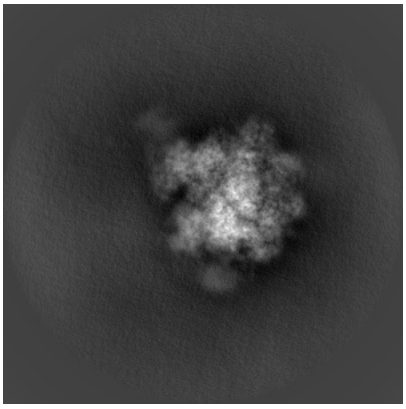


Y

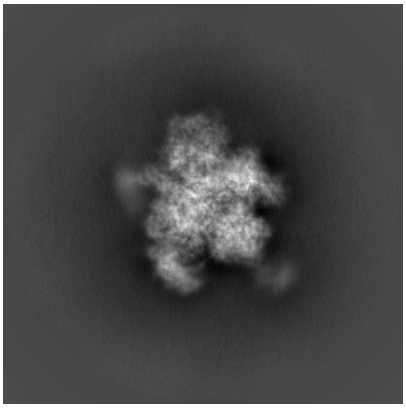


Z

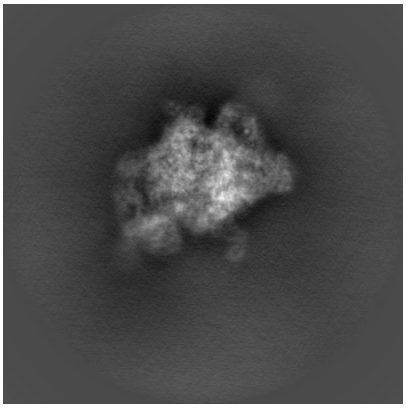
6.1.2 Raw map



X



Y

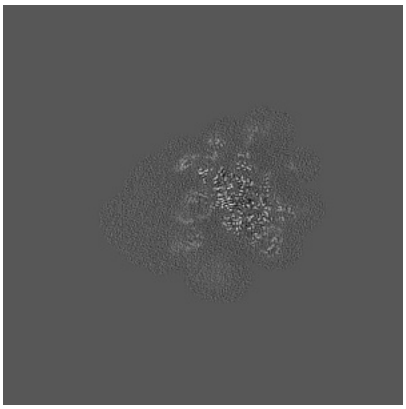


Z

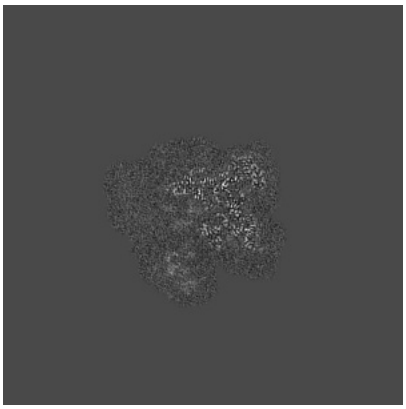
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

