wwPDB EM Validation Summary Report

Oct 24, 2026 – 10:44 am BST

PDB ID	:	9TRT / pdb_00009trt
EMDB ID	:	EMD-56197
Title	:	Structure of the Plant mitochondrial pre-initiation complex 3, (SSU,mtIF3,mRNA,tRNA)
Authors	:	Skaltsogiannis, V.; Giege, P.; Soufari, H.
Deposited on	:	2025-12-27
Resolution	:	3.05 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:

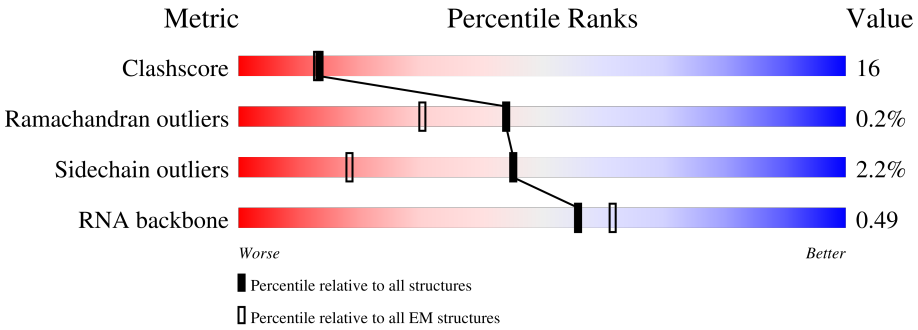
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

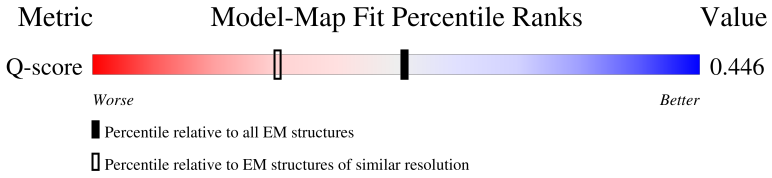
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.05 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13971 (2.55 - 3.55)

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	2	1601	7% 50% 40% 9%
2	5	77	58% 6% 51% 40% .
3	6	5	60% 40% 60%

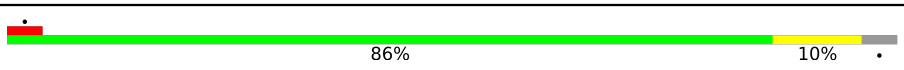
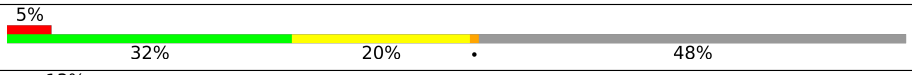
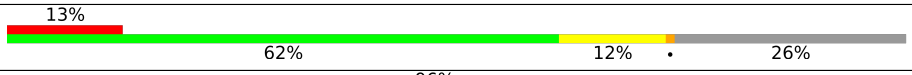
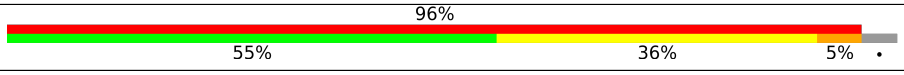
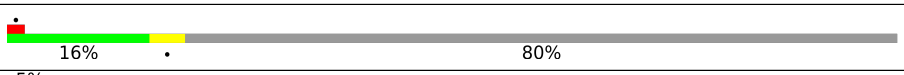
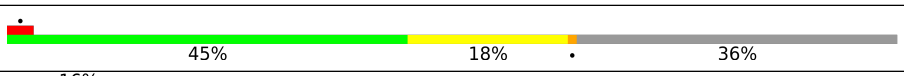
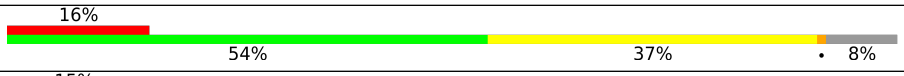
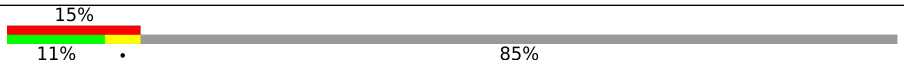
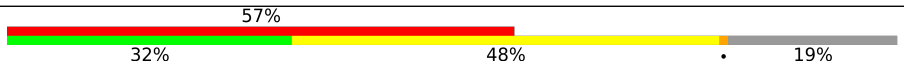
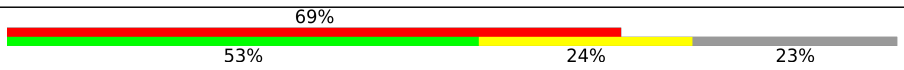
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Mol	Chain	Length	Quality of chain
4	8	520	18% 28% 9% 63%
5	A	212	60% 34%
6	B	554	13% 67% 17% 16%
7	C	362	6% 59% 31% 8%
8	D	501	15% 57% 26% 17%
9	E	138	48% 24% 27%
10	F	157	87% 82% 18%
11	G	129	73% 26%
12	H	383	12% 40% 14% 45%
13	I	228	43% 6% 50%
14	J	304	7% 24% 17% 58%
15	K	125	81% 18%
16	L	154	64% 8% 29%
17	M	155	61% 5% 35%
18	N	414	22% 5% 72%
19	O	136	60% 21% 19%
20	P	110	7% 58% 25% 17%
21	Q	237	28% 9% 62%
22	R	212	40% 62% 16% 22%
23	S	100	16% 45% 30% 25%
24	T	94	51% 47%
25	U	192	41% 35% 31% 34%
26	V	193	5% 60% 24% 15%
27	W	483	66% 13% 21%
28	X	496	32% 8% 59%

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Mol	Chain	Length	Quality of chain
29	Y	102	
30	Z	153	
31	a	424	
32	b	80	
33	c	128	
34	d	110	
35	e	383	
36	f	410	
37	g	668	
38	h	384	
39	i	725	
40	k	153	
41	l	576	

2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 92974 atoms, of which 1558 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1599	34252	15300	6247	11106	1599	0	0

- Molecule 2 is a RNA chain called initiator tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	77	1641	733	294	537	77	0	0

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	6	5	107	48	19	35	5	0	0

- Molecule 4 is a protein called Translation initiation factor IF3-1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	8	190	3075	968	1558	272	270	7	0	0

- Molecule 5 is a protein called Ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	204	1611	1032	284	285	10	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	467	3877	2520	701	643	13	0	0

- Molecule 7 is a protein called Ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	333	Total	C	N	O	S	0	0
			2806	1793	540	462	11		

- Molecule 8 is a protein called S5 DRBM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	417	Total	C	N	O	S	0	0
			3425	2146	603	664	12		

- Molecule 9 is a protein called Ribosomal protein bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	101	Total	C	N	O	S	0	0
			823	535	145	138	5		

- Molecule 10 is a protein called Small ribosomal subunit protein uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	157	Total	C	N	O	S	0	0
			1254	793	244	213	4		

- Molecule 11 is a protein called 30S ribosomal protein S8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	128	Total	C	N	O	S	0	0
			1037	652	193	189	3		

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	212	Total	C	N	O	S	0	0
			1671	1048	308	310	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS10 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	113	Total	C	N	O	S	0	0
			941	602	174	159	6		

- Molecule 14 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	127	Total 988	C 608	N 195	O 181	S 4	0	0

- Molecule 15 is a protein called Small ribosomal subunit protein uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	124	Total 993	C 614	N 209	O 166	S 4	0	0

- Molecule 16 is a protein called Ribosomal protein uS13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	110	Total 873	C 529	N 185	O 154	S 5	0	0

- Molecule 17 is a protein called Small ribosomal subunit protein uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	101	Total 843	C 524	N 174	O 140	S 5	0	0

- Molecule 18 is a protein called Small ribosomal subunit protein uS15c.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	116	Total 941	C 593	N 170	O 171	S 7	0	0

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	110	Total 869	C 550	N 169	O 144	S 6	0	0

- Molecule 20 is a protein called Small ribosomal subunit protein uS17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	91	Total 717	C 455	N 135	O 124	S 3	0	0

- Molecule 21 is a protein called Small ribosomal subunit protein bS18c.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	90	Total	C	N	O	S	0	0
			724	460	127	134	3		

- Molecule 22 is a protein called Small ribosomal subunit protein uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	166	Total	C	N	O	S	0	0
			1299	819	236	237	7		

- Molecule 23 is a protein called Ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	75	Total	C	N	O	S	0	0
			611	386	120	103	2		

- Molecule 24 is a protein called 30S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	50	Total	C	N	O	S	0	0
			408	260	79	68	1		

- Molecule 25 is a protein called Ribosomal protein mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	127	Total	C	N	O	S	0	0
			1014	647	184	178	5		

- Molecule 26 is a protein called Ribosomal protein mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	164	Total	C	N	O	S	0	0
			1399	874	266	255	4		

- Molecule 27 is a protein called Small ribosomal subunit protein mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	380	Total	C	N	O	S	0	0
			3062	1955	535	559	13		

