wwPDB EM Validation Summary Report

Dec 12, 2022 – 10:19 am GMT

PDB ID	:	6YWS
EMDB ID	:	EMD-10973
Title	:	The structure of the large subunit of the mitoribosome from Neurospora crassa
Authors	:	Amunts, A.; Itoh, Y.; Naschberger, A.
Deposited on	:	2020-04-30
Resolution	:	2.74 Å(reported)

This is a wwPDB EM Validation Summary 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:

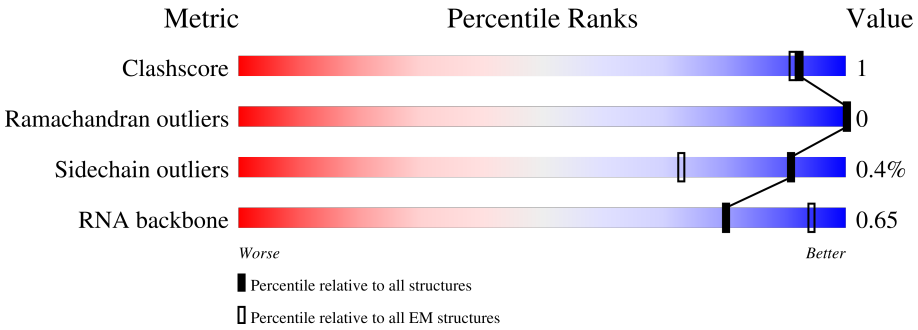
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.74 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	A	3464	6% 68% 12% · 19%
2	B	383	7% 83% · 15%
3	C	384	· 77% · 20%
4	D	325	· 75% · 22%
5	E	352	85% · 12%
6	F	255	· 76% · 21%
7	G	300	· 24% 75%

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Mol	Chain	Length	Quality of chain
8	f	347	70% 29%
9	g	158	93% 7%
10	H	183	92% 8%
11	I	131	87% 9%
12	J	312	76% 22%
13	K	249	62% 5% 33%
14	L	193	93% 6%
15	M	258	6% 72% 25%
16	N	217	58% 39%
17	O	364	9% 71% 25%
18	P	228	76% 21%
19	Q	396	86% 11%
20	R	447	12% 55% 40%
21	S	274	5% 62% 35%
22	T	263	65% 32%
23	U	161	84% 14%
24	V	219	26% 74%
25	W	129	41% 5% 54%
26	X	59	73% 8% 19%
27	Y	140	30% 67%
28	0	124	36% 63%
29	1	449	77% 18%
30	2	370	31% 67%
31	3	103	88% 8%
32	4	138	95%

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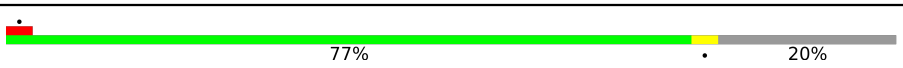
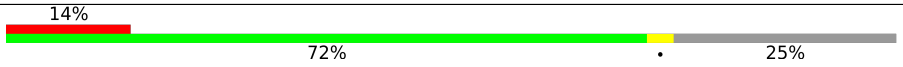
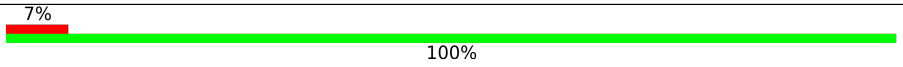
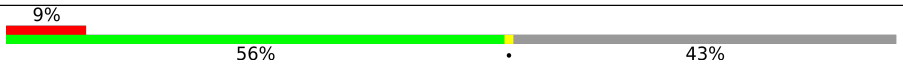
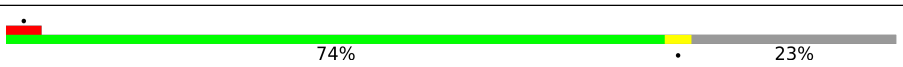
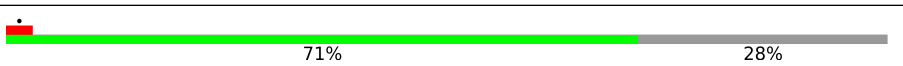
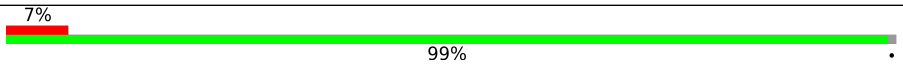
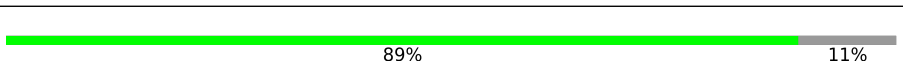
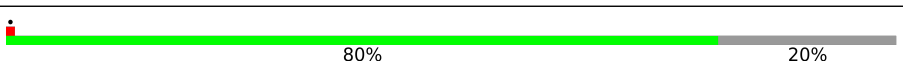
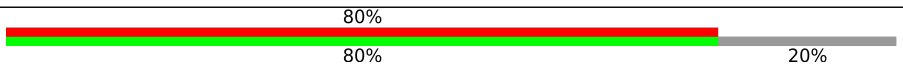
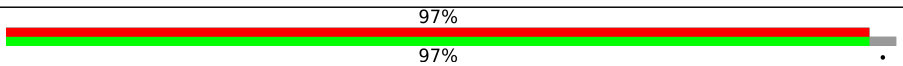
Mol	Chain	Length	Quality of chain
33	5	439	
34	6	368	
35	7	165	
36	8	443	
37	h	98	
38	i	218	
39	9	267	
40	a	225	
41	b	162	
42	c	110	
43	d	292	
44	e	303	
45	j	201	

2 Entry composition (i)

There are 50 unique types of molecules in this entry. The entry contains 223401 atoms, of which 97522 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 RNA chain called RNA (2820-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	2820	90332	26969	30189	10787	19567	2820	0	0

- Molecule 2 is a protein called 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	326	5136	1578	2592	515	436	15	0	0

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	307	4758	1468	2422	447	413	8	0	0

- Molecule 4 is a protein called 60S ribosomal protein L4, variant.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	254	4068	1280	2040	372	371	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	309	4910	1558	2461	436	443	12	0	0

- Molecule 6 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	201	3253	1022	1645	290	288	8	0	0

- Molecule 7 is a protein called RIBOSOMAL_L9 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	74	Total	C	H	N	O	S	0	0
			1245	390	627	121	104	3		

- Molecule 8 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	f	245	Total	C	H	N	O	S	0	0
			3801	1202	1925	325	346	3		

- Molecule 9 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	g	147	Total	C	H	N	O	S	0	0
			2257	700	1154	203	196	4		

- Molecule 10 is a protein called Ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	H	183	Total	C	H	N	O	S	0	0
			2885	899	1459	268	251	8		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	I	119	Total	C	H	N	O	S	0	0
			1898	564	985	182	159	8		

- Molecule 12 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	J	243	Total	C	H	N	O	S	0	0
			3827	1198	1939	346	343	1		

- Molecule 13 is a protein called 60S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	K	168	Total	C	H	N	O	S	0	0
			2751	850	1401	263	231	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	L	192	Total	C	H	N	O	S	0	0
			3135	960	1590	294	285	6		

- Molecule 15 is a protein called Mitochondrial ribosomal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	M	194	Total	C	H	N	O	S	0	0
			3164	981	1628	292	253	10		

- Molecule 16 is a protein called Aconitate hydratase.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	N	133	Total	C	H	N	O	S	0	0
			2176	673	1120	195	182	6		

- Molecule 17 is a protein called Mitochondrial large ribosomal subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	O	272	Total	C	H	N	O	S	0	0
			4532	1392	2323	424	387	6		

- Molecule 18 is a protein called Mitochondrial ribosomal protein subunit L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	P	180	Total	C	H	N	O	S	0	0
			2975	953	1494	270	254	4		

- Molecule 19 is a protein called KOW domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	Q	353	Total	C	H	N	O	S	0	0
			5829	1786	2961	547	524	11		

- Molecule 20 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	R	266	Total	C	H	N	O	S	0	0
			4499	1374	2310	441	370	4		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	S	179	Total	C	H	N	O	S	0	0
			2979	937	1507	281	252	2		

- Molecule 22 is a protein called 54S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	T	180	Total	C	H	N	O	S	0	0
			2950	937	1453	279	278	3		

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	U	138	Total	C	H	N	O	S	0	0
			2263	698	1164	213	185	3		

- Molecule 24 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	V	58	Total	C	H	N	O	S	0	0
			951	300	477	88	85	1		

- Molecule 25 is a protein called Mitochondrial ribosomal protein subunit L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	W	59	Total	C	H	N	O	S	0	0
			949	282	489	98	72	8		

- Molecule 26 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	X	48	Total	C	H	N	O	S	0	0
			836	263	433	71	65	4		

- Molecule 27 is a protein called Related to ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Y	46	Total	C	H	N	O	S	0	0
			777	224	412	84	56	1		

- Molecule 28 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	0	46	Total	C	H	N	O	S	0	0
			797	240	409	86	58	4		

- Molecule 29 is a protein called Mitochondrial large ribosomal subunit YmL35.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	1	367	Total	C	H	N	O	S	0	0
			6014	1899	3029	547	531	8		

- Molecule 30 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	2	123	Total	C	H	N	O	S	0	0
			2101	660	1055	211	171	4		

- Molecule 31 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	3	95	Total	C	H	N	O	S	0	0
			1536	489	773	135	137	2		

- Molecule 32 is a protein called Mitochondrial ribosomal protein L43.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	4	137	Total	C	H	N	O	S	0	0
			2139	671	1087	192	183	6		

- Molecule 33 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	5	350	Total	C	H	N	O	S	0	0
			5429	1740	2710	477	493	9		

- Molecule 34 is a protein called 50S ribosomal subunit L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	6	273	Total	C	H	N	O	S	0	0
			4474	1418	2248	399	401	8		

- Molecule 35 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	7	84	Total	C	H	N	O	0	0
			1383	431	709	130	113		

- Molecule 36 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	8	331	Total	C	H	N	O	S	0	0
			5374	1683	2714	480	489	8		

- Molecule 37 is a protein called Mitochondrial ribosomal protein L44.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	h	98	Total	C	H	N	O	S	0	0
			1577	490	798	139	146	4		

- Molecule 38 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	i	124	Total	C	H	N	O	S	0	0
			1998	613	1022	181	177	5		

- Molecule 39 is a protein called RNase III domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	9	206	Total	C	H	N	O	S	0	0
			3341	1051	1698	295	290	7		

- Molecule 40 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	a	161	Total	C	H	N	O	S	0	0
			2671	837	1340	253	235	6		

- Molecule 41 is a protein called Mitoc_mL59 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	b	161	Total	C	H	N	O	S	0	0
			2693	840	1379	249	221	4		

- Molecule 42 is a protein called 54S ribosomal protein L31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	c	98	Total	C	H	N	O	S	0	0
			1700	528	873	162	134	3		

- Molecule 43 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	d	235	Total	C	H	N	O	S	0	0
			3797	1180	1909	363	339	6		

- Molecule 44 is a protein called 60S ribosomal protein L1.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	e	242	Total	C	H	N	O	S	0	0
			3821	1189	1935	332	353	12		

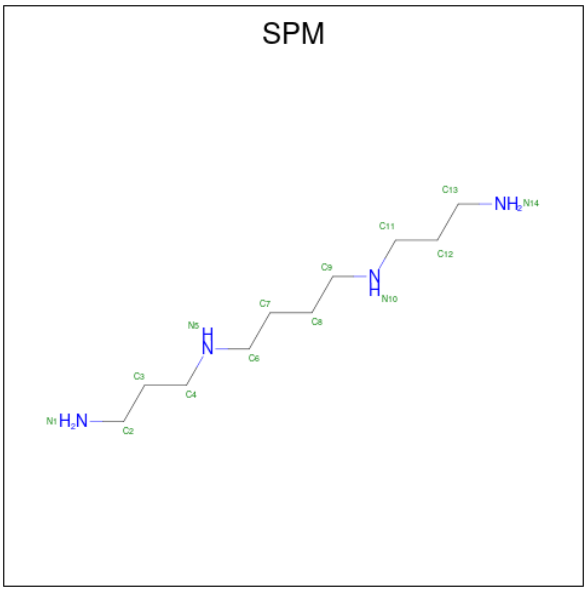
- Molecule 45 is a protein called L51_S25_CI-B8 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	j	195	Total	C	H	N	O	S	0	0
			3133	970	1582	290	283	8		

- Molecule 46 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
46	A	160	Total	Mg	0
			160	160	
46	K	1	Total	Mg	0
			1	1	
46	2	1	Total	Mg	0
			1	1	
46	3	1	Total	Mg	0
			1	1	

- Molecule 47 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms				AltConf
47	A	1	Total	C	H	N	0
			40	10	26	4	

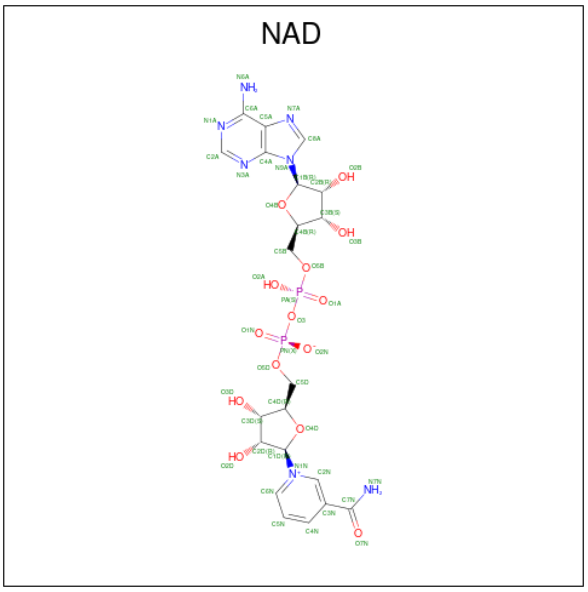
- Molecule 48 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
48	A	12	Total	K	0
			12	12	

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
49	W	1	Total	Zn	0
			1	1	
49	0	1	Total	Zn	0
			1	1	