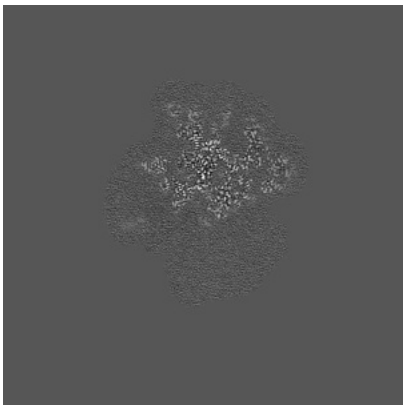
6.2.1 Primary map



X Index: 256

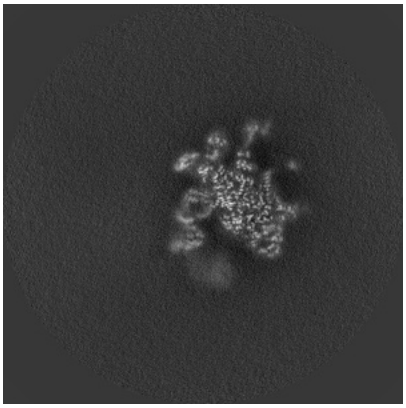


Y Index: 256

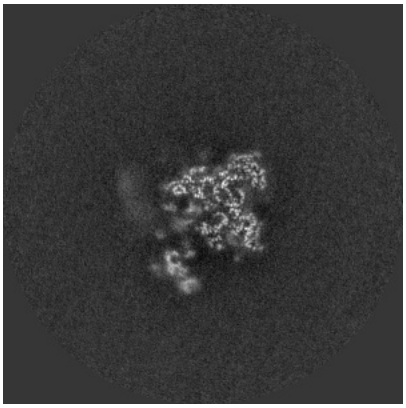


Z Index: 256

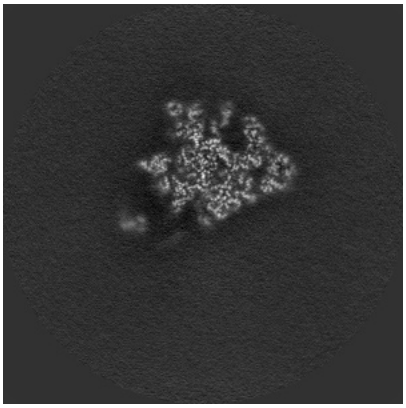
6.2.2 Raw map



X Index: 256



Y Index: 256

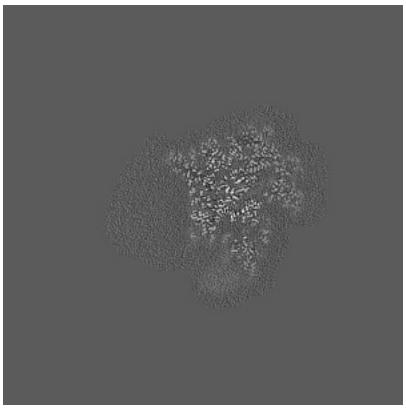


Z Index: 256

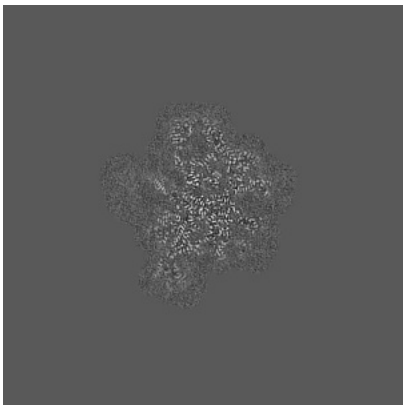
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