- Molecule 28 is a protein called RRM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	204	Total	C	N	O	S	0	0
			1613	1011	262	329	11		

- Molecule 29 is a protein called MOSC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	98	Total	C	N	O	S	0	0
			793	495	159	137	2		

- Molecule 30 is a protein called Ribosomal Protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	80	Total	C	N	O	S	0	0
			649	422	121	104	2		

- Molecule 31 is a protein called Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	315	Total	C	N	O	S	0	0
			2486	1546	448	482	10		

- Molecule 32 is a protein called CBS domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	77	Total	C	N	O	S	0	0
			610	378	116	108	8		

- Molecule 33 is a protein called Small ribosomal subunit protein mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	26	Total	C	N	O	S	0	0
			232	145	54	32	1		

- Molecule 34 is a protein called IGR domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	78	Total	C	N	O	S	0	0
			616	403	110	102	1		

- Molecule 35 is a protein called Ribosomal protein mS45.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	246	Total	C	N	O	S	0	0
			2074	1310	374	380	10		

- Molecule 36 is a protein called Ribosomal protein mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	377	Total	C	N	O	S	0	0
			2922	1843	486	573	20		

- Molecule 37 is a protein called Small ribosomal subunit protein mS81 (rPPR8).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	103	Total	C	N	O	S	0	0
			814	524	132	151	7		

- Molecule 38 is a protein called Adenylyl cyclase.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	310	Total	C	N	O	S	0	0
			2463	1557	438	455	13		

- Molecule 39 is a protein called PROP1-like PPR domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	336	Total	C	N	O	S	0	0
			2722	1716	458	533	15		

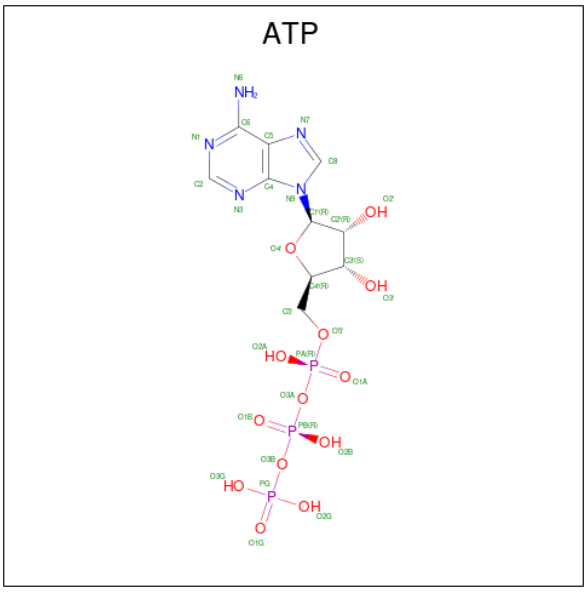
- Molecule 40 is a protein called RRM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	28	Total	C	N	O	S	0	0
			220	139	42	35	4		

- Molecule 41 is a protein called Small ribosomal subunit protein mS80 (rPPR6).

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	442	Total	C	N	O	S	0	0
			3468	2209	573	663	23		

- Molecule 42 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
42	W	1	Total	C	N	O	P	0
			31	10	5	13	3	

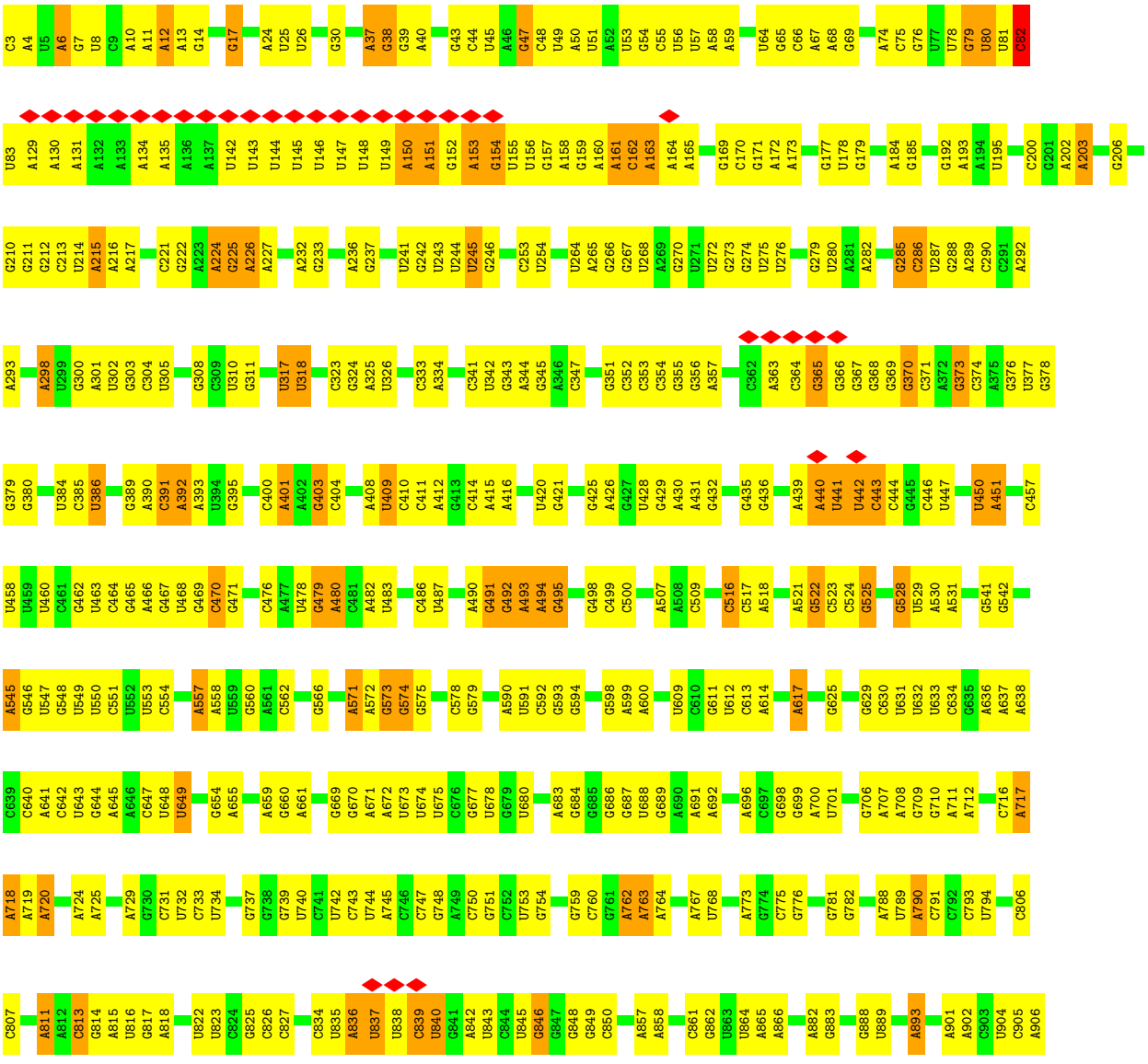
3 Residue-property plots (i)