- Molecule 50 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



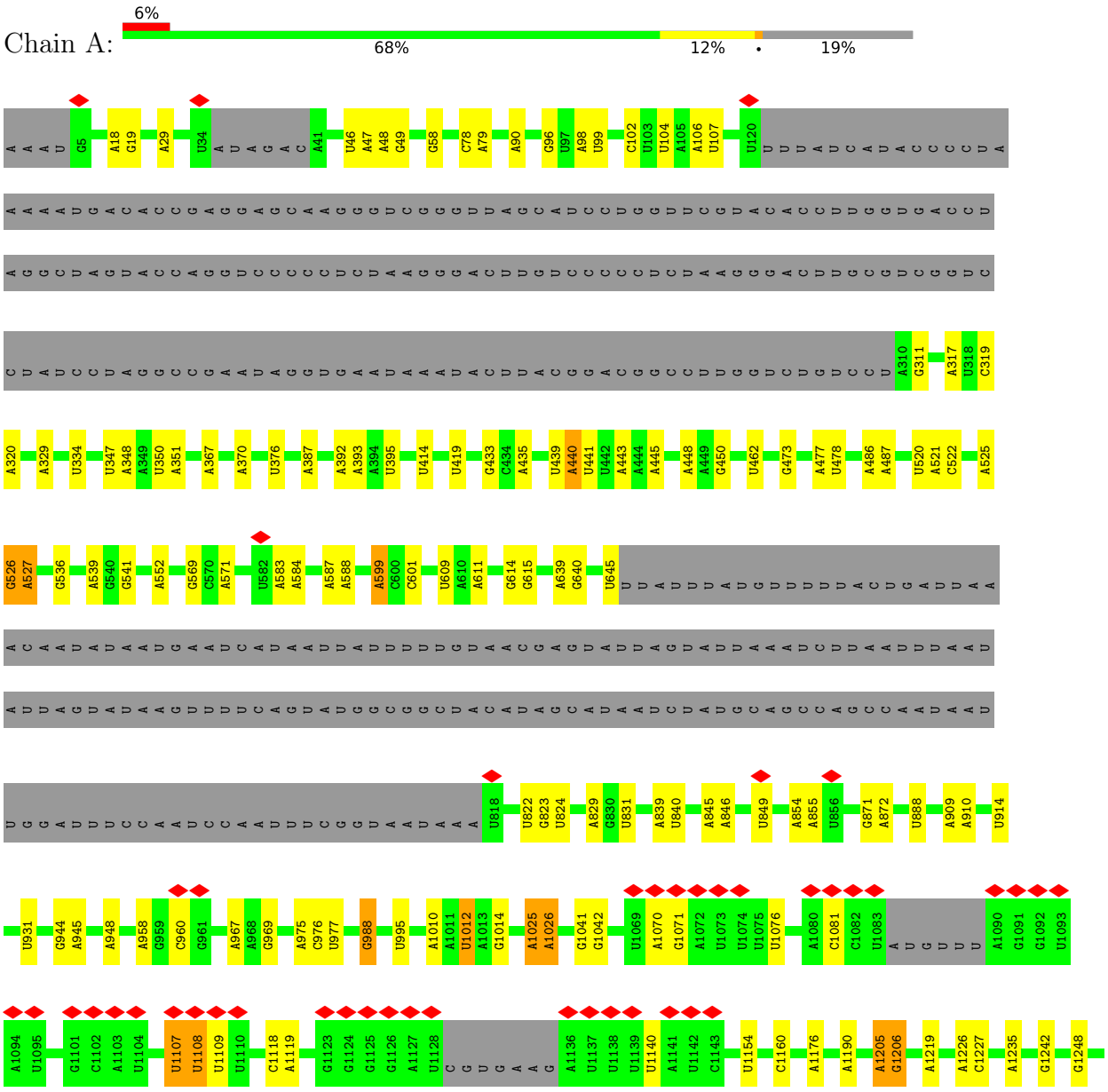
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
50	2	1	70	21	26	7	14	2	0

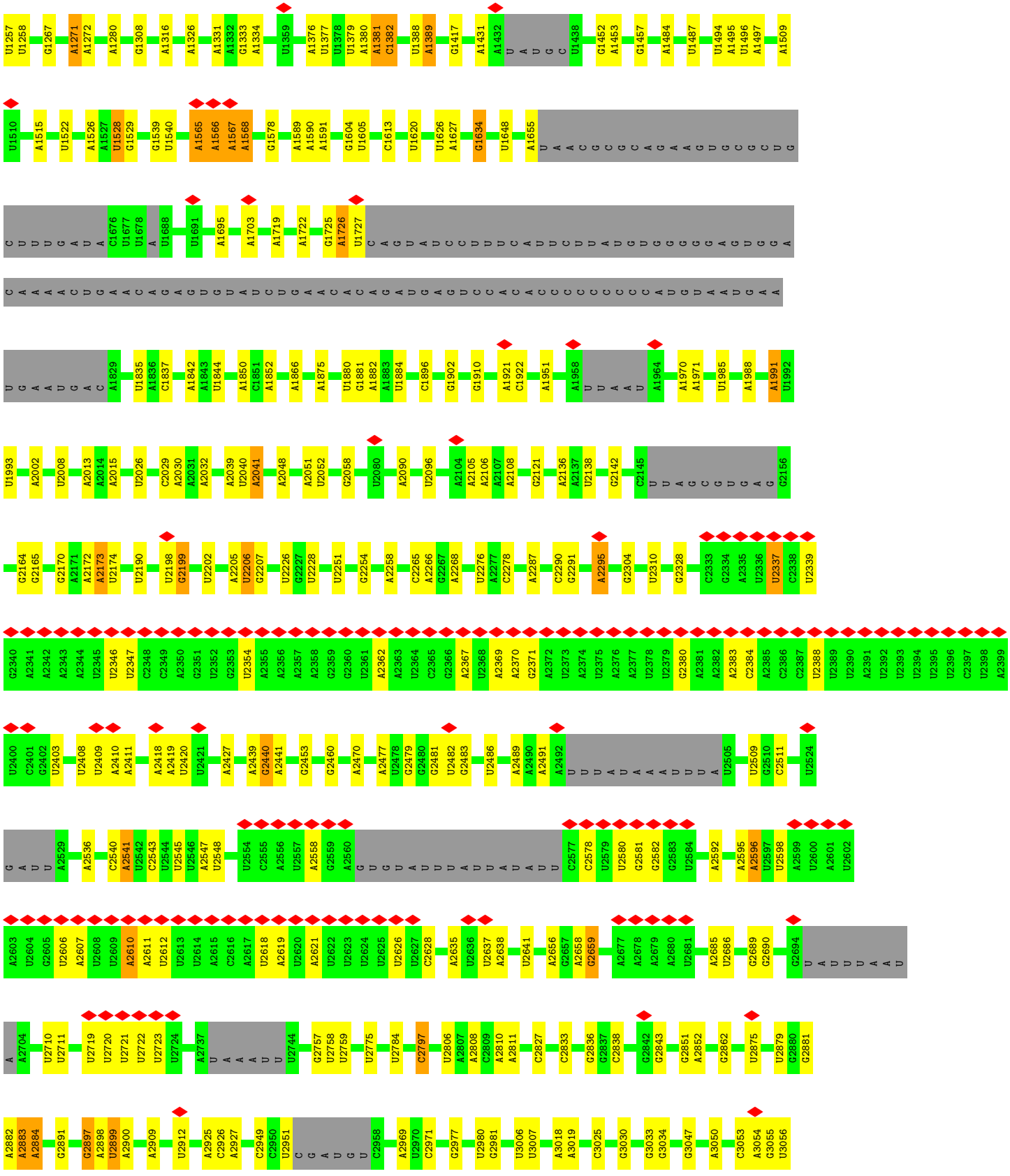
3 Residue-property plots (i)

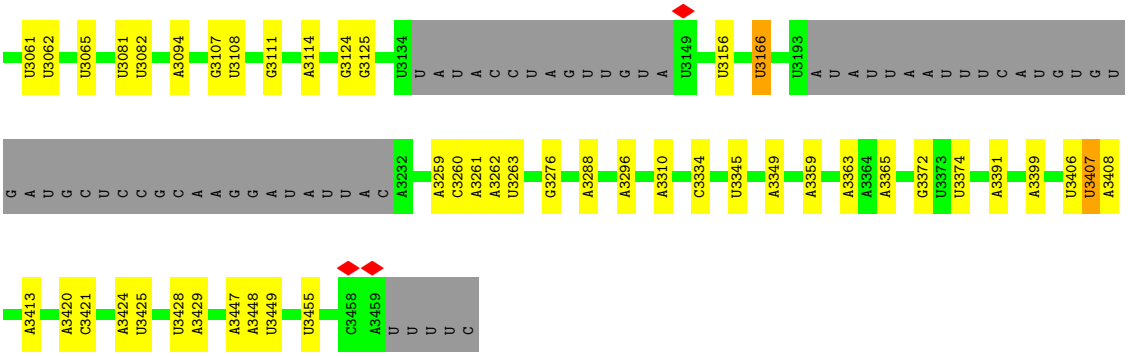
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: RNA (2820-MER)

Chain A:

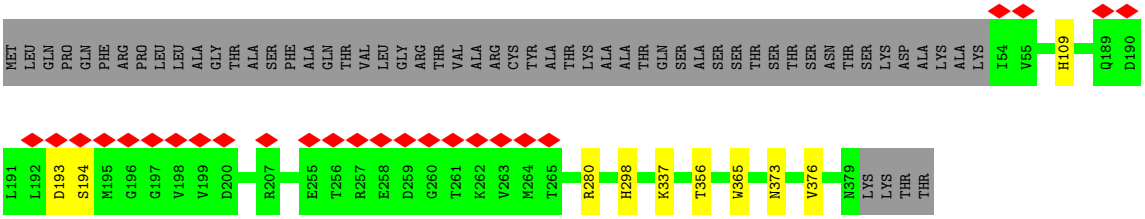






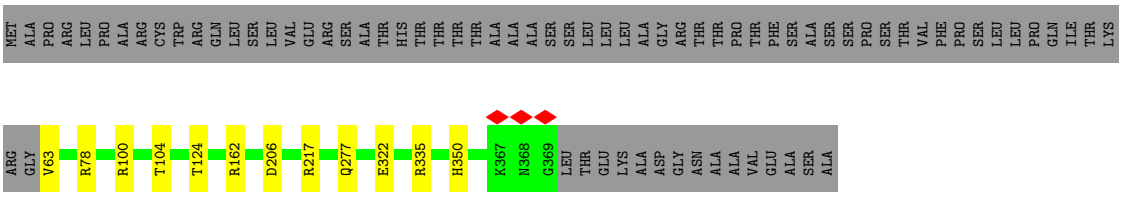
• Molecule 2: 60S ribosomal protein L2

Chain B:



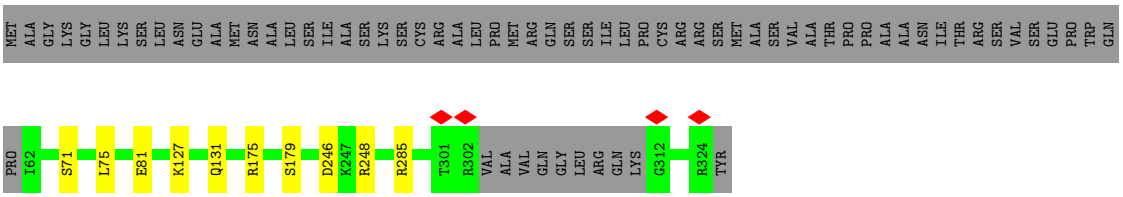
• Molecule 3: 60S ribosomal protein L3

Chain C:



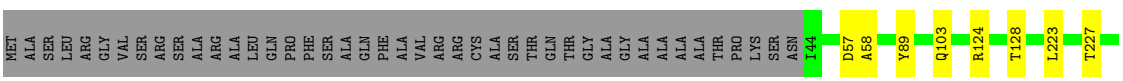
• Molecule 4: 60S ribosomal protein L4, variant

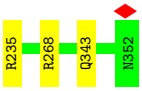
Chain D:



• Molecule 5: 50S ribosomal protein L5

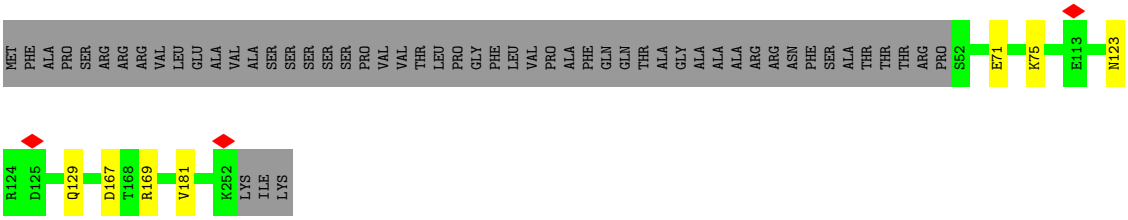
Chain E:





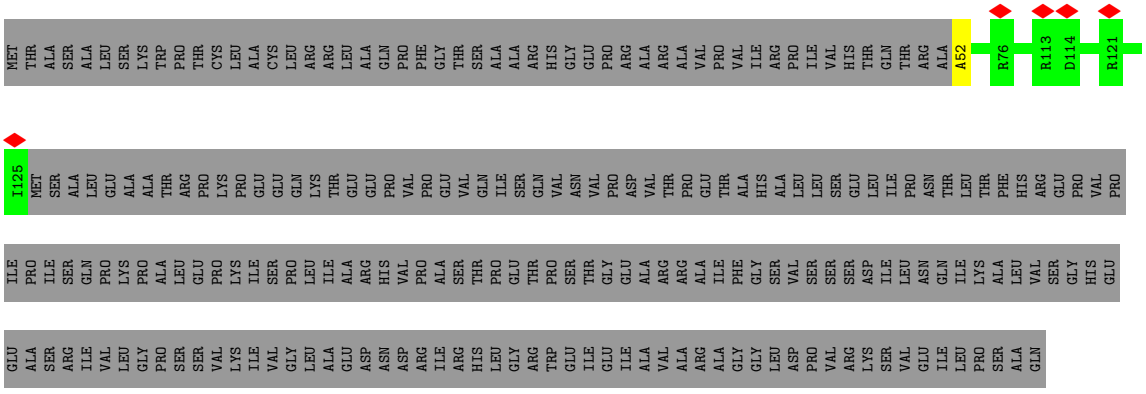
• Molecule 6: 60S ribosomal protein L6

Chain F:



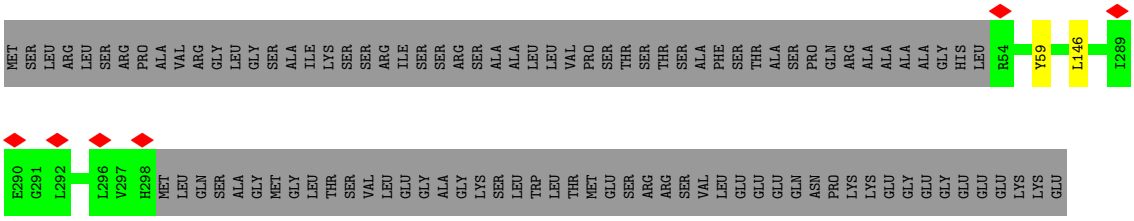
• Molecule 7: RIBOSOMAL_L9 domain-containing protein

Chain G:



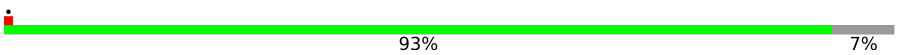
• Molecule 8: Uncharacterized protein

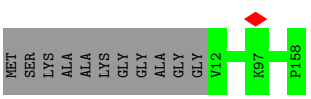
Chain f:



• Molecule 9: 60S ribosomal protein L19

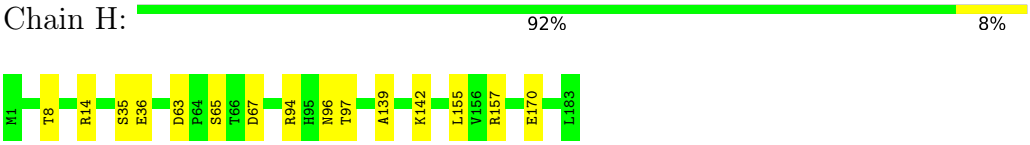
Chain g:





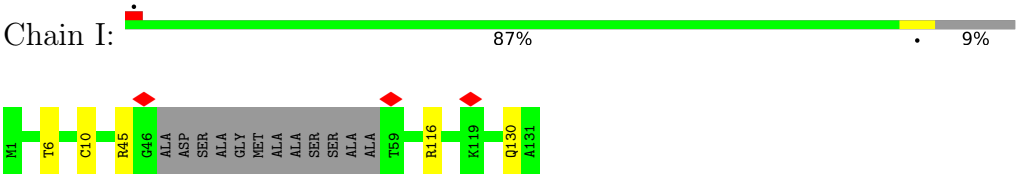
• Molecule 10: Ribosomal protein L13

Chain H:



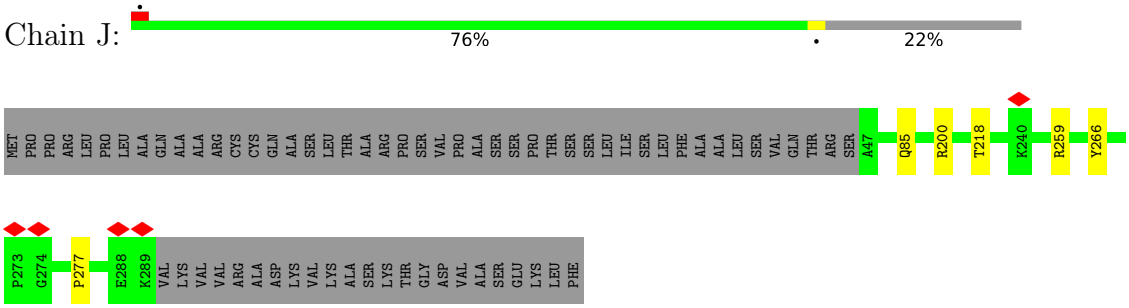
• Molecule 11: 50S ribosomal protein L14

Chain I:



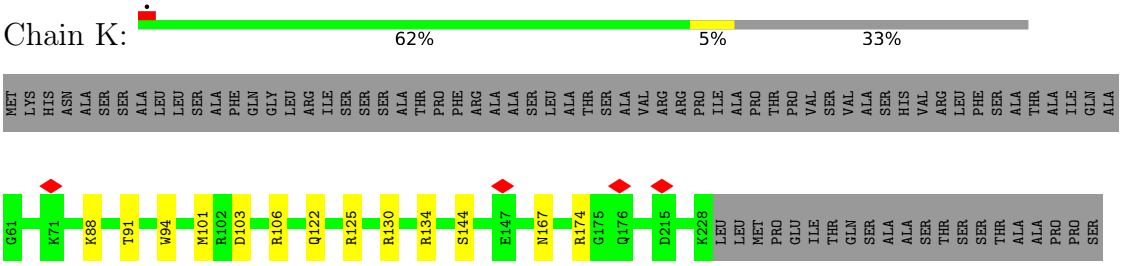
• Molecule 12: Ribosomal protein L15

Chain J:



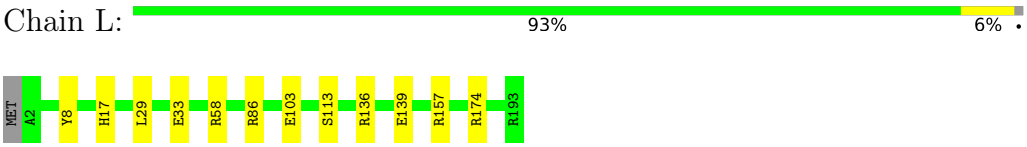
• Molecule 13: 60S ribosomal protein L16

Chain K:



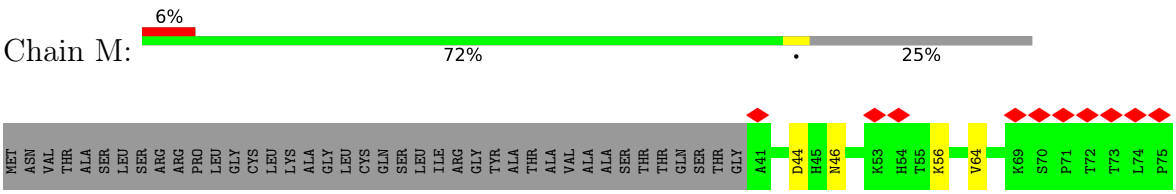
• Molecule 14: 50S ribosomal protein L17

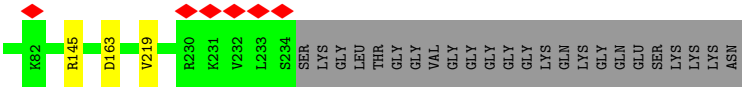
Chain L:



• Molecule 15: Mitochondrial ribosomal protein

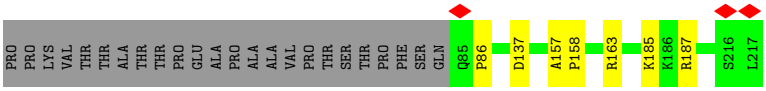
Chain M:





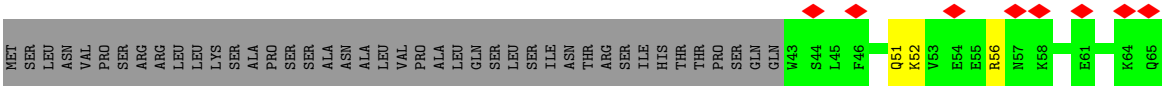
• Molecule 16: Aconitate hydratase

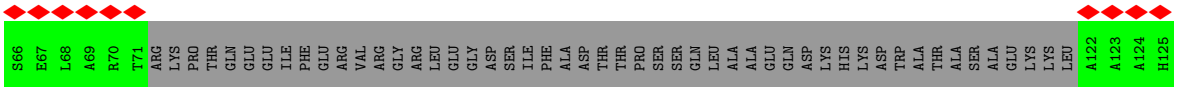
Chain N:

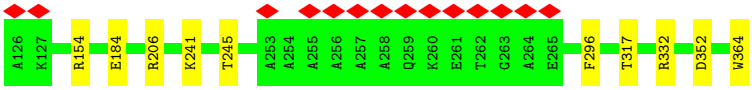


• Molecule 17: Mitochondrial large ribosomal subunit

Chain O:

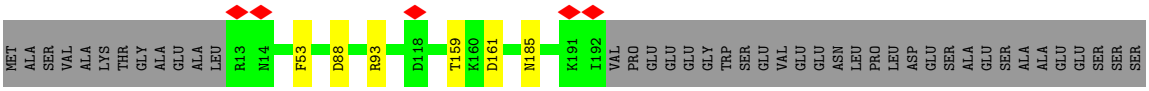






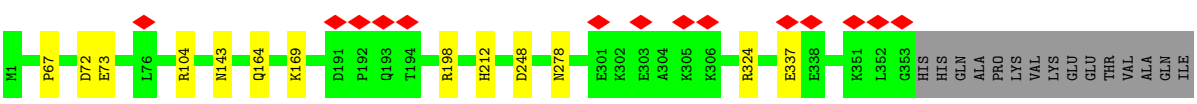
• Molecule 18: Mitochondrial ribosomal protein subunit L23

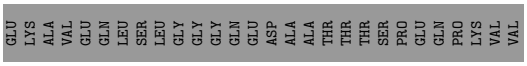
Chain P:



• Molecule 19: KOW domain-containing protein

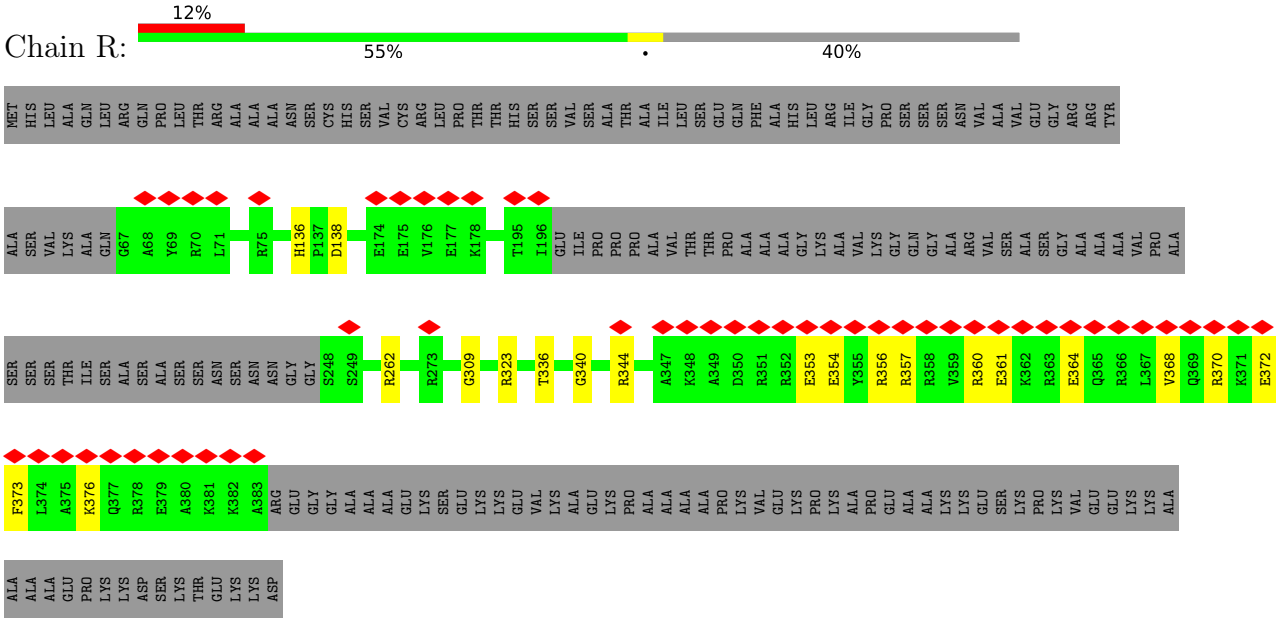
Chain Q:





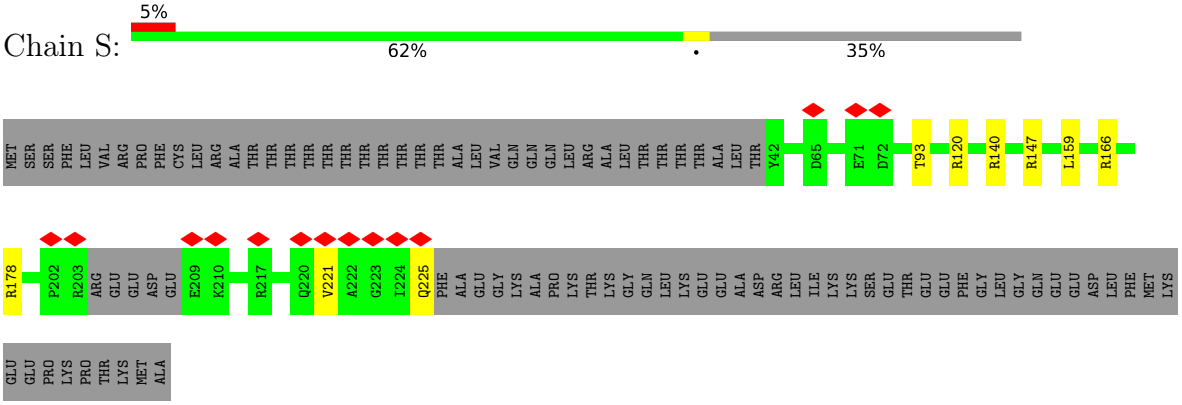
• Molecule 20: Uncharacterized protein

Chain R:



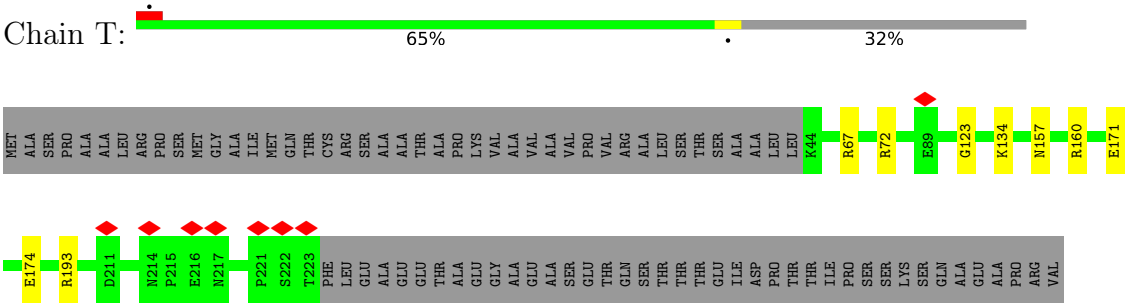
• Molecule 21: 50S ribosomal protein L24

Chain S:



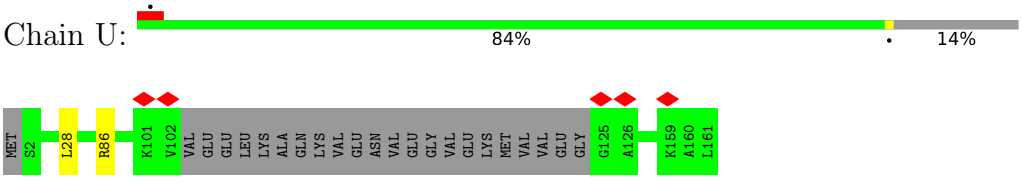
• Molecule 22: 54S ribosomal protein L4, mitochondrial

Chain T:



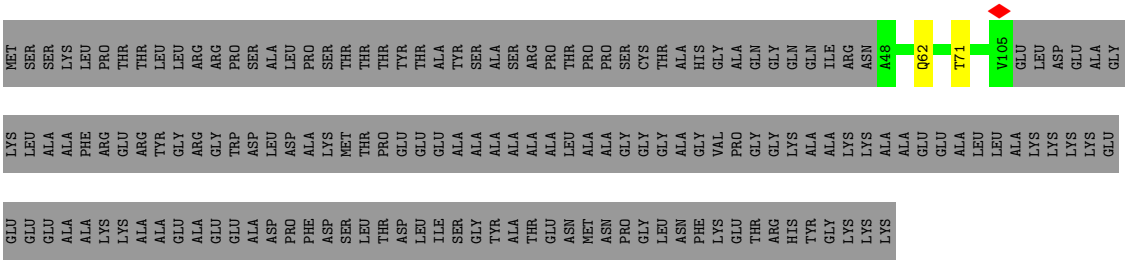
• Molecule 23: 50S ribosomal protein L30