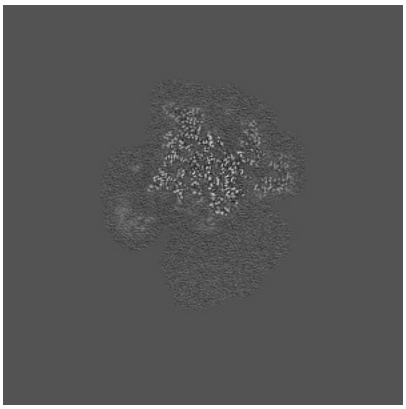
6.3.1 Primary map



X Index: 284

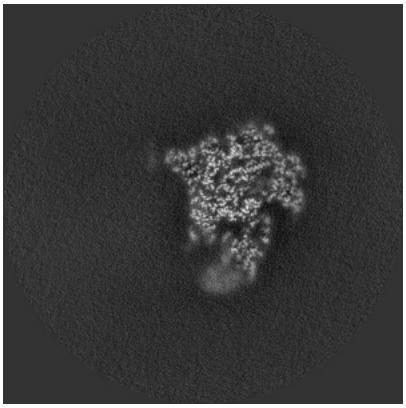


Y Index: 293

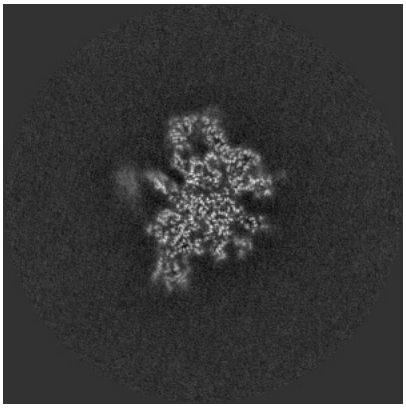


Z Index: 246

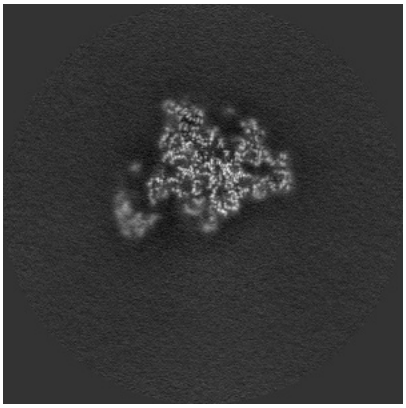
6.3.2 Raw map



X Index: 285



Y Index: 293



Z Index: 243

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.11. 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.

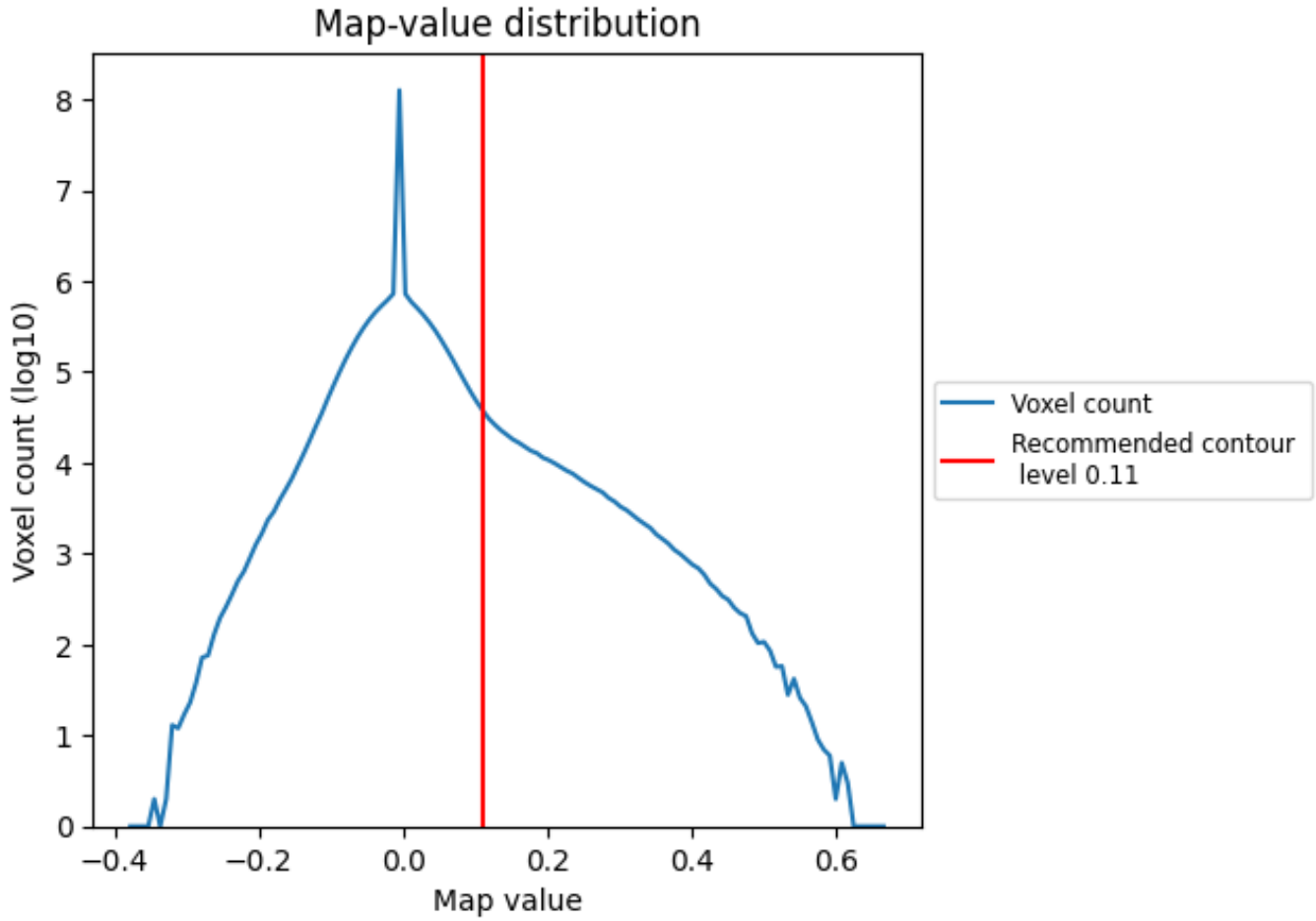
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