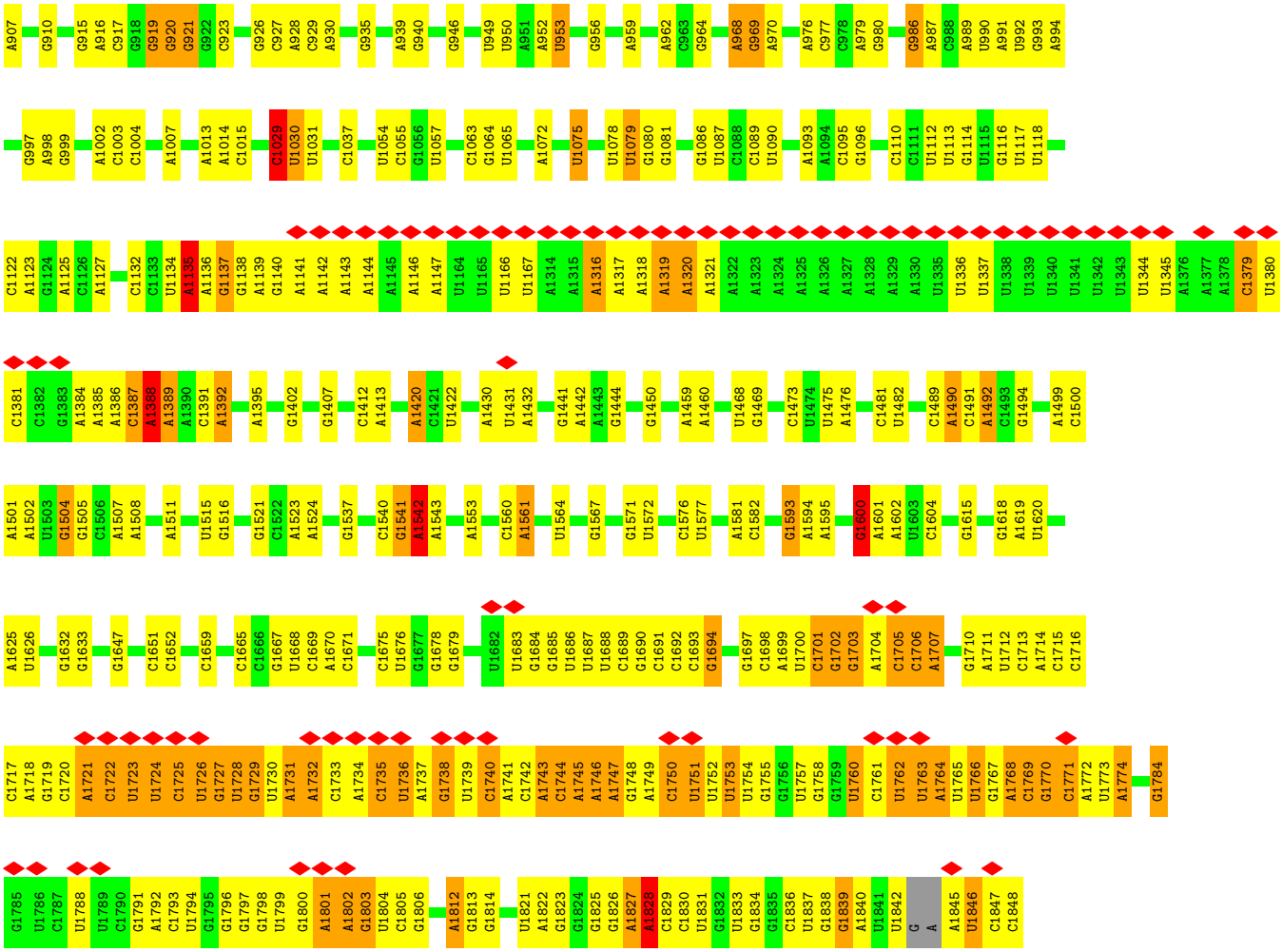
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 18S rRNA

Chain 2:



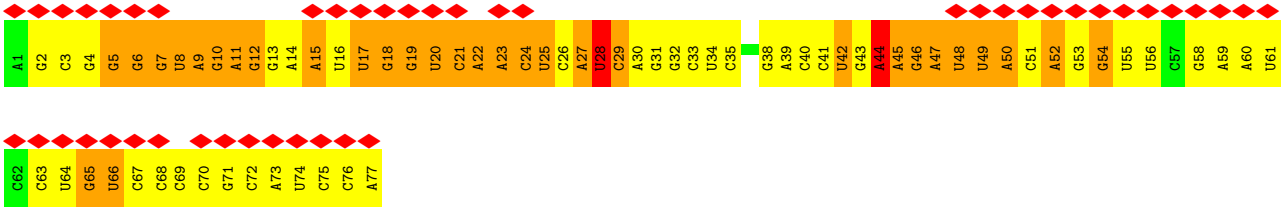




• Molecule 2: initiator tRNA

Chain 5:

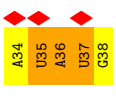




• Molecule 3: mRNA

Chain 6:

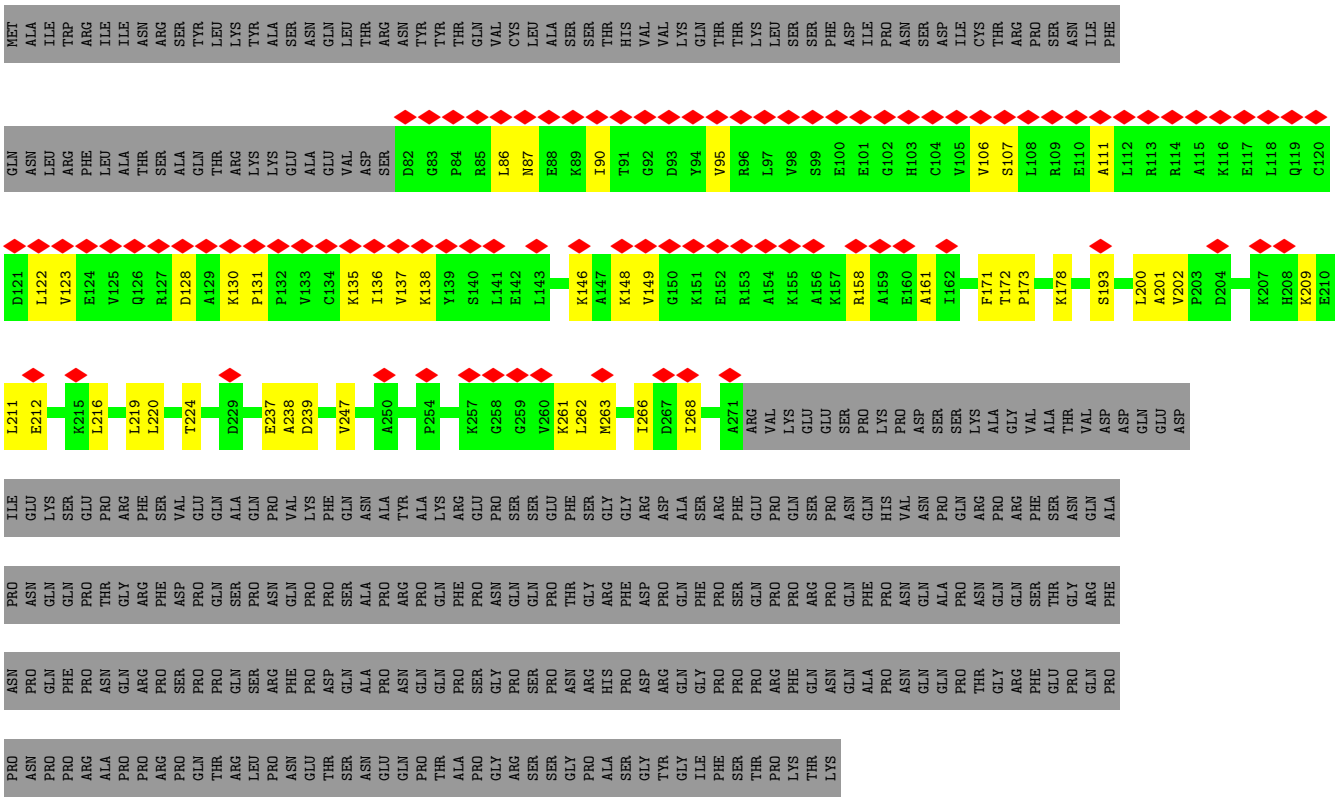




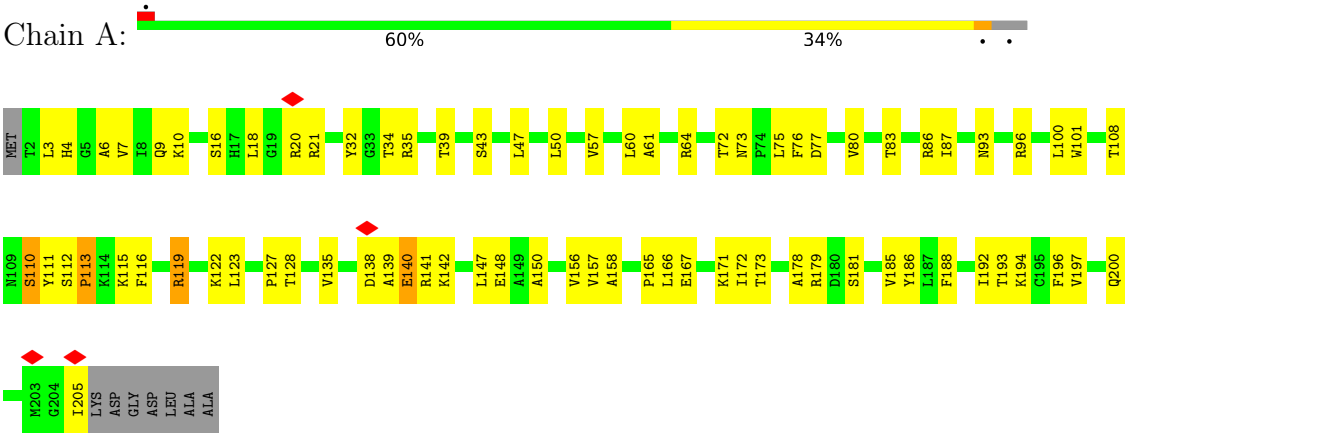
• Molecule 4: Translation initiation factor IF3-1, mitochondrial

Chain 8:

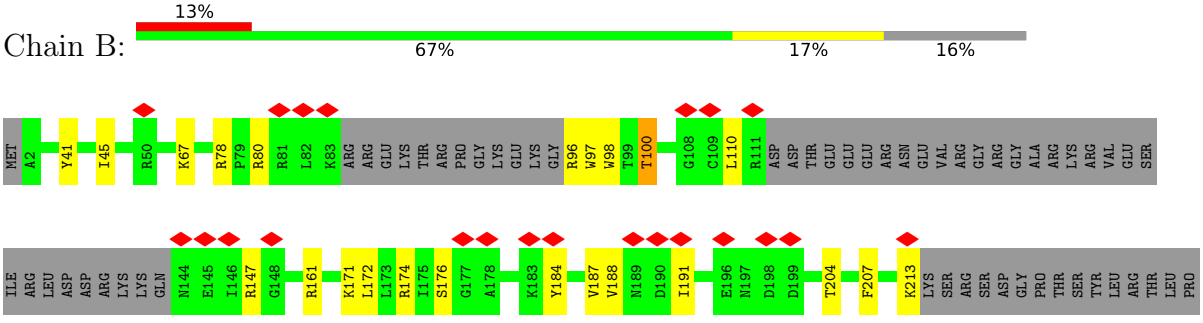


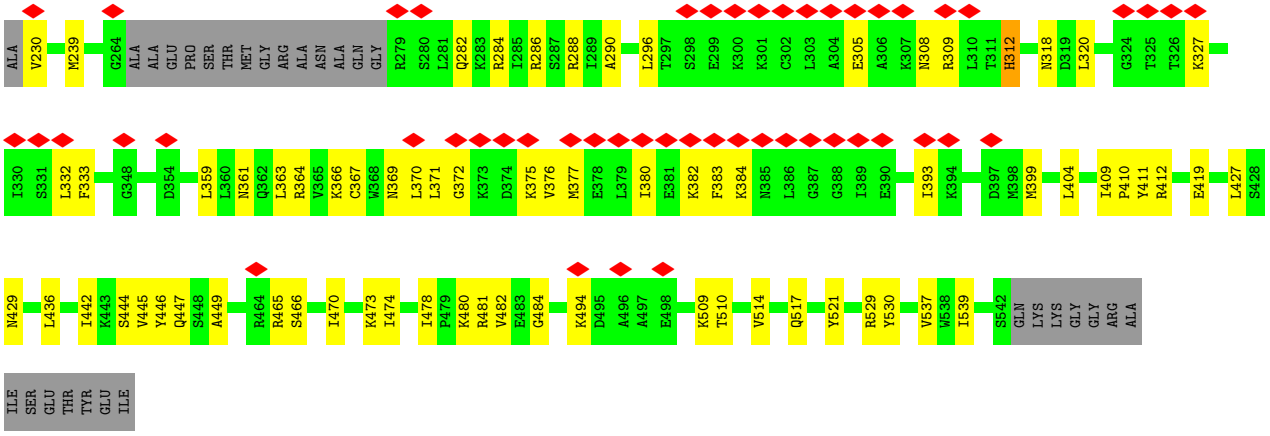


• Molecule 5: Ribosomal protein S2



• Molecule 6: Small ribosomal subunit protein uS3m

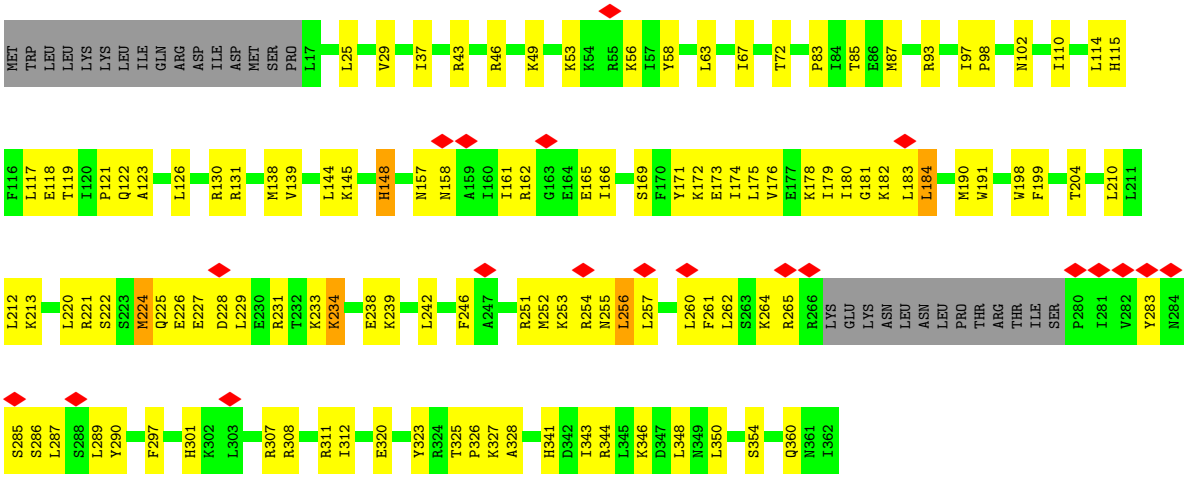




• Molecule 7: Ribosomal protein S4

Chain C:

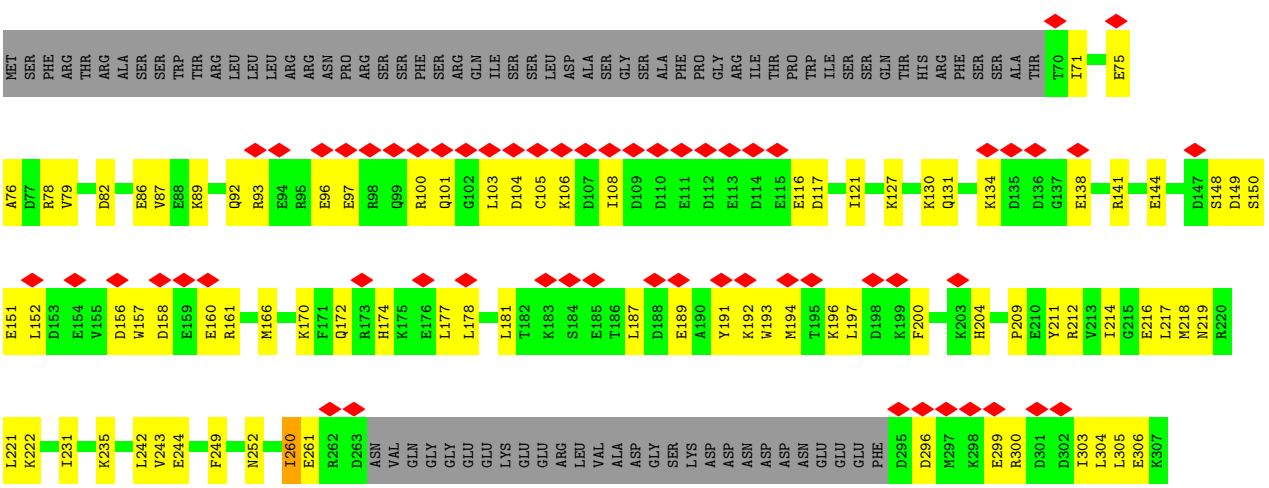


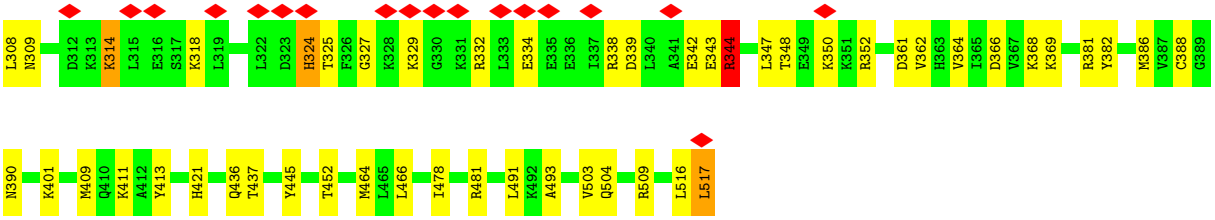


• Molecule 8: S5 DRBM domain-containing protein

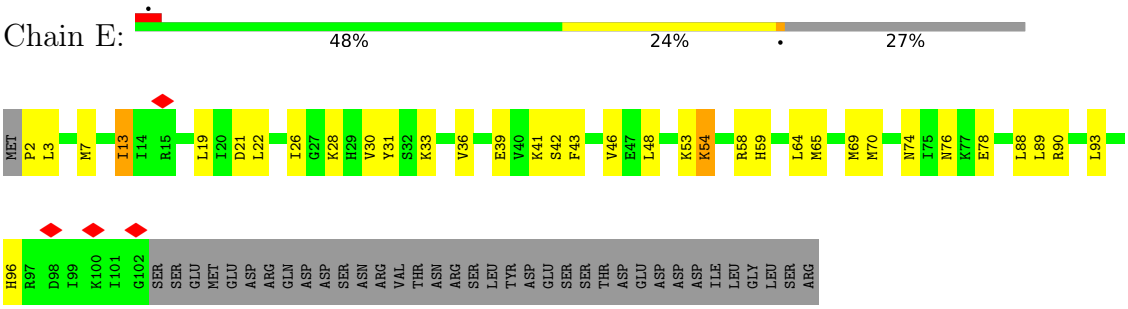
Chain D:



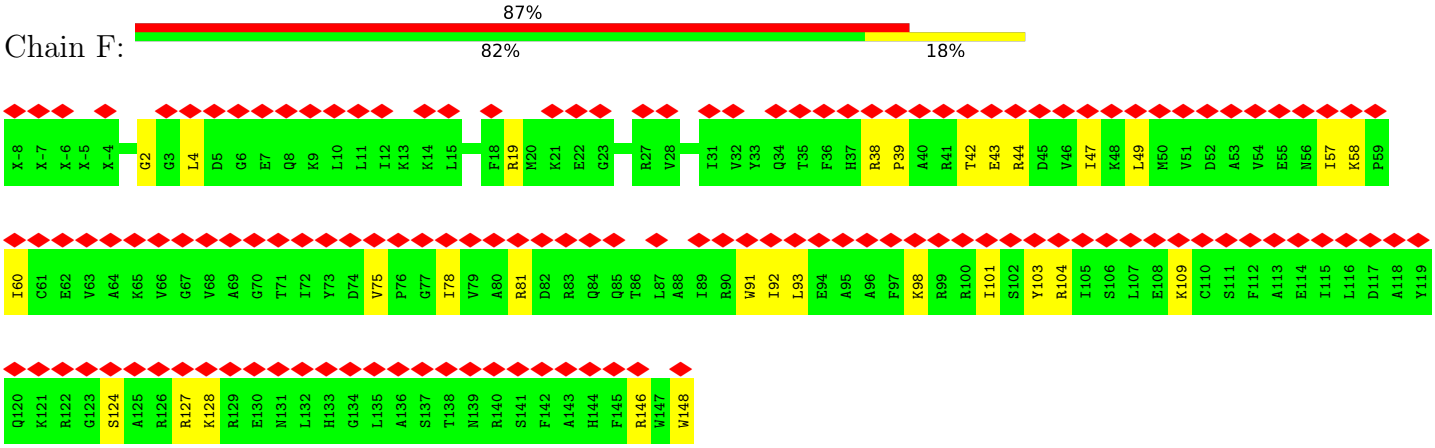




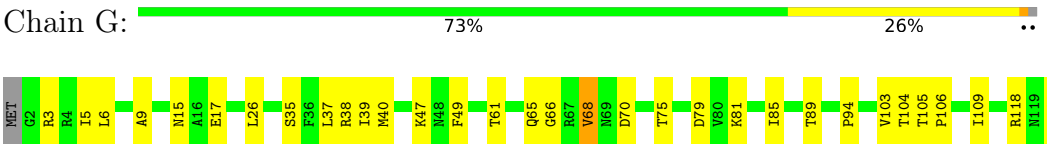
• Molecule 9: Ribosomal protein bS6m



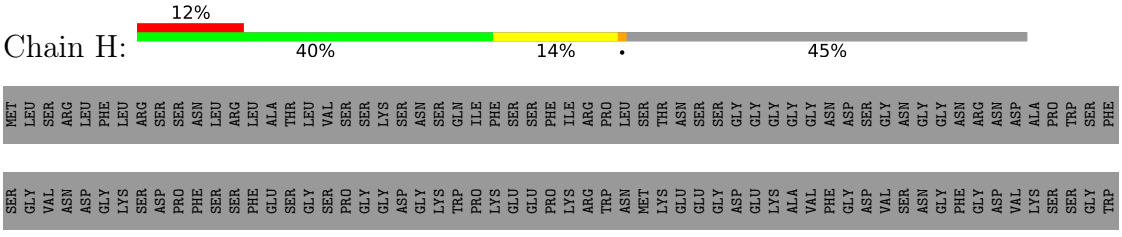
• Molecule 10: Small ribosomal subunit protein uS7m

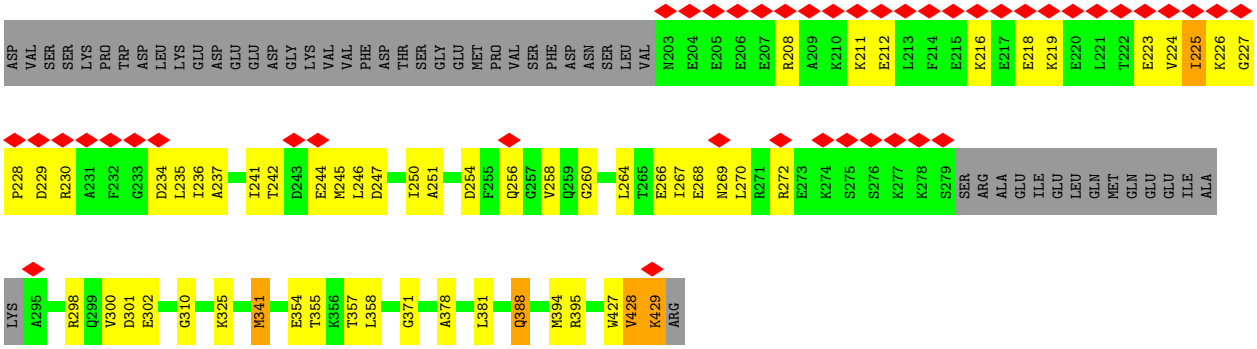


• Molecule 11: 30S ribosomal protein S8, chloroplastic



• Molecule 12: 30S ribosomal protein S9

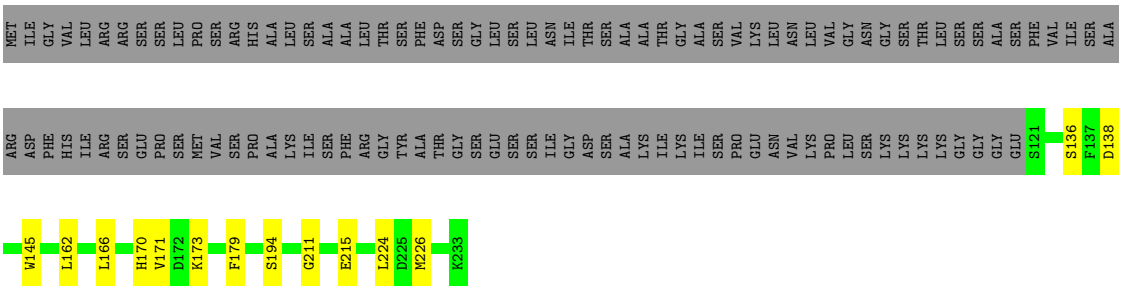




• Molecule 13: Small ribosomal subunit protein uS10 domain-containing protein

Chain I:

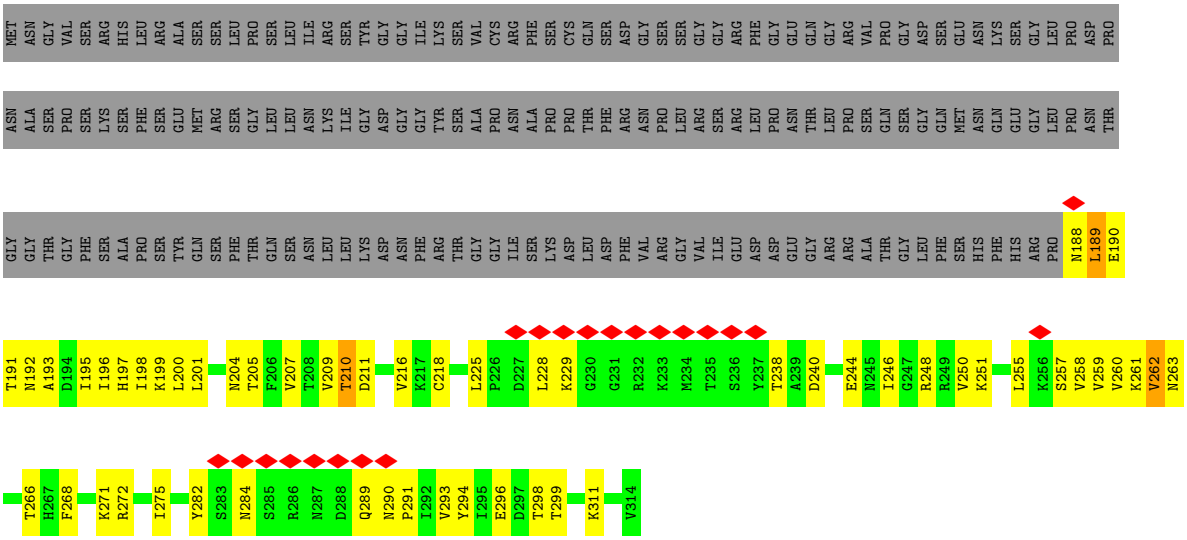




• Molecule 14: Ribosomal protein S11

Chain J:

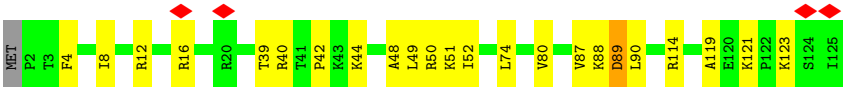




• Molecule 15: Small ribosomal subunit protein uS12m

Chain K:

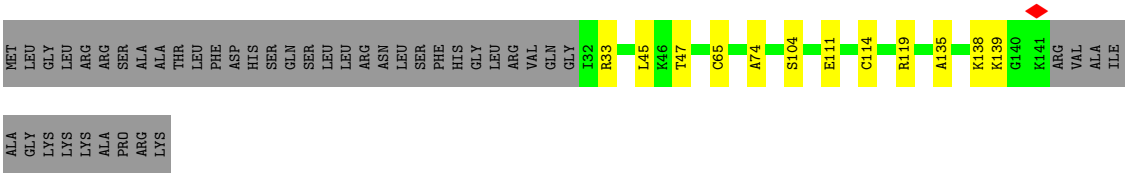




• Molecule 16: Ribosomal protein uS13m

Chain L:

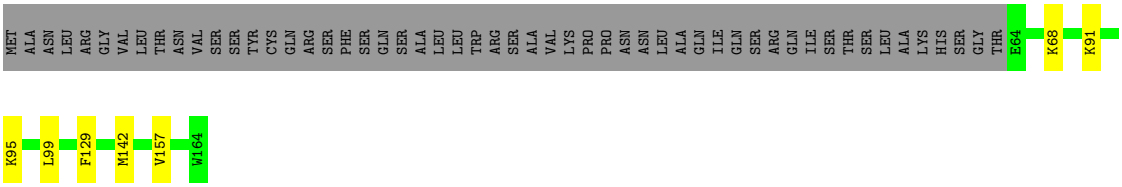




• Molecule 17: Small ribosomal subunit protein uS14m

Chain M:

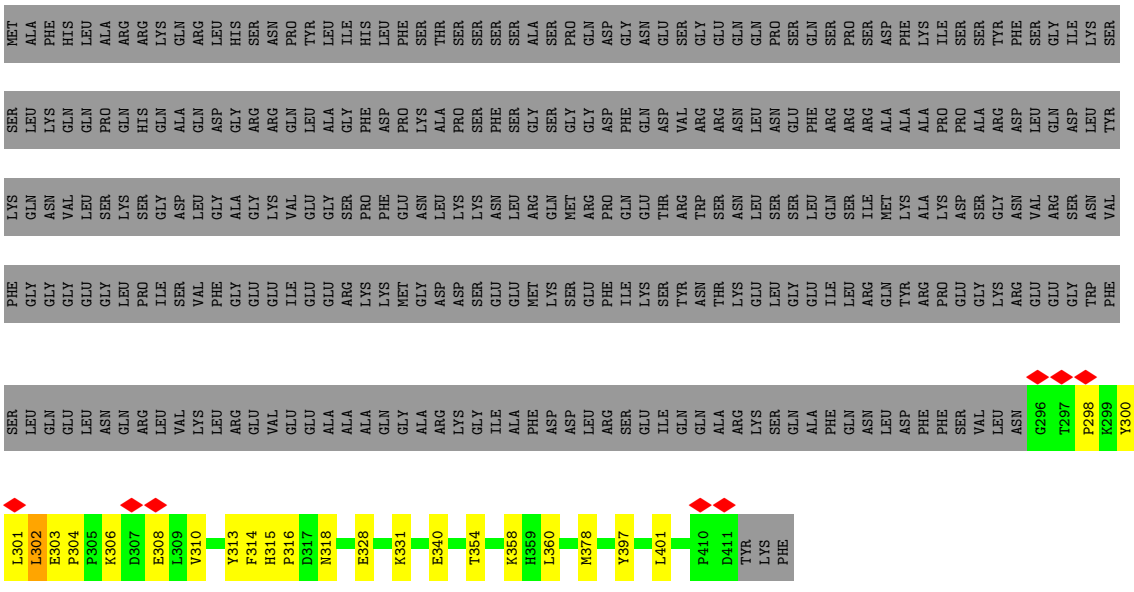




• Molecule 18: Small ribosomal subunit protein uS15c

Chain N:

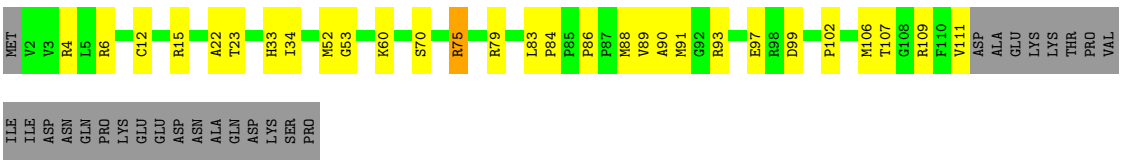




• Molecule 19: 30S ribosomal protein S16

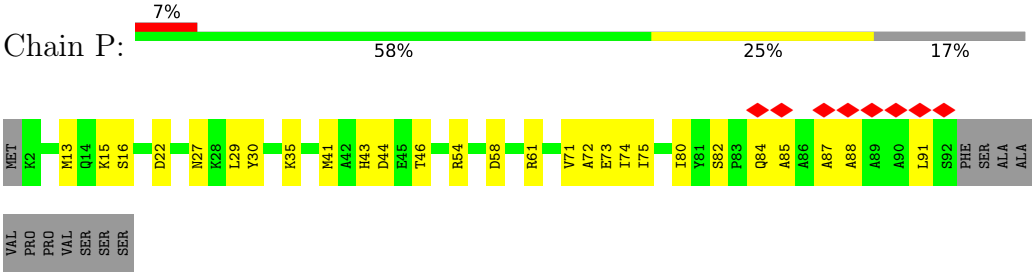
Chain O:





• Molecule 20: Small ribosomal subunit protein uS17c

Chain P:



• Molecule 21: Small ribosomal subunit protein bS18c

Chain Q:



• Molecule 22: Small ribosomal subunit protein uS19m

Chain R:



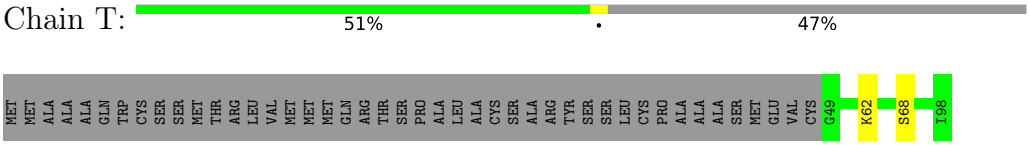
• Molecule 23: Ribosomal protein S21

Chain S:



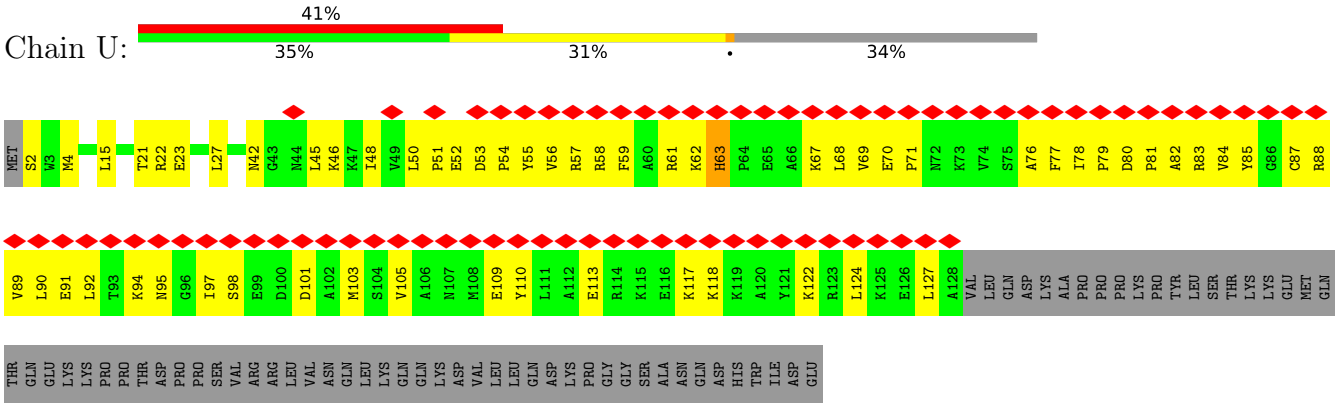
• Molecule 24: 30S ribosomal protein S31, mitochondrial

Chain T:



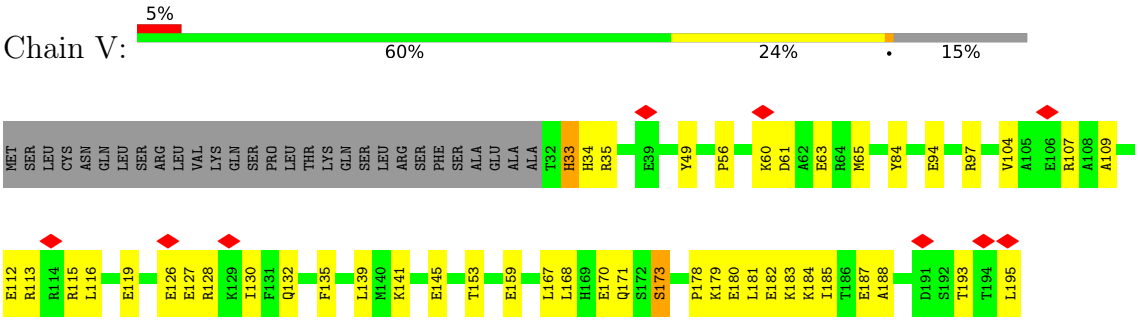
• Molecule 25: Ribosomal protein mS23

Chain U:



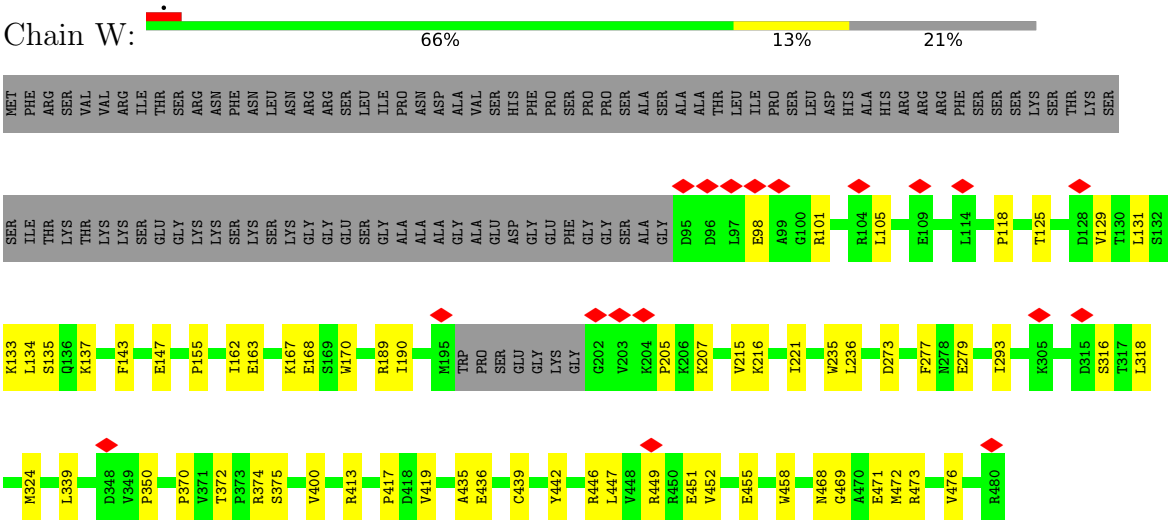
• Molecule 26: Ribosomal protein mS26

Chain V:



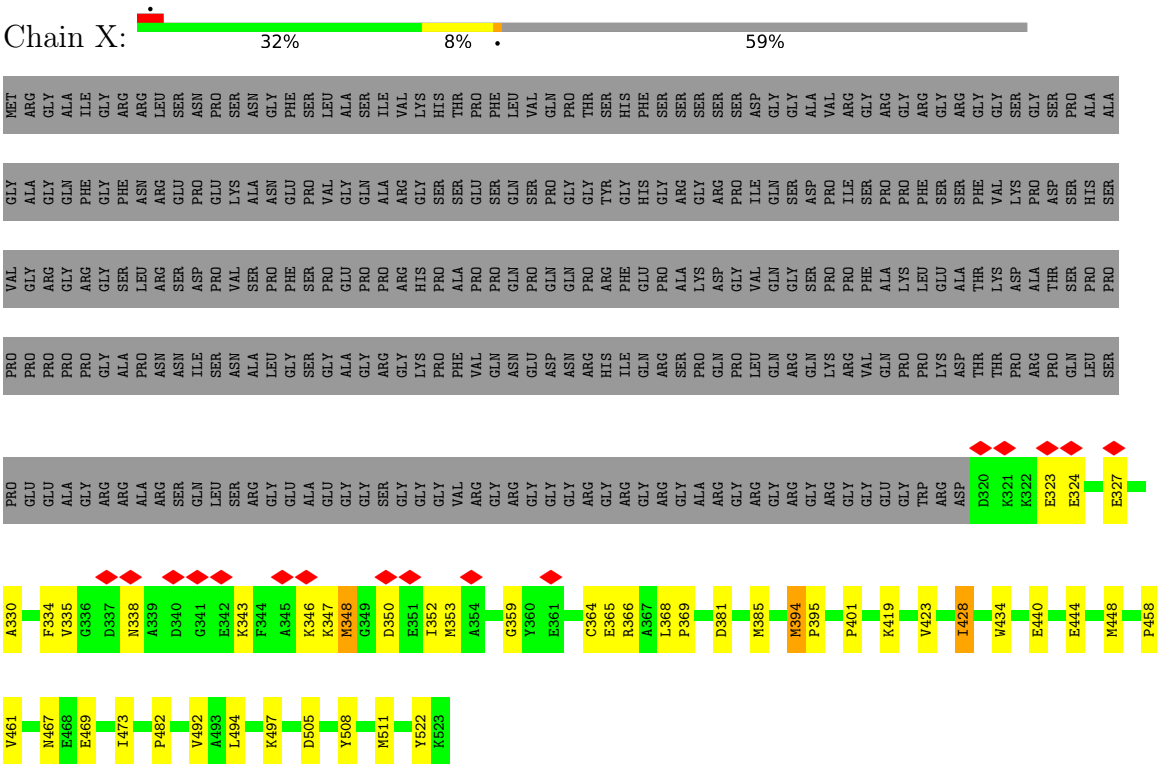
• Molecule 27: Small ribosomal subunit protein mS29

Chain W:



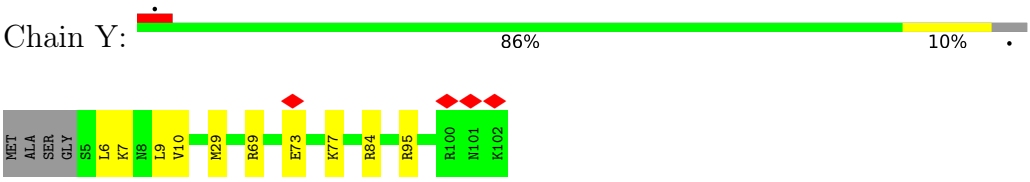
• Molecule 28: RRM domain-containing protein

Chain X:



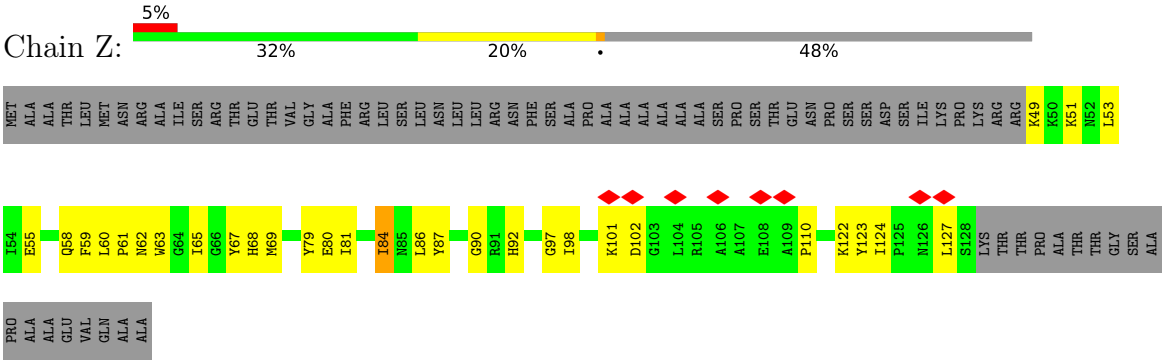
• Molecule 29: MOSC domain-containing protein

Chain Y:



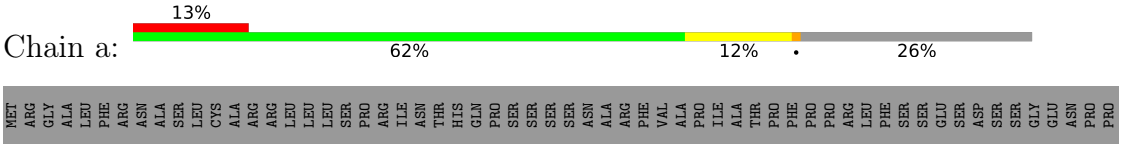
• Molecule 30: Ribosomal Protein S34, mitochondrial