Chain U:



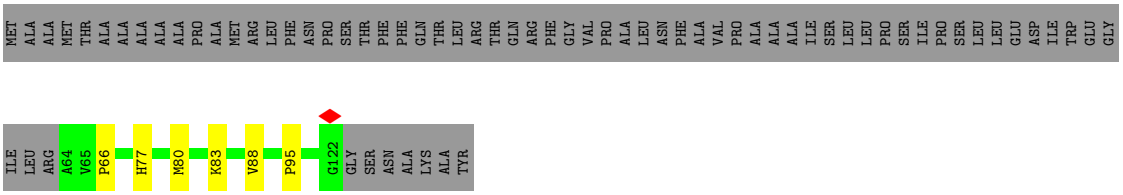
• Molecule 24: Uncharacterized protein

Chain V:



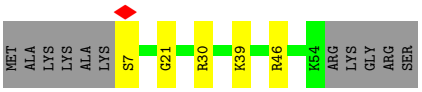
• Molecule 25: Mitochondrial ribosomal protein subunit L32

Chain W:



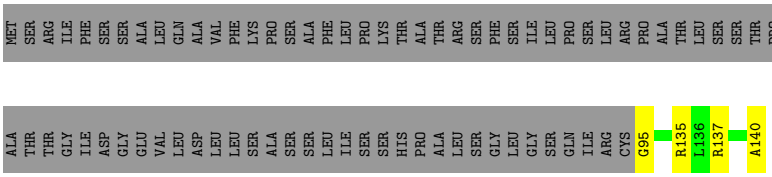
• Molecule 26: Uncharacterized protein

Chain X:



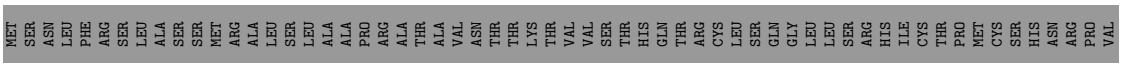
• Molecule 27: Related to ribosomal protein L34, mitochondrial

Chain Y:



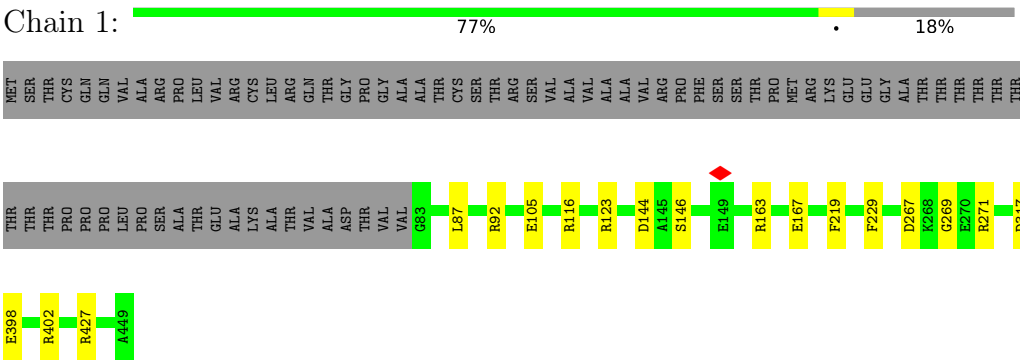
• Molecule 28: Ribosomal protein

Chain 0:



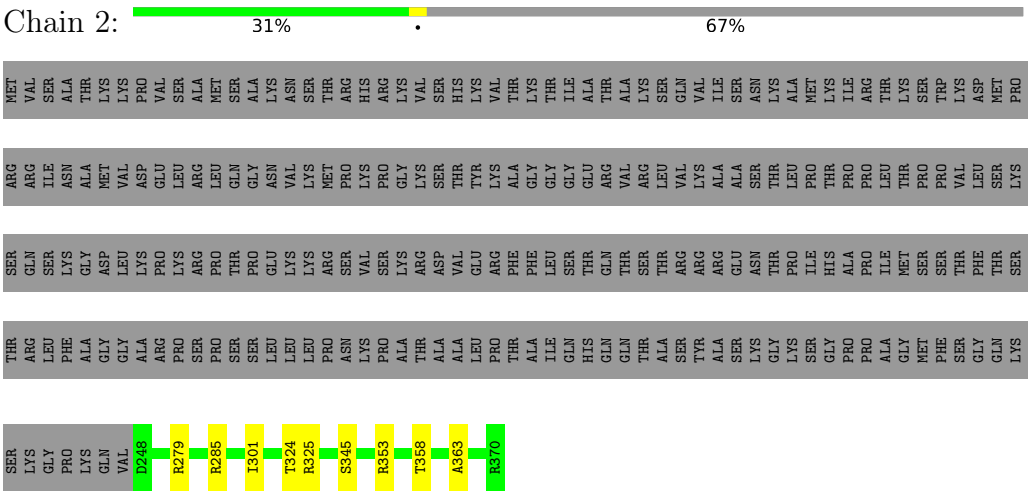
• Molecule 29: Mitochondrial large ribosomal subunit YmL35

Chain 1:



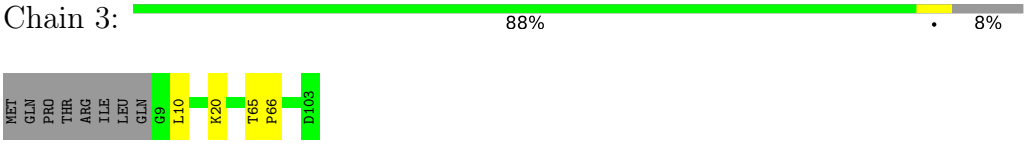
• Molecule 30: Uncharacterized protein

Chain 2:



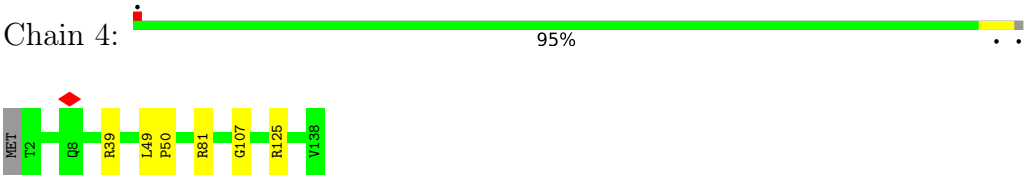
• Molecule 31: Uncharacterized protein

Chain 3:



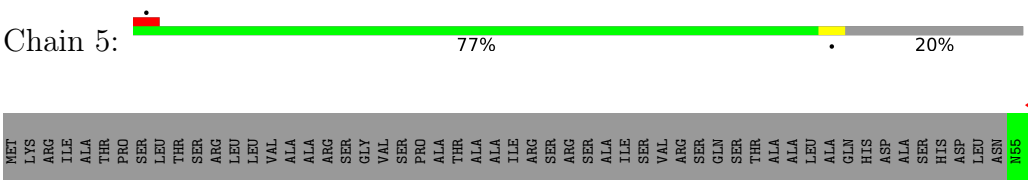
• Molecule 32: Mitochondrial ribosomal protein L43

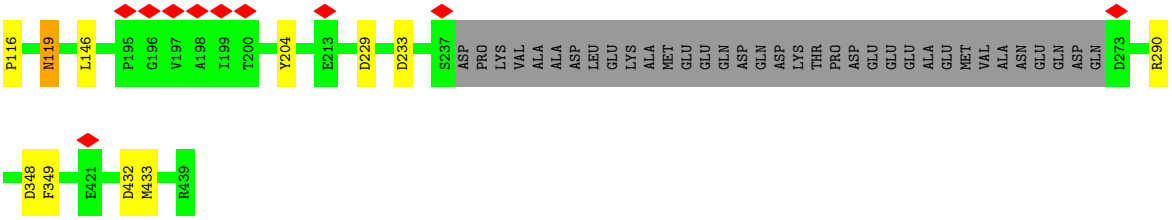
Chain 4:



• Molecule 33: 60S ribosomal protein L3

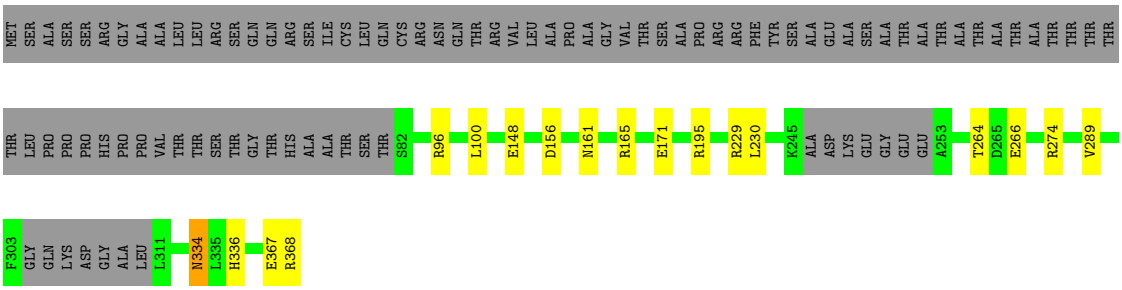
Chain 5:





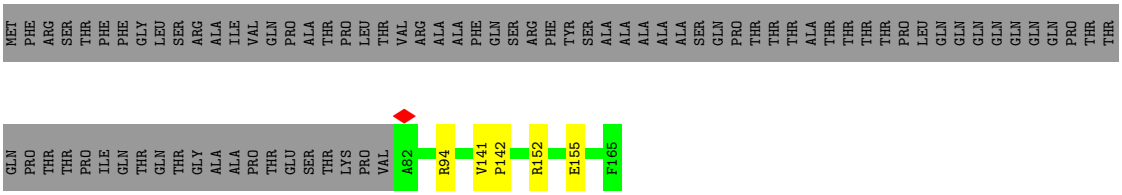
• Molecule 34: 50S ribosomal subunit L30

Chain 6:



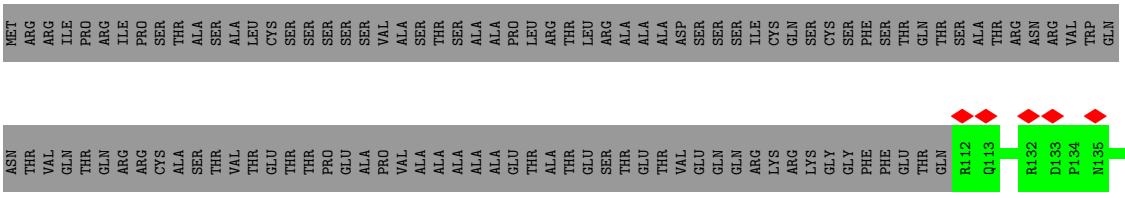
• Molecule 35: Uncharacterized protein

Chain 7:



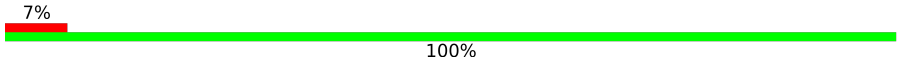
• Molecule 36: Uncharacterized protein

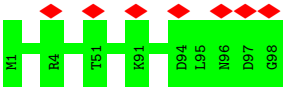
Chain 8:



• Molecule 37: Mitochondrial ribosomal protein L44

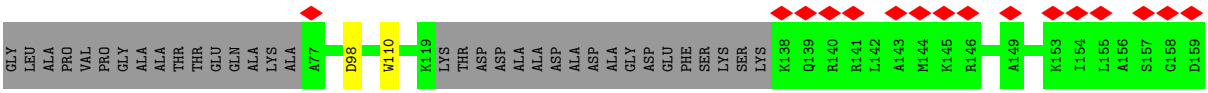
Chain h:

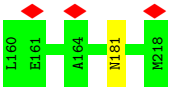




• Molecule 38: Uncharacterized protein

Chain i:



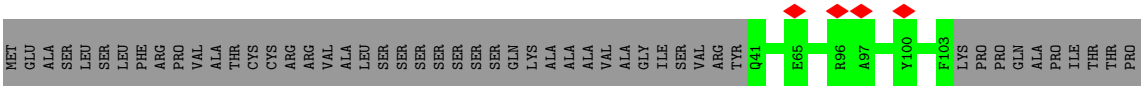


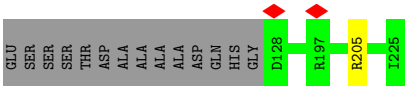
• Molecule 39: RNase III domain-containing protein

Chain 9:

• Molecule 40: 60S ribosomal protein L20

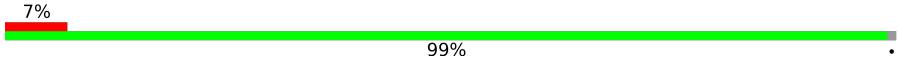
Chain a:

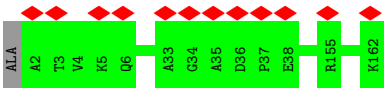




• Molecule 41: Mitoc_mL59 domain-containing protein

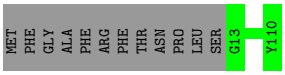
Chain b:





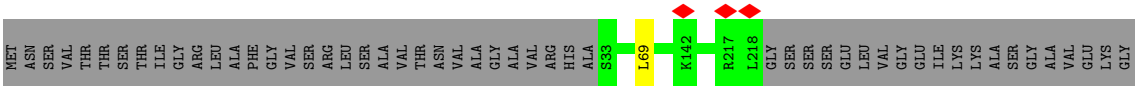
• Molecule 42: 54S ribosomal protein L31, mitochondrial

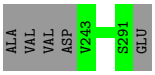
Chain c:



• Molecule 43: Uncharacterized protein

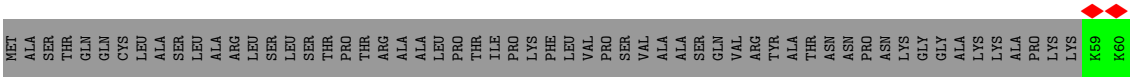
Chain d:

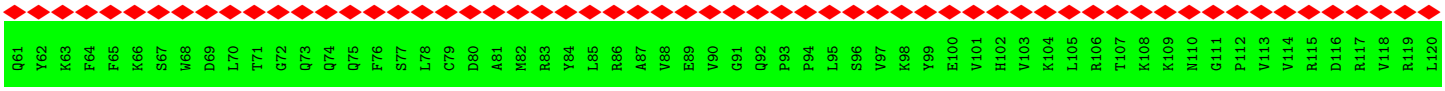


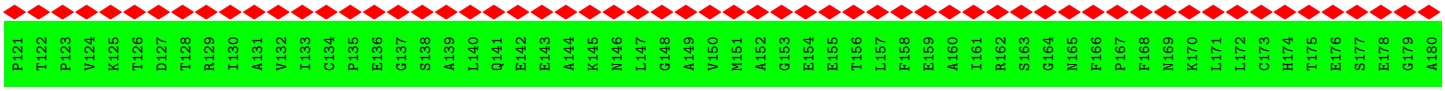


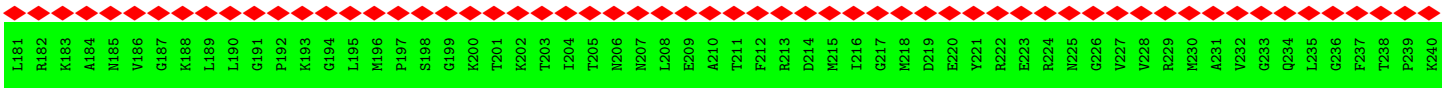
• Molecule 44: 60S ribosomal protein L1

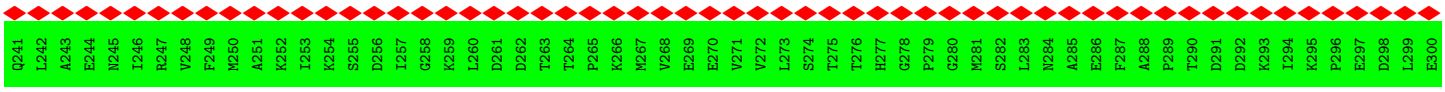
Chain e:





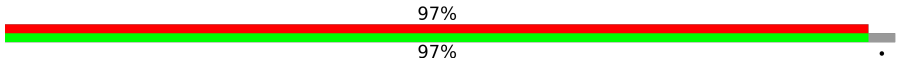


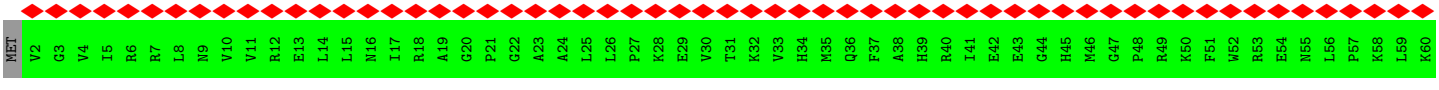


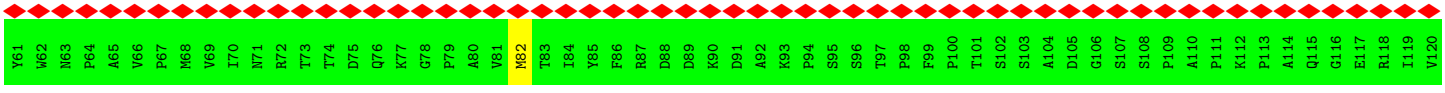


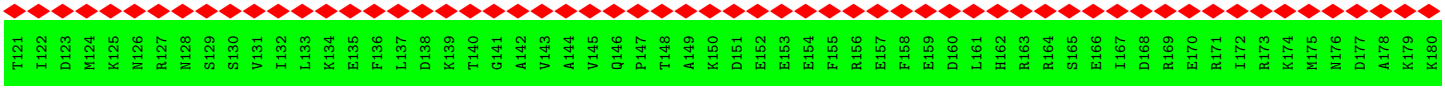
• Molecule 45: L51_S25_CI-B8 domain-containing protein

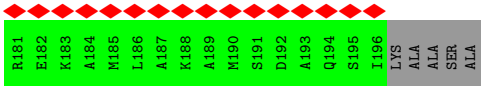
Chain j:








T121 I122 D123 M124 K125 N126 R127 N128 S129 S130 V131 I132 L133 K134 E135 F136 L137 D138 K139 T140 G141 A142 V143 A144 V145 Q146 P147 T148 A149 K150 D151 E152 E153 E154 F155 R156 E157 F158 E159 D160 L161 H162 R163 R164 S165 E166 I167 D168 R169 E170 R171 I172 R173 K174 M175 N176 D177 A178 K179 K180


R181 E182 K183 A184 M185 L186 A187 K188 A189 M190 S191 D192 A193 Q194 S195 I196 LYS ALA ALA SER ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131806	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 ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	41.788	Depositor
Minimum map value	-22.612	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.105	Depositor
Recommended contour level	3.35	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SPM, K, NAD, ZN

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	A	0.20	0/67352	0.67	0/104875
2	B	0.24	0/2603	0.44	0/3508
3	C	0.24	0/2380	0.44	0/3209
4	D	0.23	0/2072	0.41	0/2794
5	E	0.25	0/2518	0.41	0/3427
6	F	0.24	0/1644	0.41	0/2218
7	G	0.24	0/630	0.44	0/842
8	f	0.24	0/1923	0.41	0/2631
9	g	0.24	0/1126	0.41	0/1525
10	H	0.24	0/1460	0.42	0/1975
11	I	0.24	0/918	0.45	0/1225
12	J	0.24	0/1931	0.41	0/2597
13	K	0.24	0/1376	0.42	0/1842
14	L	0.23	0/1569	0.40	0/2106
15	M	0.24	0/1572	0.43	0/2117
16	N	0.24	0/1077	0.45	0/1452
17	O	0.23	0/2248	0.39	0/3015
18	P	0.24	0/1523	0.39	0/2058
19	Q	0.24	0/2916	0.40	0/3927
20	R	0.24	0/2227	0.41	0/2978
21	S	0.23	0/1510	0.40	0/2042
22	T	0.23	0/1538	0.39	0/2086
23	U	0.23	0/1117	0.42	0/1496
24	V	0.25	0/486	0.44	0/659
25	W	0.23	0/467	0.41	0/616
26	X	0.24	0/411	0.42	0/551
27	Y	0.23	0/368	0.44	0/485
28	0	0.25	0/395	0.45	0/523
29	1	0.24	0/3053	0.39	0/4108
30	2	0.25	0/1074	0.40	0/1449
31	3	0.25	0/783	0.44	0/1056
32	4	0.25	0/1077	0.42	0/1453

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	5	0.25	0/2790	0.39	0/3794
34	6	0.25	0/2274	0.42	0/3062
35	7	0.23	0/686	0.42	0/919
36	8	0.24	0/2714	0.40	0/3657
37	h	0.24	0/791	0.40	0/1065
38	i	0.24	0/989	0.39	0/1324
39	9	0.23	0/1678	0.38	0/2267
40	a	0.23	0/1364	0.40	0/1842
41	b	0.23	0/1348	0.37	0/1816
42	c	0.23	0/846	0.41	0/1134
43	d	0.23	0/1930	0.41	0/2597
44	e	0.24	0/1918	0.41	0/2582
45	j	0.23	0/1581	0.40	0/2127
All	All	0.22	0/134253	0.56	0/195031

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60143	30189	30189	109	0
2	B	2544	2592	2592	5	0
3	C	2336	2422	2420	10	0
4	D	2028	2040	2040	5	0
5	E	2449	2461	2461	8	0
6	F	1608	1645	1645	4	0
7	G	618	627	627	1	0
8	f	1876	1925	1925	0	0
9	g	1103	1154	1154	0	0
10	H	1426	1459	1459	9	0
11	I	913	985	985	3	0
12	J	1888	1939	1939	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	K	1350	1401	1401	7	0
14	L	1545	1590	1590	6	0
15	M	1536	1628	1628	7	0
16	N	1056	1120	1120	6	0
17	O	2209	2323	2323	9	0
18	P	1481	1494	1494	4	0
19	Q	2868	2961	2961	9	0
20	R	2189	2310	2310	14	0
21	S	1472	1507	1507	6	0
22	T	1497	1453	1453	6	0
23	U	1099	1164	1164	2	0
24	V	474	477	477	2	0
25	W	460	489	488	5	0
26	X	403	433	433	4	0
27	Y	365	412	412	3	0
28	0	388	409	409	1	0
29	1	2985	3029	3029	13	0
30	2	1046	1055	1055	8	0
31	3	763	773	773	2	0
32	4	1052	1087	1087	4	0
33	5	2719	2710	2710	9	0
34	6	2226	2248	2248	12	0
35	7	674	709	709	3	0
36	8	2660	2714	2714	7	0
37	h	779	798	798	0	0
38	i	976	1022	1022	0	0
39	9	1643	1698	1698	7	0
40	a	1331	1340	1340	0	0
41	b	1314	1379	1379	0	0
42	c	827	873	873	0	0
43	d	1888	1909	1909	0	0
44	e	1886	1935	1935	0	0
45	j	1551	1582	1581	0	0
46	2	1	0	0	0	0
46	3	1	0	0	0	0
46	A	160	0	0	0	0
46	K	1	0	0	0	0
47	A	14	26	26	0	0
48	A	12	0	0	0	0
49	0	1	0	0	0	0
49	W	1	0	0	0	0
50	2	44	26	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	125879	97522	97518	245	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 245 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2276:U:OP1	3:C:63:VAL:N	2.09	0.85
1:A:2580:U:O2	20:R:360:ARG:NH1	2.11	0.84
17:O:296:PHE:O	17:O:317:THR:OG1	2.00	0.80
1:A:2337:U:O2'	1:A:2339:U:OP1	2.00	0.80
1:A:3094:A:OP1	10:H:94:ARG:NH1	2.15	0.79

There are no symmetry-related clashes.

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	
2	B	324/383 (85%)	316 (98%)	8 (2%)	0	100	100
3	C	305/384 (79%)	300 (98%)	5 (2%)	0	100	100
4	D	250/325 (77%)	246 (98%)	4 (2%)	0	100	100
5	E	307/352 (87%)	302 (98%)	5 (2%)	0	100	100
6	F	199/255 (78%)	197 (99%)	2 (1%)	0	100	100
7	G	72/300 (24%)	72 (100%)	0	0	100	100
8	f	243/347 (70%)	239 (98%)	4 (2%)	0	100	100
9	g	145/158 (92%)	141 (97%)	4 (3%)	0	100	100
10	H	181/183 (99%)	179 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	I	115/131 (88%)	112 (97%)	3 (3%)	0	100	100
12	J	241/312 (77%)	236 (98%)	5 (2%)	0	100	100
13	K	166/249 (67%)	164 (99%)	2 (1%)	0	100	100
14	L	190/193 (98%)	189 (100%)	1 (0%)	0	100	100
15	M	192/258 (74%)	190 (99%)	2 (1%)	0	100	100
16	N	131/217 (60%)	126 (96%)	5 (4%)	0	100	100
17	O	268/364 (74%)	266 (99%)	2 (1%)	0	100	100
18	P	178/228 (78%)	177 (99%)	1 (1%)	0	100	100
19	Q	351/396 (89%)	350 (100%)	1 (0%)	0	100	100
20	R	262/447 (59%)	258 (98%)	4 (2%)	0	100	100
21	S	175/274 (64%)	168 (96%)	7 (4%)	0	100	100
22	T	178/263 (68%)	174 (98%)	4 (2%)	0	100	100
23	U	134/161 (83%)	133 (99%)	1 (1%)	0	100	100
24	V	56/219 (26%)	56 (100%)	0	0	100	100
25	W	57/129 (44%)	56 (98%)	1 (2%)	0	100	100
26	X	46/59 (78%)	45 (98%)	1 (2%)	0	100	100
27	Y	44/140 (31%)	44 (100%)	0	0	100	100
28	0	44/124 (36%)	42 (96%)	2 (4%)	0	100	100
29	1	365/449 (81%)	358 (98%)	7 (2%)	0	100	100
30	2	121/370 (33%)	121 (100%)	0	0	100	100
31	3	93/103 (90%)	87 (94%)	6 (6%)	0	100	100
32	4	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
33	5	346/439 (79%)	345 (100%)	1 (0%)	0	100	100
34	6	267/368 (73%)	265 (99%)	2 (1%)	0	100	100
35	7	82/165 (50%)	81 (99%)	1 (1%)	0	100	100
36	8	329/443 (74%)	325 (99%)	4 (1%)	0	100	100
37	h	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
38	i	120/218 (55%)	113 (94%)	7 (6%)	0	100	100
39	9	204/267 (76%)	201 (98%)	3 (2%)	0	100	100
40	a	157/225 (70%)	156 (99%)	1 (1%)	0	100	100
41	b	159/162 (98%)	156 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	c	96/110 (87%)	95 (99%)	1 (1%)	0	100	100
43	d	231/292 (79%)	226 (98%)	5 (2%)	0	100	100
44	e	240/303 (79%)	233 (97%)	7 (3%)	0	100	100
45	j	193/201 (96%)	186 (96%)	7 (4%)	0	100	100
All	All	8088/11202 (72%)	7954 (98%)	134 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	B	267/312 (86%)	265 (99%)	2 (1%)	84	90
3	C	242/303 (80%)	241 (100%)	1 (0%)	91	94
4	D	216/274 (79%)	216 (100%)	0	100	100
5	E	267/296 (90%)	267 (100%)	0	100	100
6	F	173/216 (80%)	172 (99%)	1 (1%)	86	91
7	G	64/254 (25%)	64 (100%)	0	100	100
8	f	206/287 (72%)	204 (99%)	2 (1%)	76	85
9	g	120/124 (97%)	120 (100%)	0	100	100
10	H	149/149 (100%)	149 (100%)	0	100	100
11	I	100/105 (95%)	100 (100%)	0	100	100
12	J	198/255 (78%)	197 (100%)	1 (0%)	88	92
13	K	142/205 (69%)	141 (99%)	1 (1%)	84	90
14	L	164/165 (99%)	162 (99%)	2 (1%)	71	83
15	M	164/209 (78%)	164 (100%)	0	100	100
16	N	119/188 (63%)	119 (100%)	0	100	100
17	O	235/315 (75%)	235 (100%)	0	100	100
18	P	158/196 (81%)	157 (99%)	1 (1%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	Q	312/347 (90%)	311 (100%)	1 (0%)	92 95
20	R	226/359 (63%)	226 (100%)	0	100 100
21	S	159/242 (66%)	159 (100%)	0	100 100
22	T	161/224 (72%)	160 (99%)	1 (1%)	86 91
23	U	118/138 (86%)	118 (100%)	0	100 100
24	V	54/170 (32%)	54 (100%)	0	100 100
25	W	50/102 (49%)	49 (98%)	1 (2%)	55 72
26	X	46/54 (85%)	46 (100%)	0	100 100
27	Y	38/116 (33%)	38 (100%)	0	100 100
28	0	41/108 (38%)	41 (100%)	0	100 100
29	1	316/384 (82%)	314 (99%)	2 (1%)	86 91
30	2	109/317 (34%)	109 (100%)	0	100 100
31	3	83/91 (91%)	82 (99%)	1 (1%)	71 83
32	4	113/114 (99%)	113 (100%)	0	100 100
33	5	279/351 (80%)	278 (100%)	1 (0%)	91 94
34	6	238/310 (77%)	236 (99%)	2 (1%)	81 89
35	7	69/136 (51%)	69 (100%)	0	100 100
36	8	285/378 (75%)	283 (99%)	2 (1%)	84 90
37	h	88/88 (100%)	88 (100%)	0	100 100
38	i	101/162 (62%)	98 (97%)	3 (3%)	41 61
39	9	176/225 (78%)	176 (100%)	0	100 100
40	a	146/196 (74%)	145 (99%)	1 (1%)	84 90
41	b	141/141 (100%)	141 (100%)	0	100 100
42	c	86/96 (90%)	86 (100%)	0	100 100
43	d	201/243 (83%)	200 (100%)	1 (0%)	88 92
44	e	207/256 (81%)	207 (100%)	0	100 100
45	j	167/171 (98%)	166 (99%)	1 (1%)	86 91
All	All	6994/9372 (75%)	6966 (100%)	28 (0%)	91 94