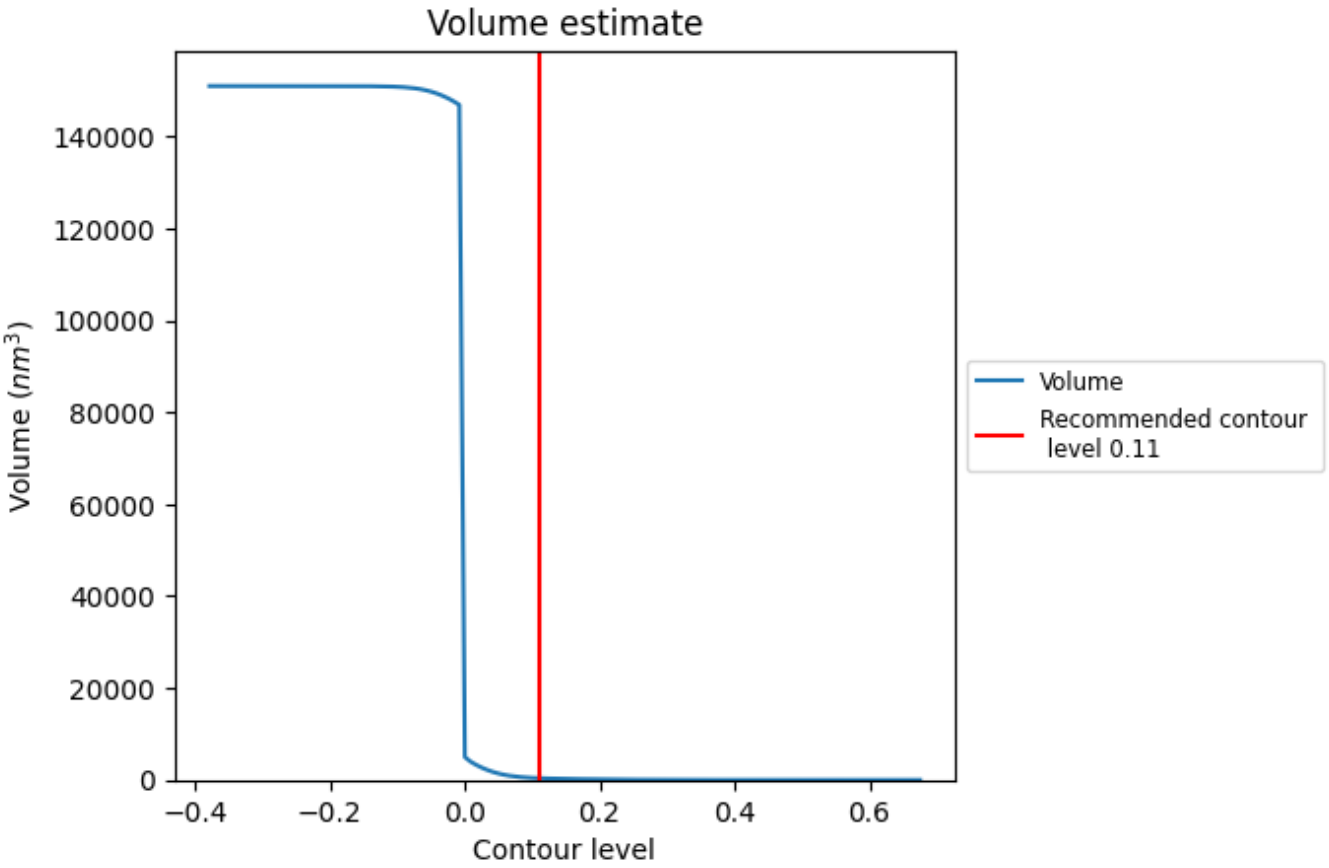
This section contains the results of statistical analysis of the map.

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.

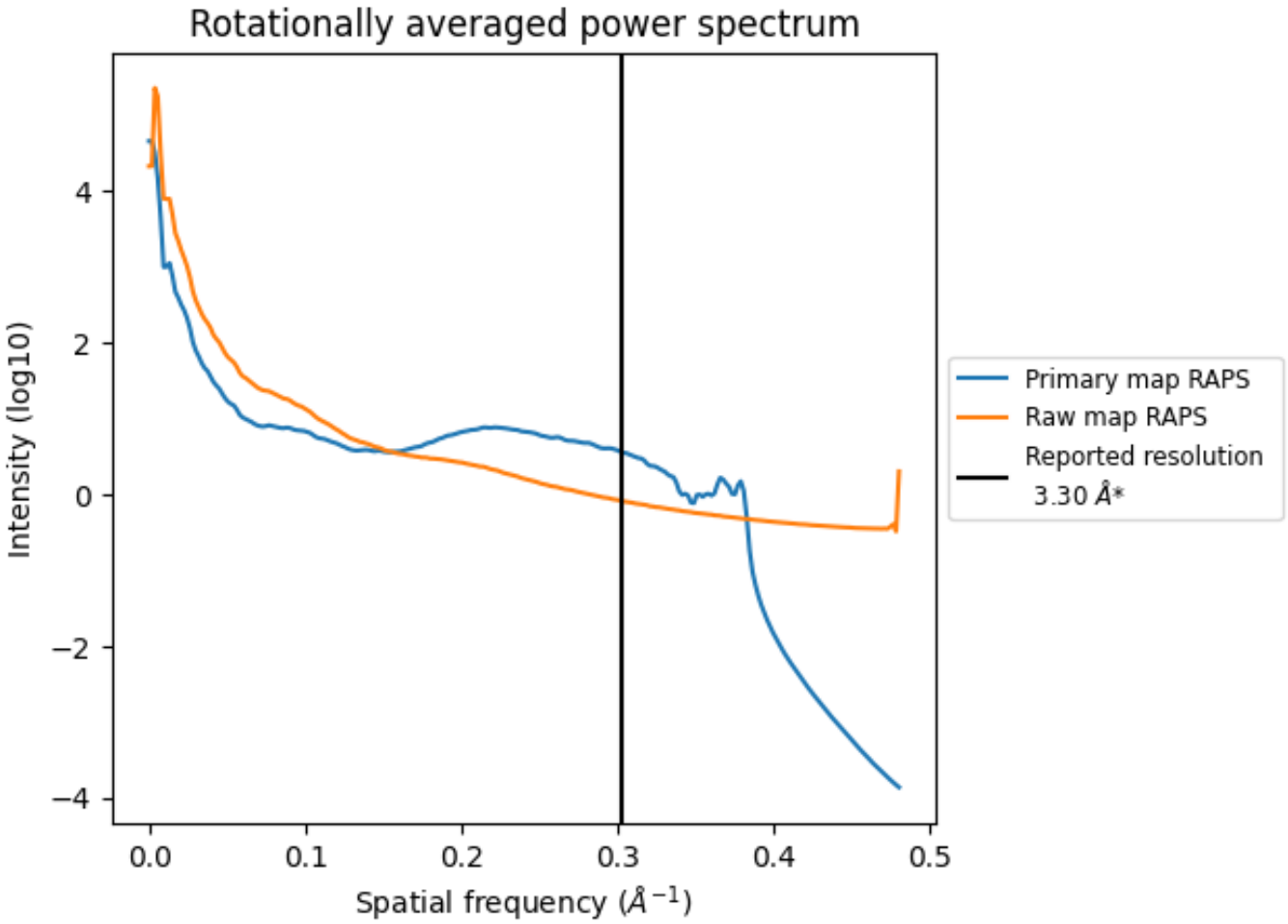
7.2 Volume estimate



The volume at the recommended contour level is 383 nm^3; this corresponds to an approximate mass of 346 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 (i)