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	1	229	PHE

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Mol	Chain	Res	Type
45	j	82	MET
33	5	119	ASN
38	i	181	ASN
31	3	10	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
6	F	189	HIS
17	O	293	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2800/3464 (80%)	345 (12%)	10 (0%)

5 of 345 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	18	A
1	A	19	G
1	A	29	A
1	A	46	U
1	A	47	A

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2481	G
1	A	2720	U
1	A	2883	A
1	A	1107	U
1	A	1205	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 179 ligands modelled in this entry, 177 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
50	NAD	2	4301	46	42,48,48	0.74	1 (2%)	50,73,73	0.93	2 (4%)
47	SPM	A	3661	-	13,13,13	0.32	0	12,12,12	0.75	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
50	NAD	2	4301	46	-	3/26/62/62	0/5/5/5
47	SPM	A	3661	-	-	2/11/11/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	2	4301	NAD	C2N-N1N	-2.09	1.32	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	2	4301	NAD	O4B-C1B-C2B	-3.23	102.21	106.93
50	2	4301	NAD	N3A-C2A-N1A	-2.66	124.52	128.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	2	4301	NAD	C3D-C4D-C5D-O5D
50	2	4301	NAD	O4D-C4D-C5D-O5D
50	2	4301	NAD	C4B-C5B-O5B-PA
47	A	3661	SPM	N10-C11-C12-C13
47	A	3661	SPM	C12-C11-N10-C9

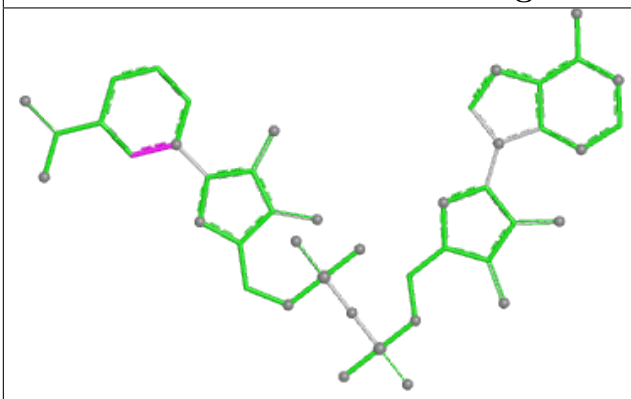
There are no ring outliers.

1 monomer is involved in 2 short contacts:

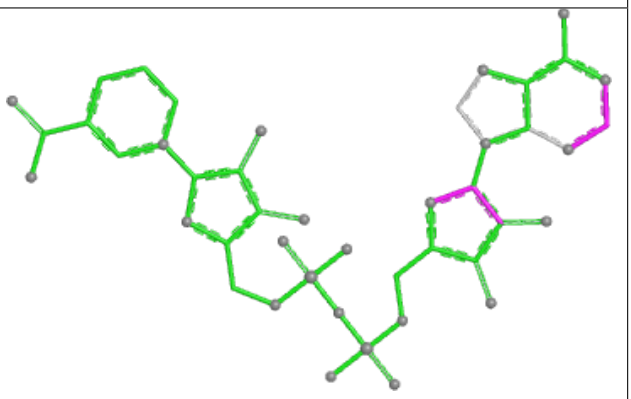
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	2	4301	NAD	2	0

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

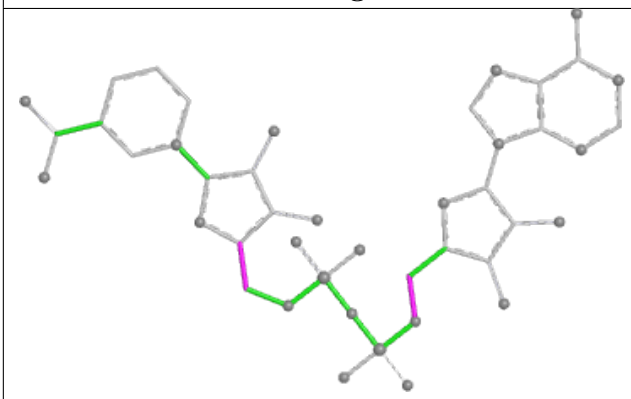
Ligand NAD 2 4301



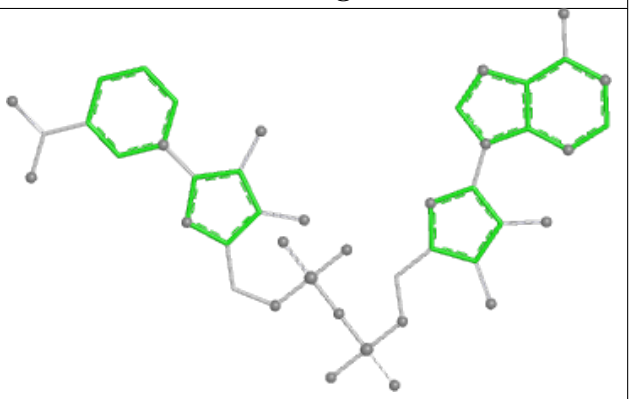
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

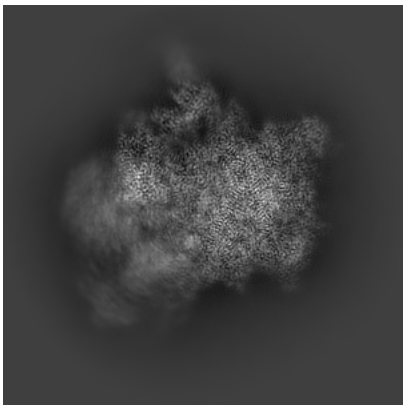
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10973. These allow visual inspection of the internal detail of the map and identification of artifacts.

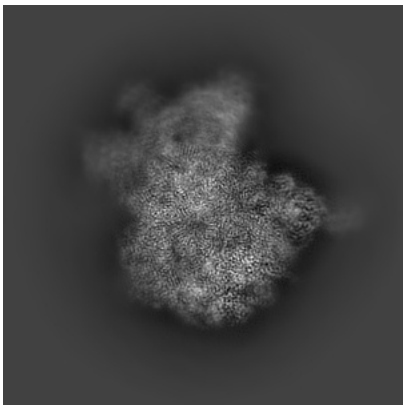
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

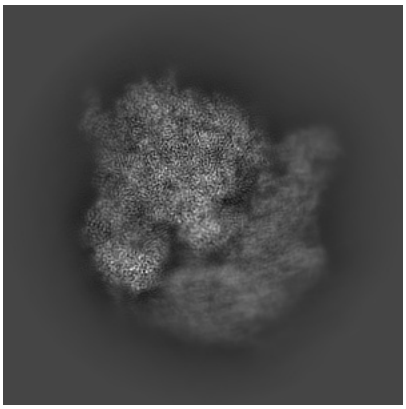
6.1.1 Primary map



X

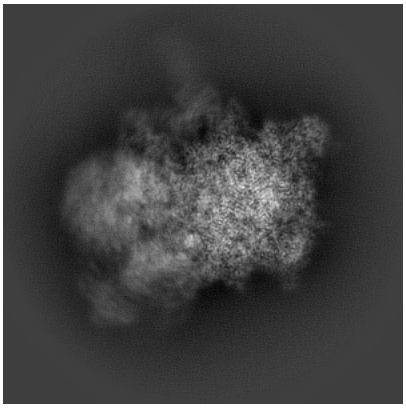


Y

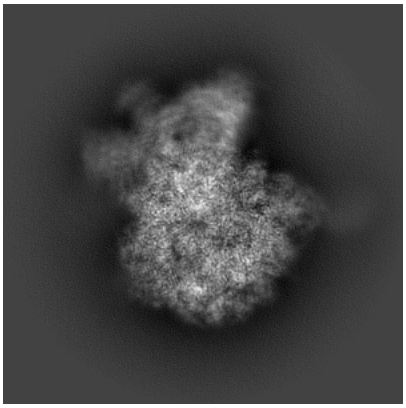


Z

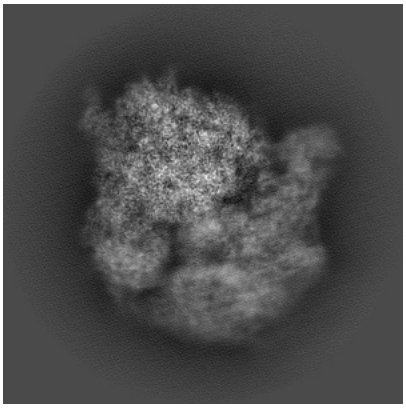
6.1.2 Raw map



X



Y

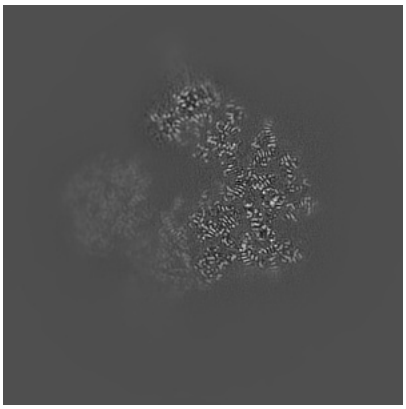


Z

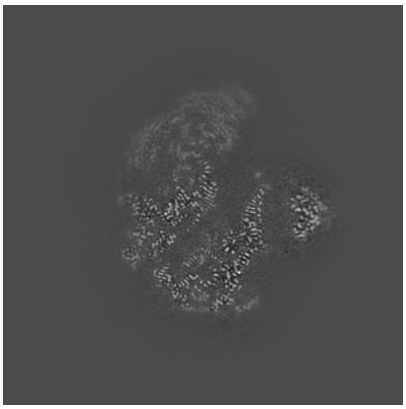
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



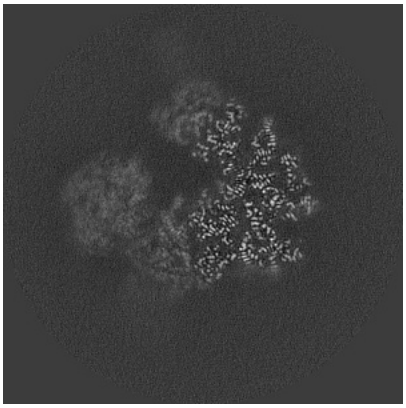
X Index: 200



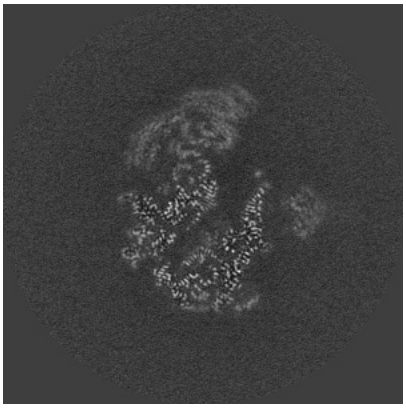
Y Index: 200

Z Index: 200

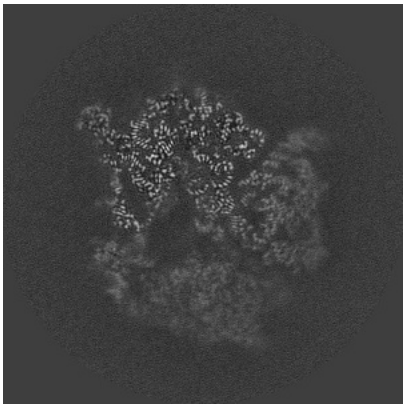
6.2.2 Raw map



X Index: 200



Y Index: 200

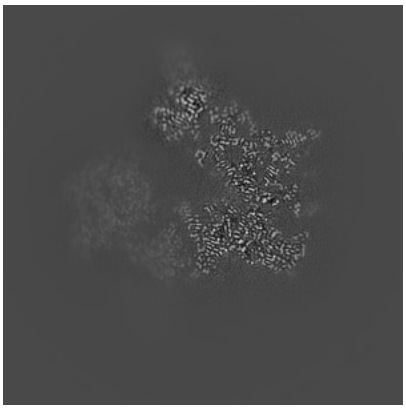


Z Index: 200

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

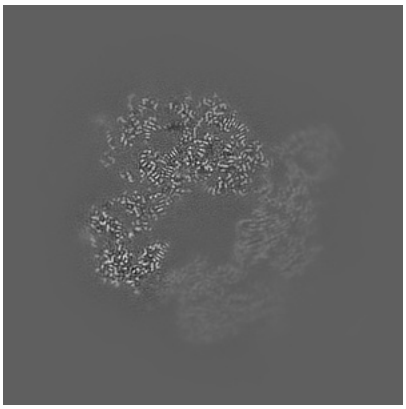
6.3 Largest variance slices (i)

6.3.1 Primary map



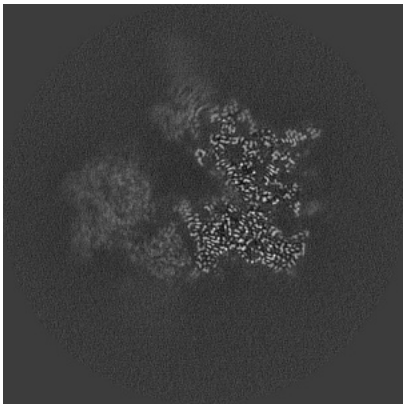
X Index: 192

Y Index: 228



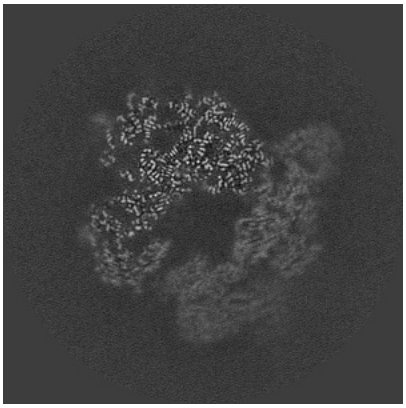
Z Index: 220

6.3.2 Raw map



X Index: 192

Y Index: 228

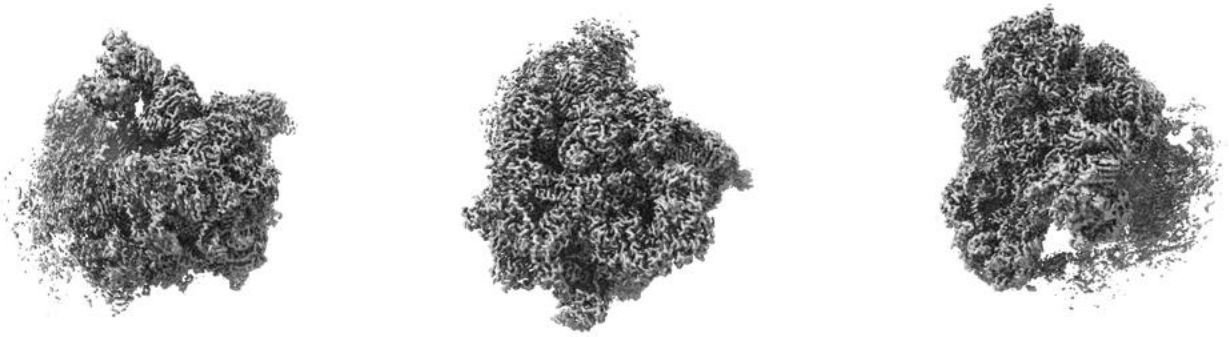


Z Index: 220

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

6.4 Orthogonal surface views (i)

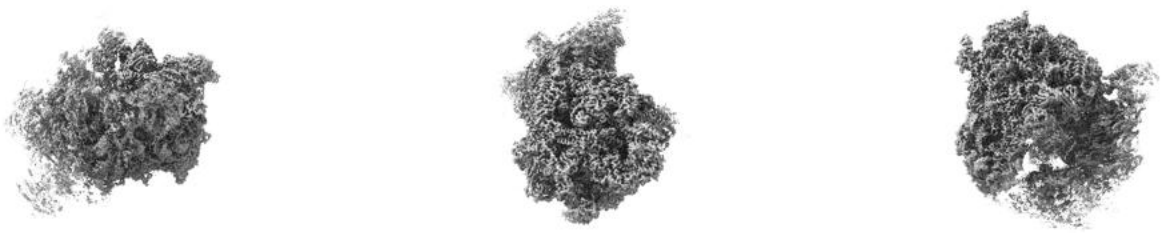
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.35. 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.

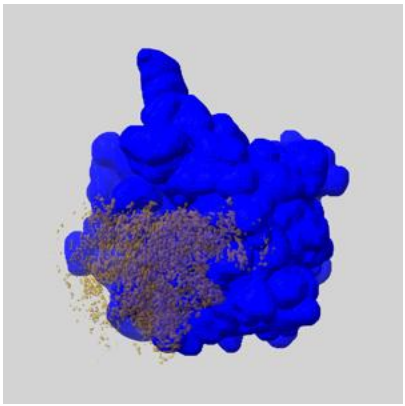
6.5 Mask visualisation (i)

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

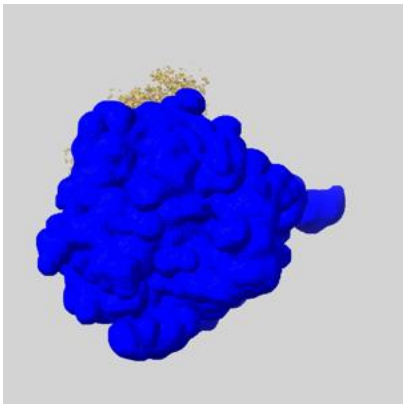
A mask typically either:

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

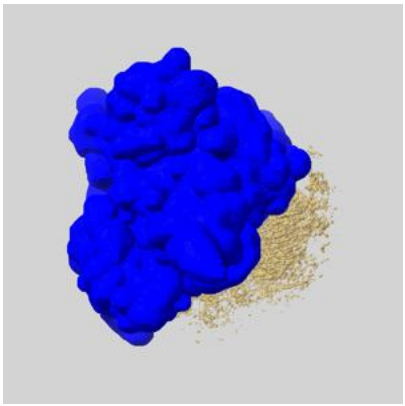
6.5.1 emd_10973_msk_1.map (i)



X



Y

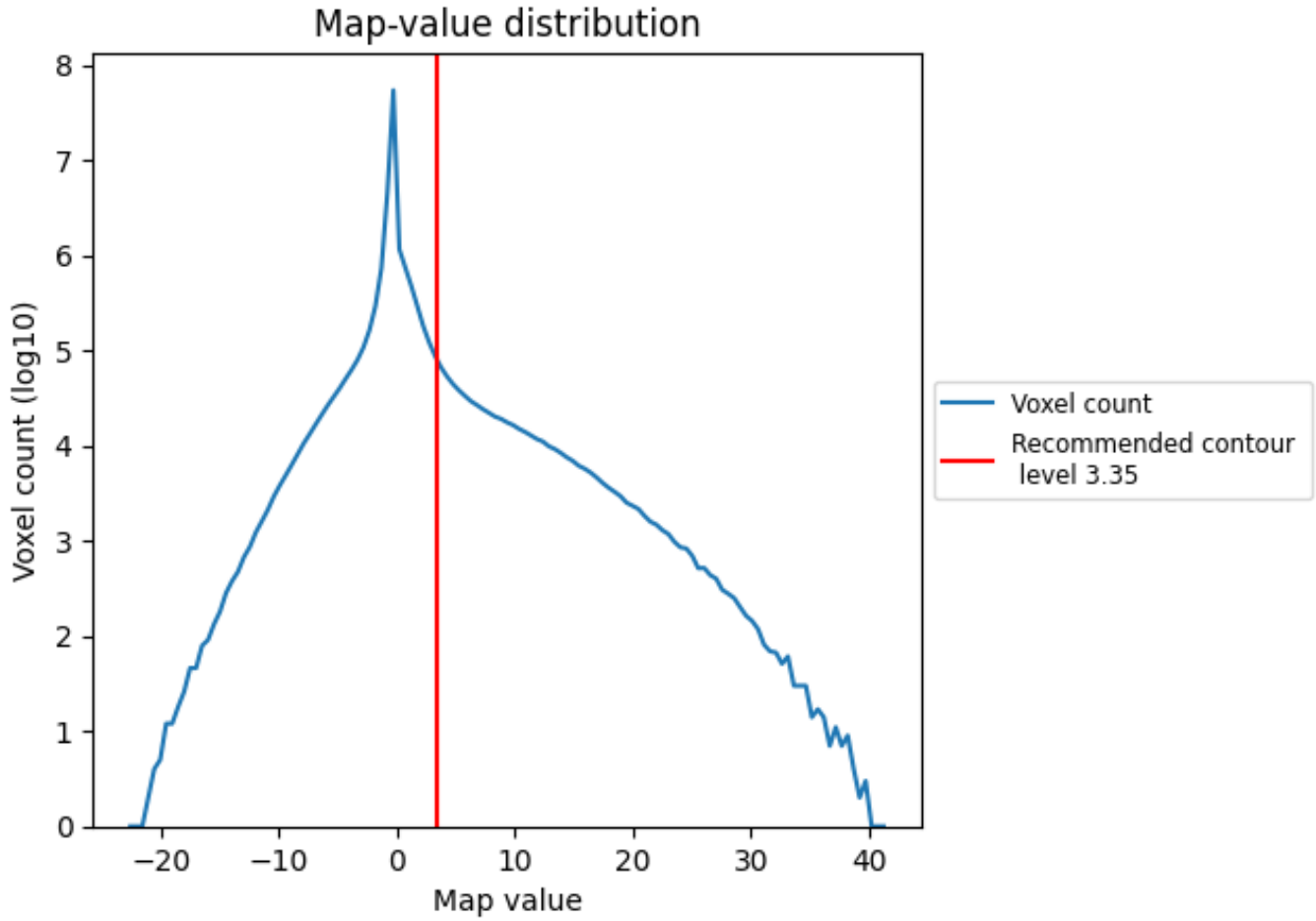


Z

7 Map analysis

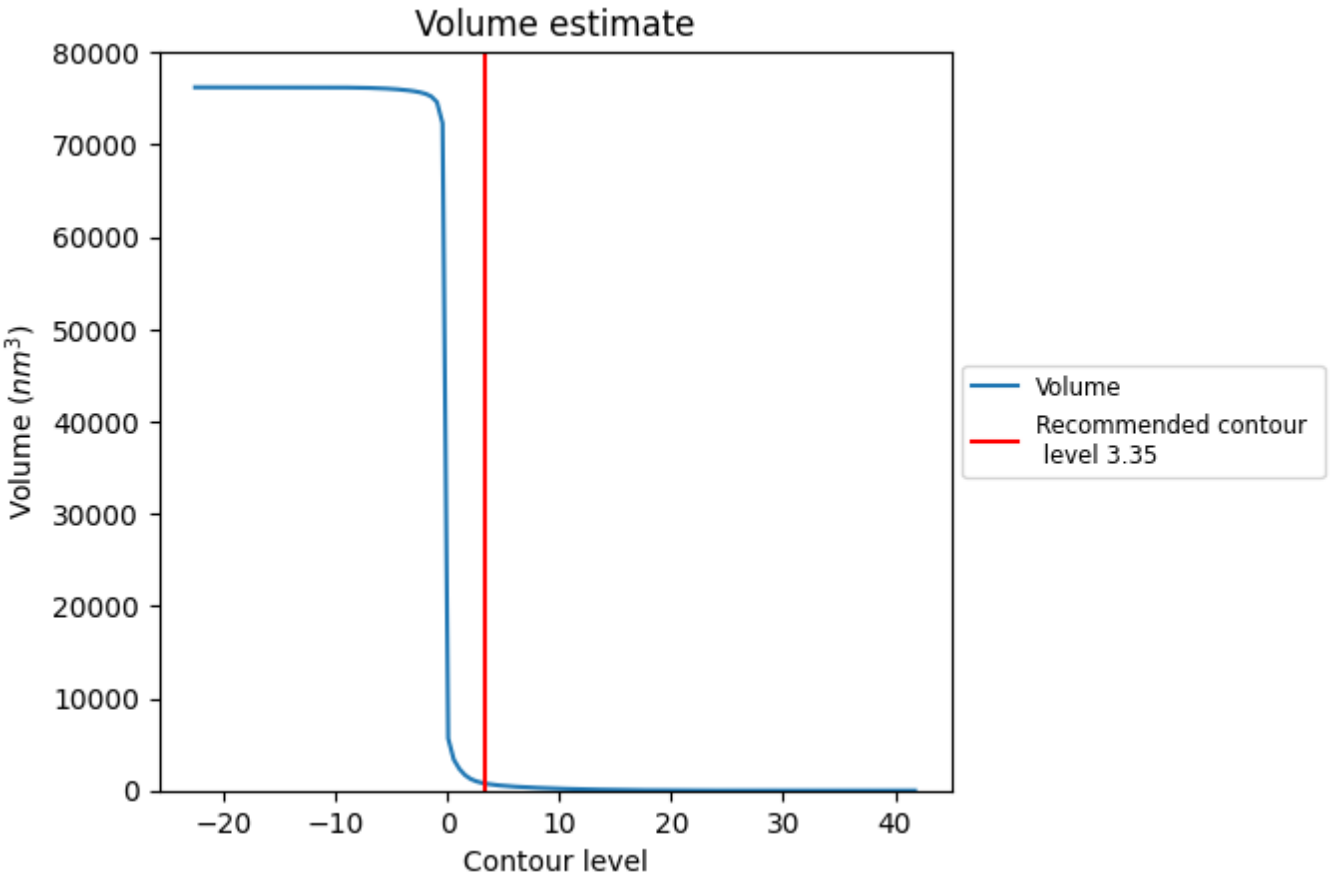
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

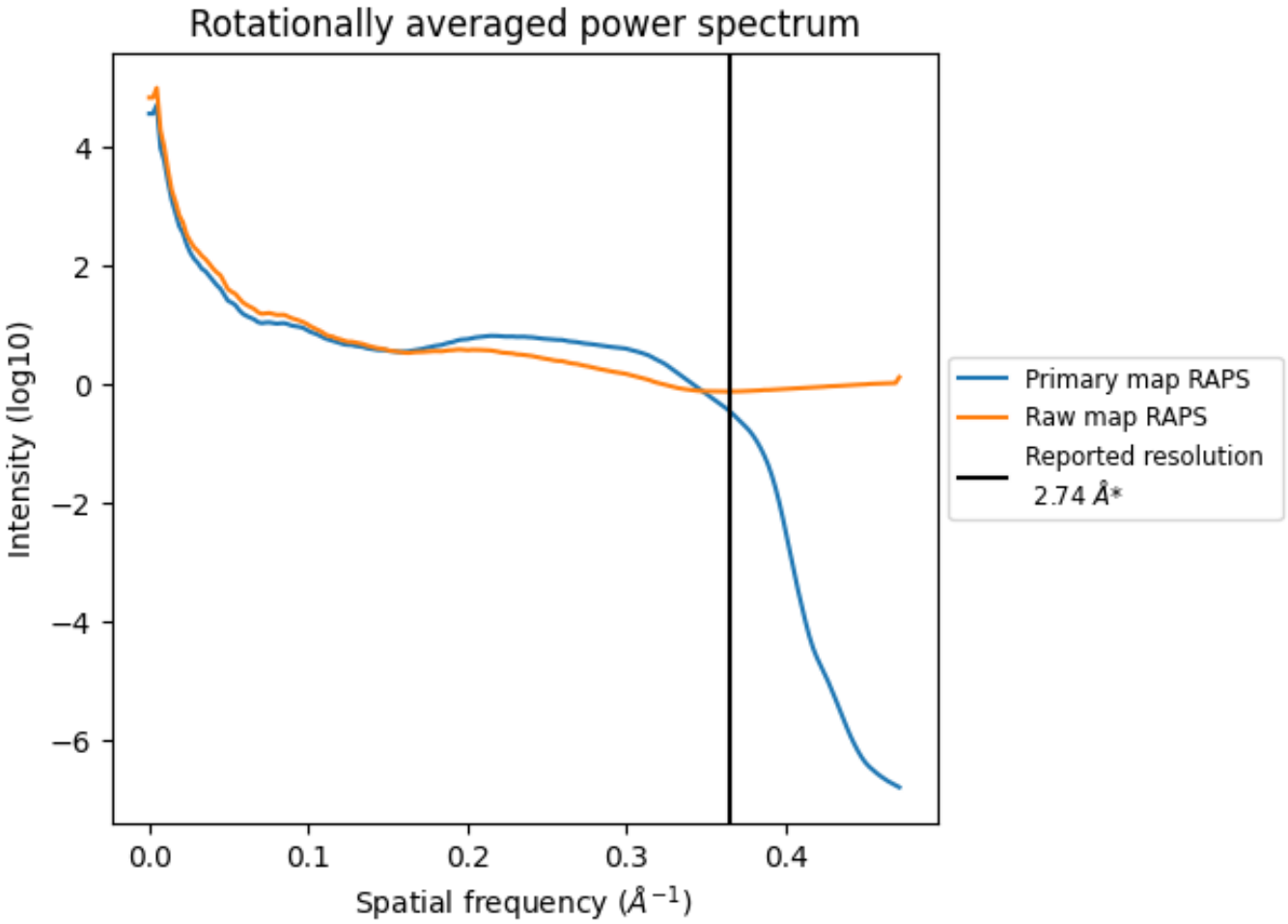
7.2 Volume estimate (i)