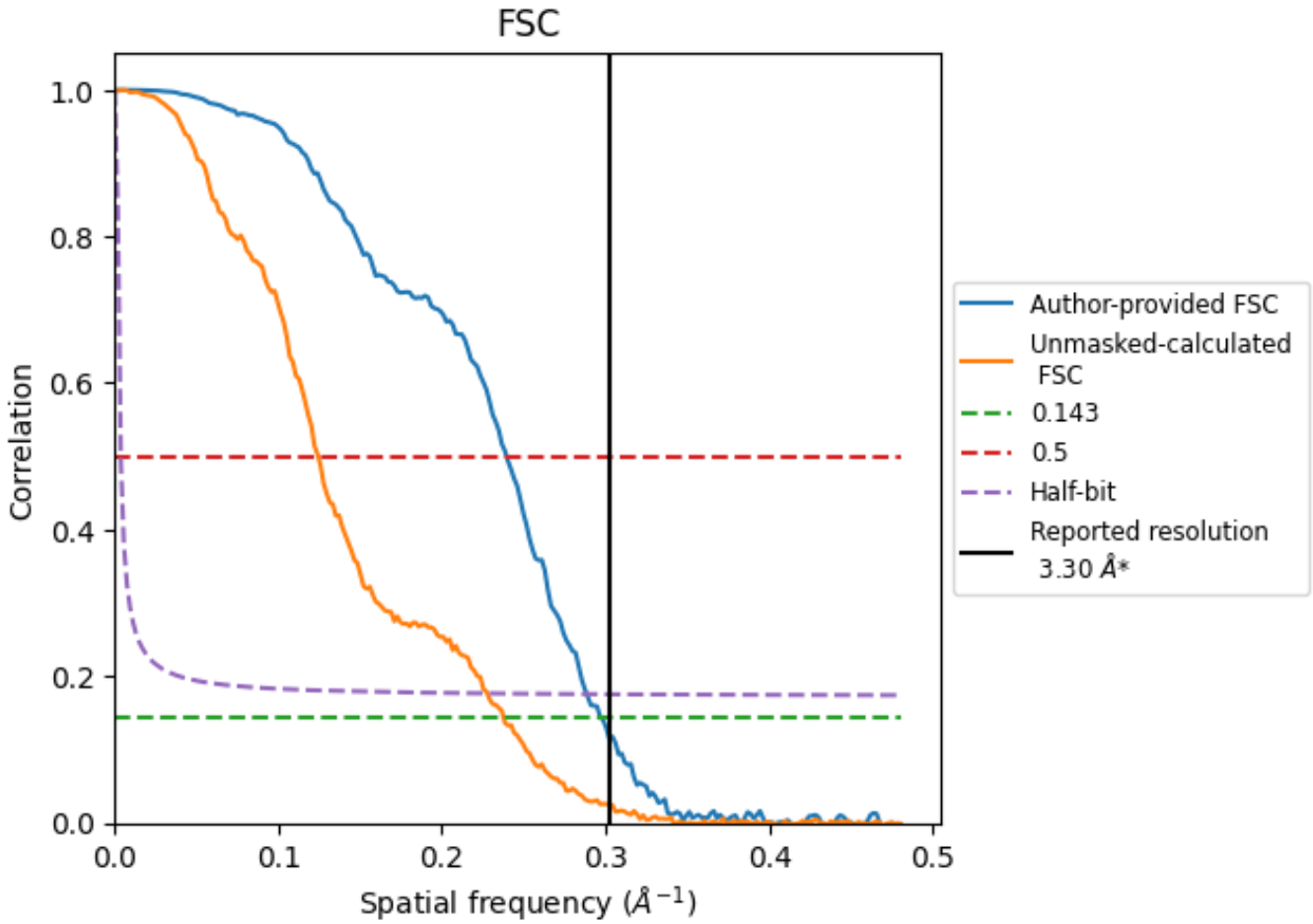


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

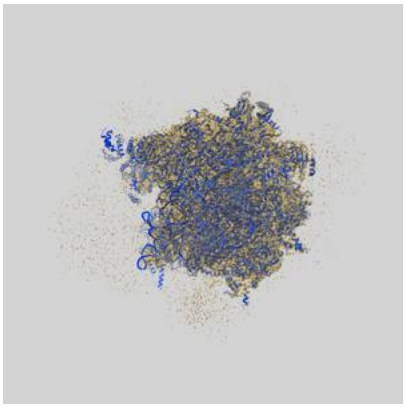
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.36	4.18	3.47
Unmasked-calculated*	4.21	8.05	4.39