The volume at the recommended contour level is 767 nm^3; this corresponds to an approximate mass of 693 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)

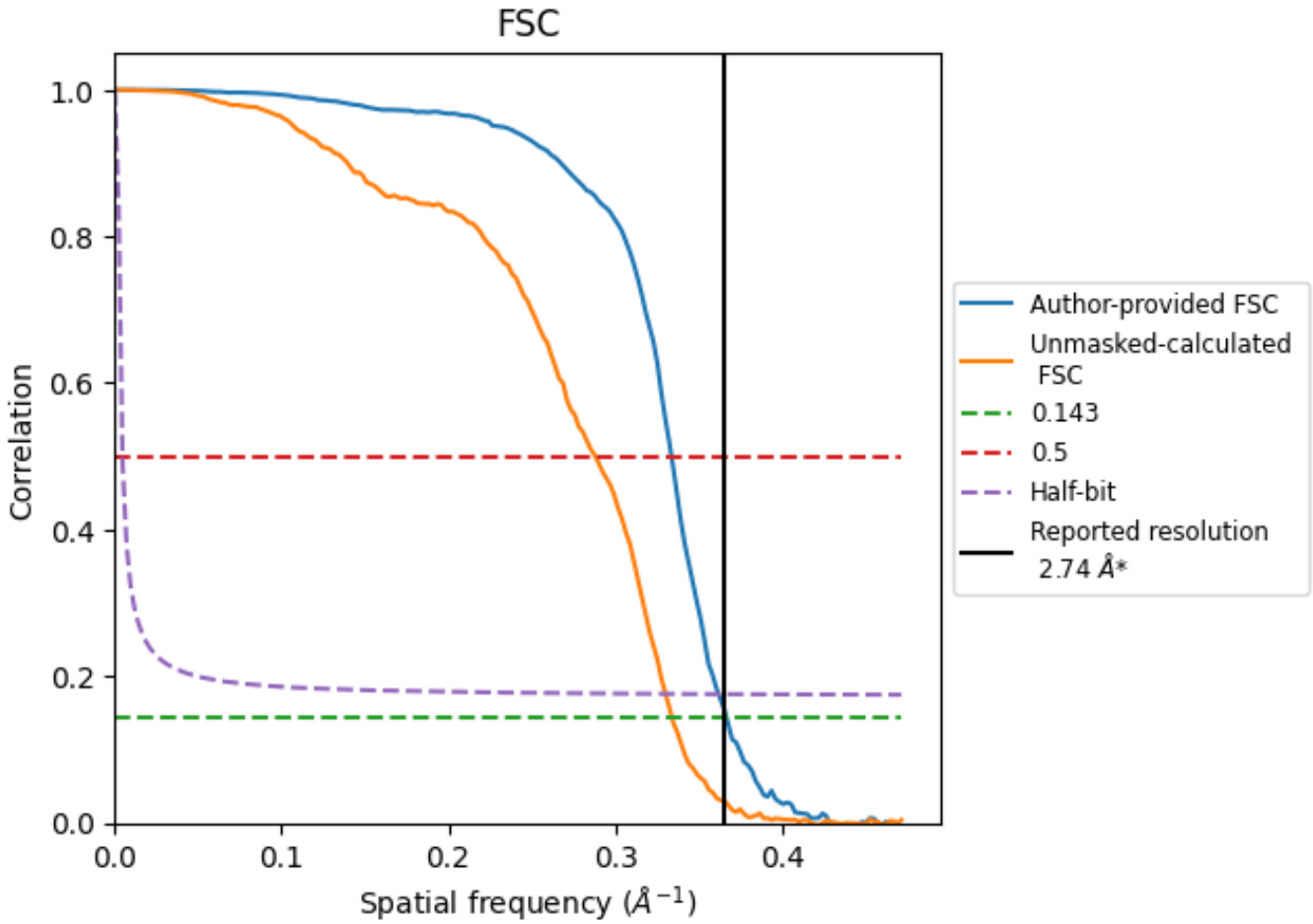


*Reported resolution corresponds to spatial frequency of 0.365 Å^{-1}

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 0.365 Å^{-1}

8.2 Resolution estimates (i)

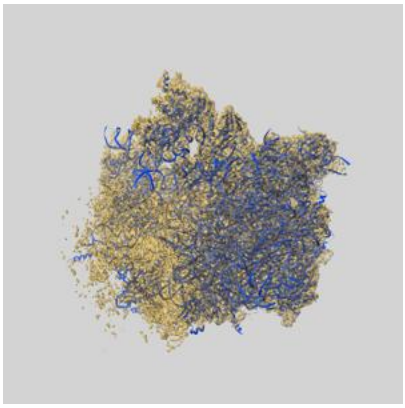
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.73	2.99	2.76
Unmasked-calculated*	2.99	3.47	3.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

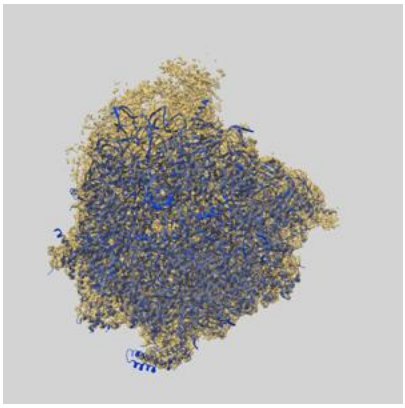
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10973 and PDB model 6YWS. Per-residue inclusion information can be found in section 3 on page 14.

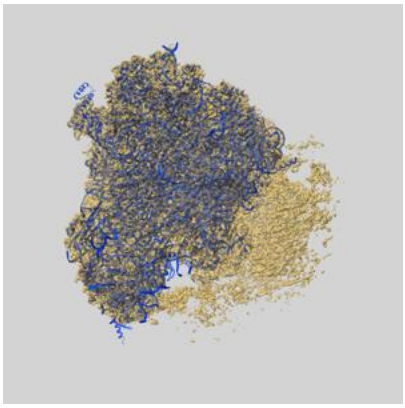
9.1 Map-model overlay



X



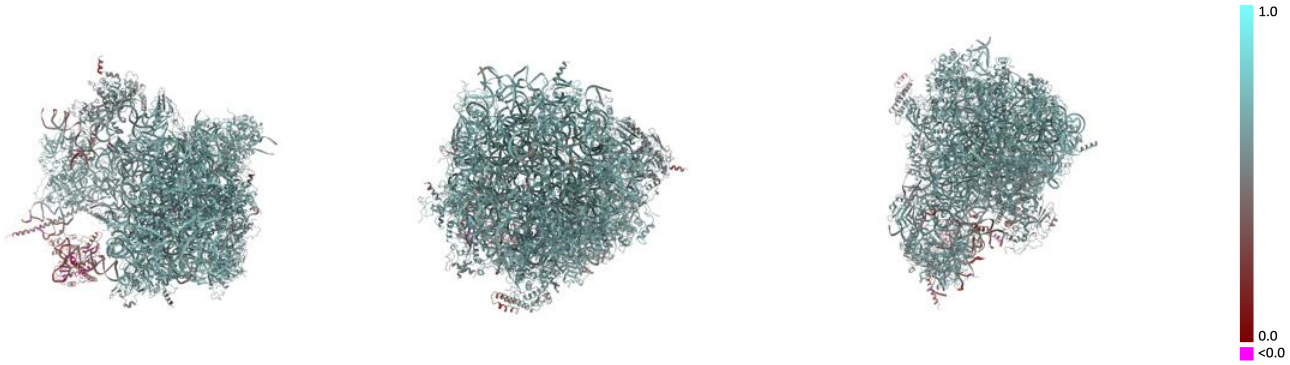
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.35 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.

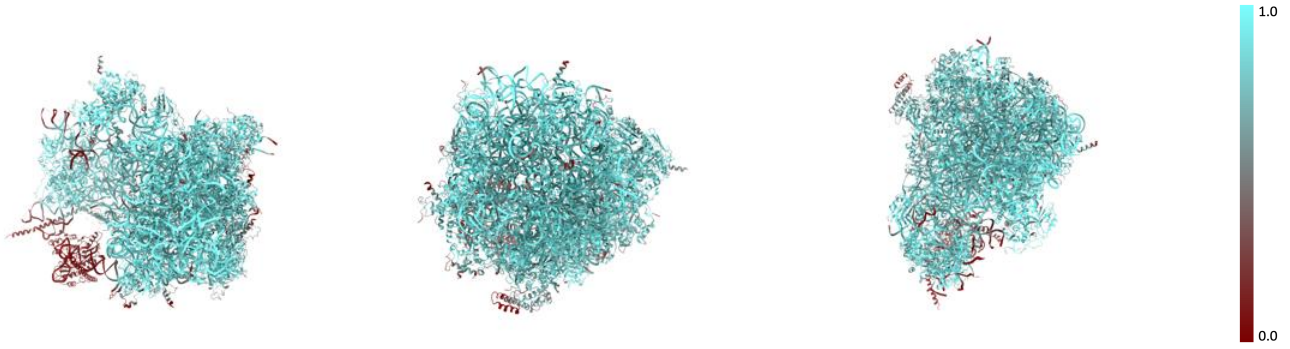
9.2 Q-score mapped to coordinate model



X Y Z

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

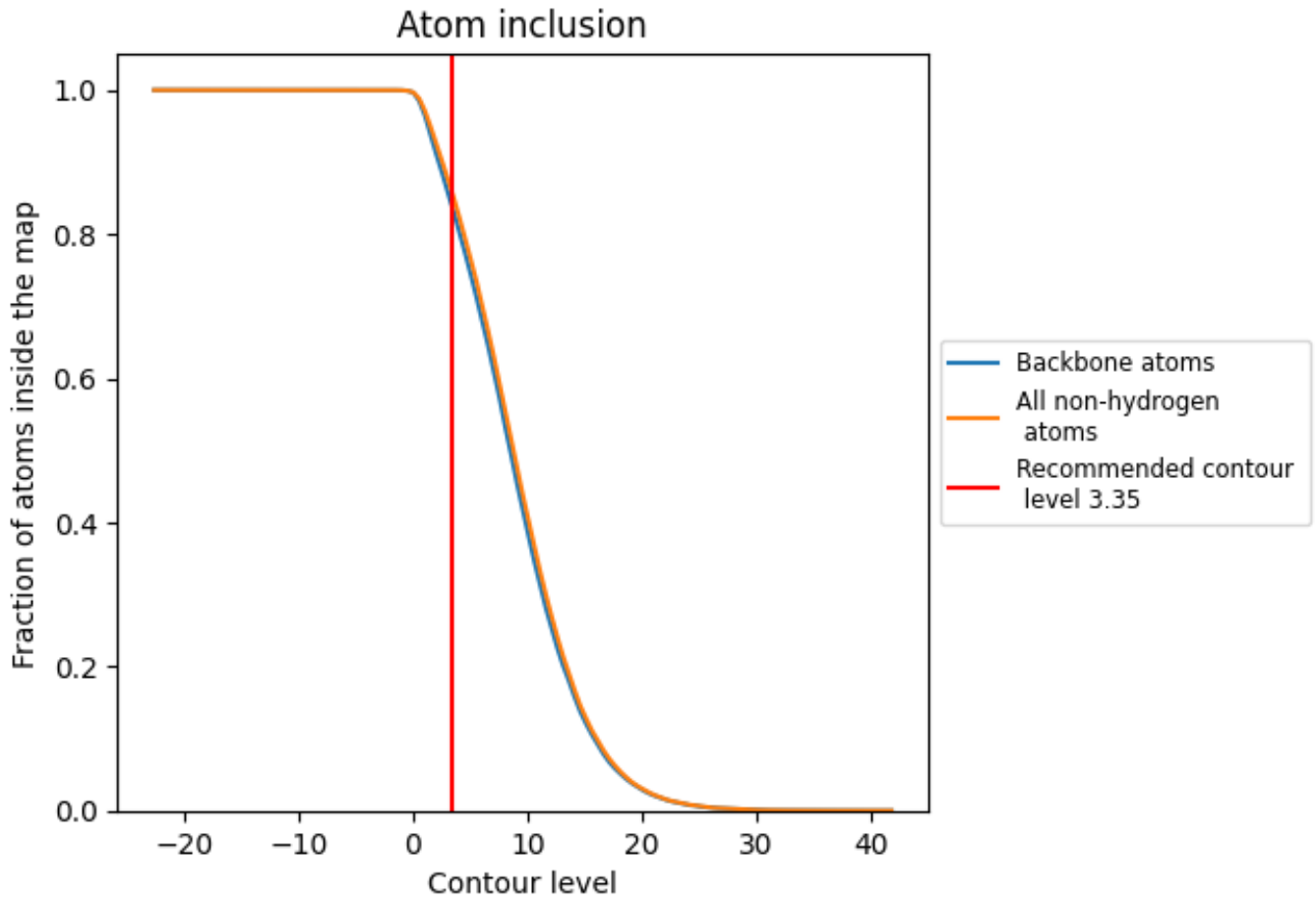
9.3 Atom inclusion mapped to coordinate model



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 (3.35).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 86% 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 (3.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8605	0.6010
0	0.9651	0.6630
1	0.9304	0.6160
2	0.9674	0.6390
3	0.8898	0.6290
4	0.9322	0.6580
5	0.8664	0.6230
6	0.9400	0.6120
7	0.8733	0.6250
8	0.6329	0.5420
9	0.7675	0.5890
A	0.8975	0.6160
B	0.8804	0.6370
C	0.9264	0.6560
D	0.8683	0.6270
E	0.9284	0.6210
F	0.8342	0.5930
G	0.7660	0.5860
H	0.9452	0.6600
I	0.8888	0.6410
J	0.8839	0.6350
K	0.8793	0.6360
L	0.9057	0.6450
M	0.8266	0.6210
N	0.8895	0.6430
O	0.8277	0.6280
P	0.8832	0.6360
Q	0.8191	0.6110
R	0.6841	0.5420
S	0.8370	0.6180
T	0.8606	0.6250
U	0.8565	0.6280
V	0.9588	0.6290
W	0.9357	0.6510
X	0.9072	0.6260

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	0.9625	0.6680
a	0.8446	0.6110
b	0.8055	0.6050
c	0.9433	0.6610
d	0.8625	0.6270
e	0.0000	0.1970
f	0.8893	0.5140
g	0.8937	0.5240
h	0.7709	0.5010
i	0.7587	0.4790
j	0.0000	0.1220