*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 4.21 differs from the reported value 3.3 by more than 10 %

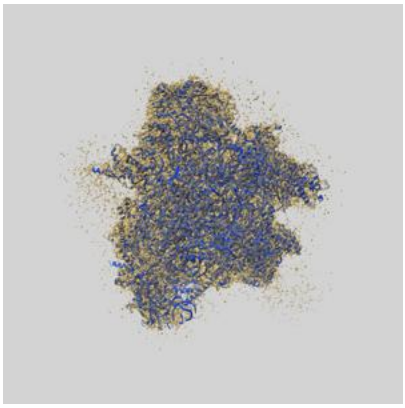
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11643 and PDB model 7A5H. Per-residue inclusion information can be found in section 3 on page 16.

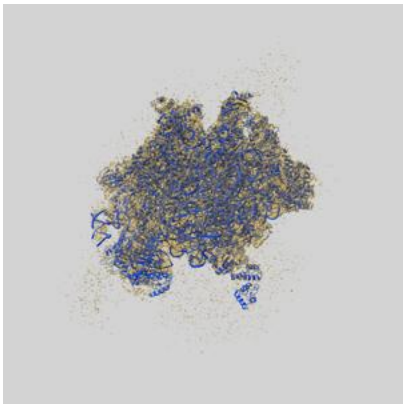
9.1 Map-model overlay



X



Y



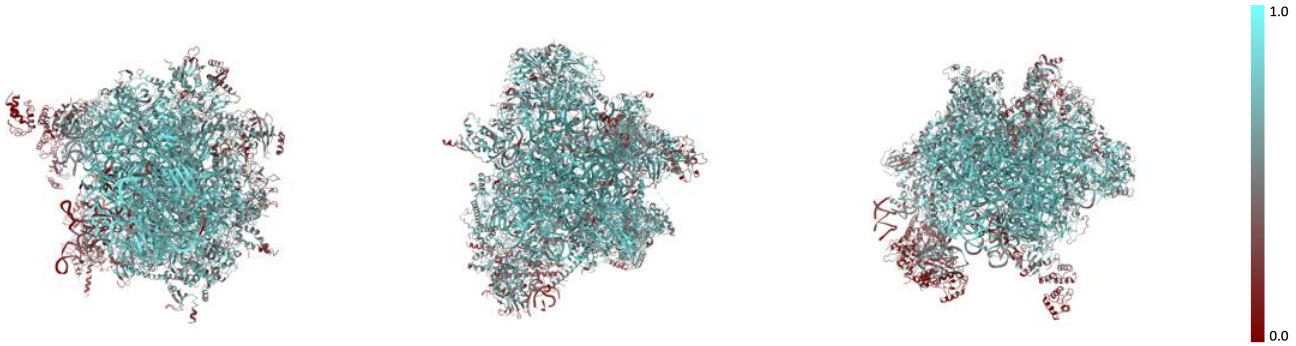
Z

The images above show the 3D surface view of the map at the recommended contour level 0.11 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

This section was not generated.

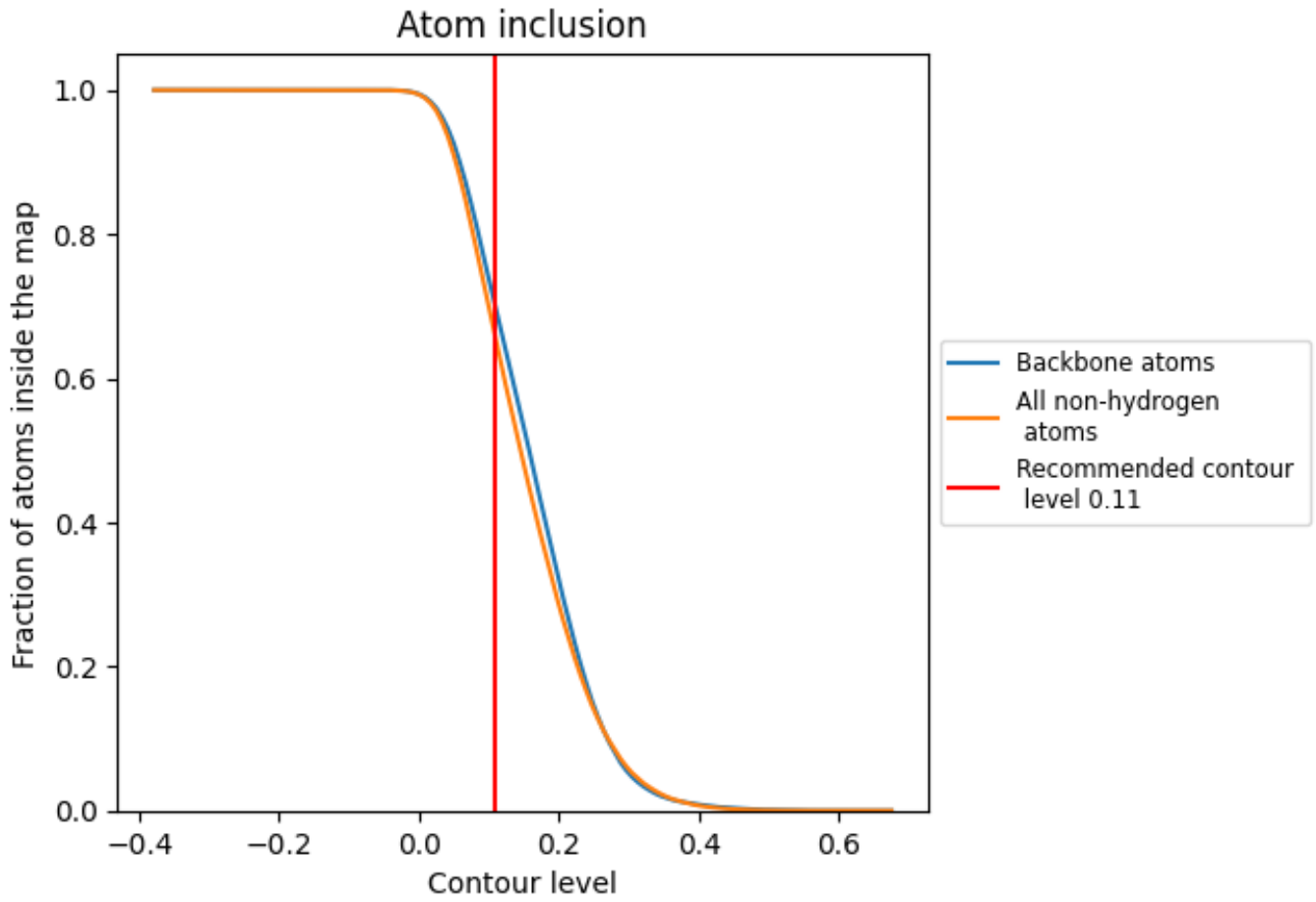
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.11).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 65% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.6530
0	0.6354
1	0.6476
2	0.8262
24	0.1939
3	0.7895
5	0.6453
6	0.5386
7	0.5052
8	0.1424
9	0.6121
A	0.8363
B	0.3871
C	0.3123
D	0.7186
E	0.7118
F	0.7101
G	0.3443
H	0.5317
I	0.3493
J	0.1800
K	0.7509
L	0.6889
M	0.7257
N	0.6970
O	0.7350
P	0.6258
Q	0.6394
R	0.7599
S	0.7226
T	0.7106
U	0.6158
V	0.4917
W	0.7476
X	0.6307

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Chain	Atom inclusion
Y	0.6853
Y2	0.1083
Z	0.7375
a	0.6842
b	0.7267
c	0.6196
d	0.4407
e	0.0626
f	0.2608
g	0.6852
h	0.4981
i	0.7686
j	0.6475
k	0.3736
l	0.5097
m	0.1331
o	0.7608
p	0.5088
q	0.4952
r	0.7203
s	0.6889
t	0.1429
u	0.4298
v	0.2289
w	0.0474