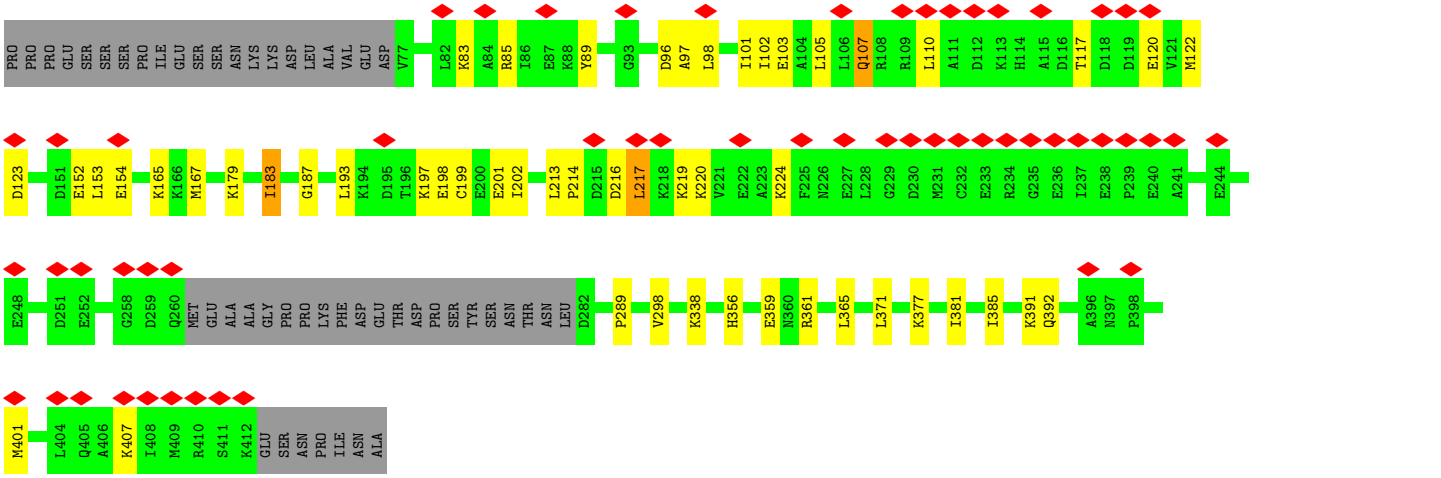
Chain Z:



• Molecule 31: Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein

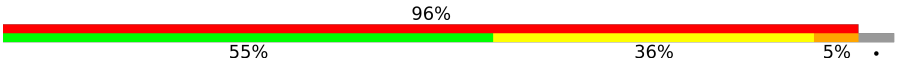
Chain a:

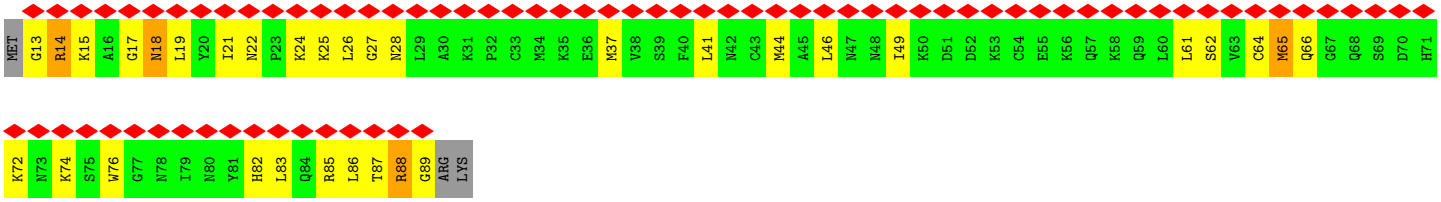




• Molecule 32: CBS domain-containing protein

Chain b:

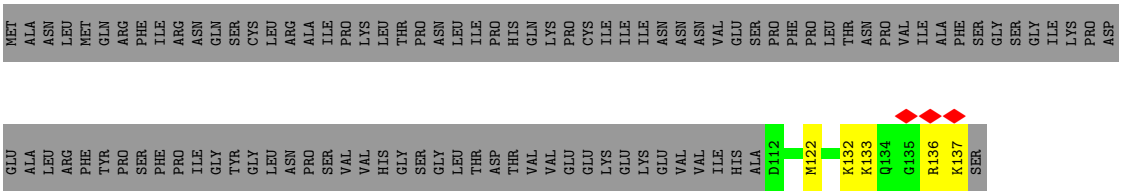




• Molecule 33: Small ribosomal subunit protein mS38

Chain c:

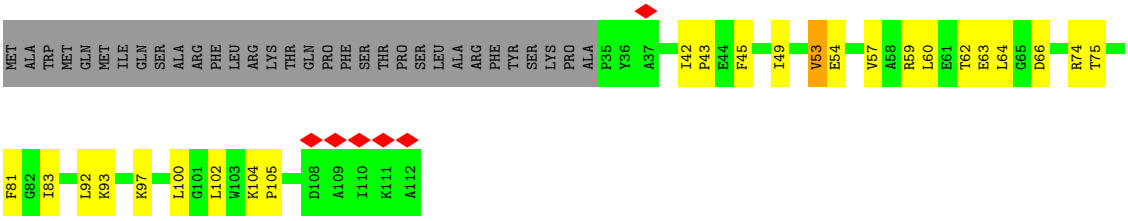




• Molecule 34: IGR domain-containing protein

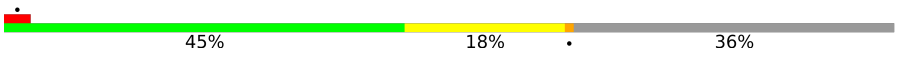
Chain d:

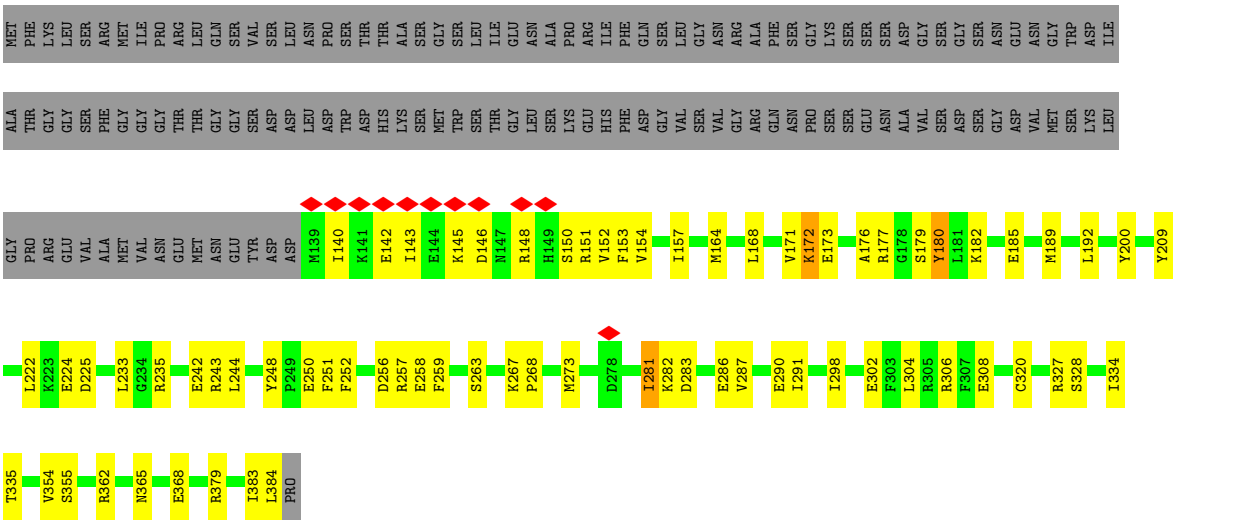




• Molecule 35: Ribosomal protein mS45

Chain e:

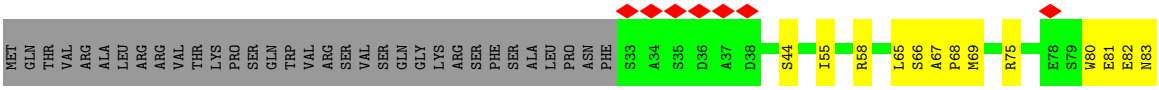




• Molecule 36: Ribosomal protein mS47

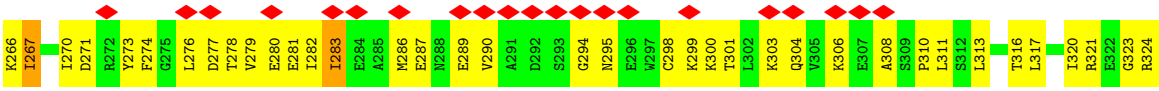
Chain f:

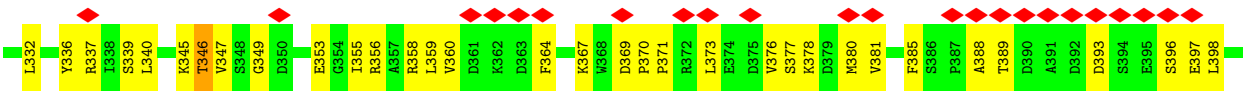




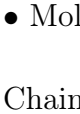








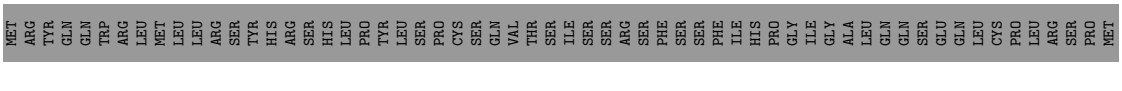




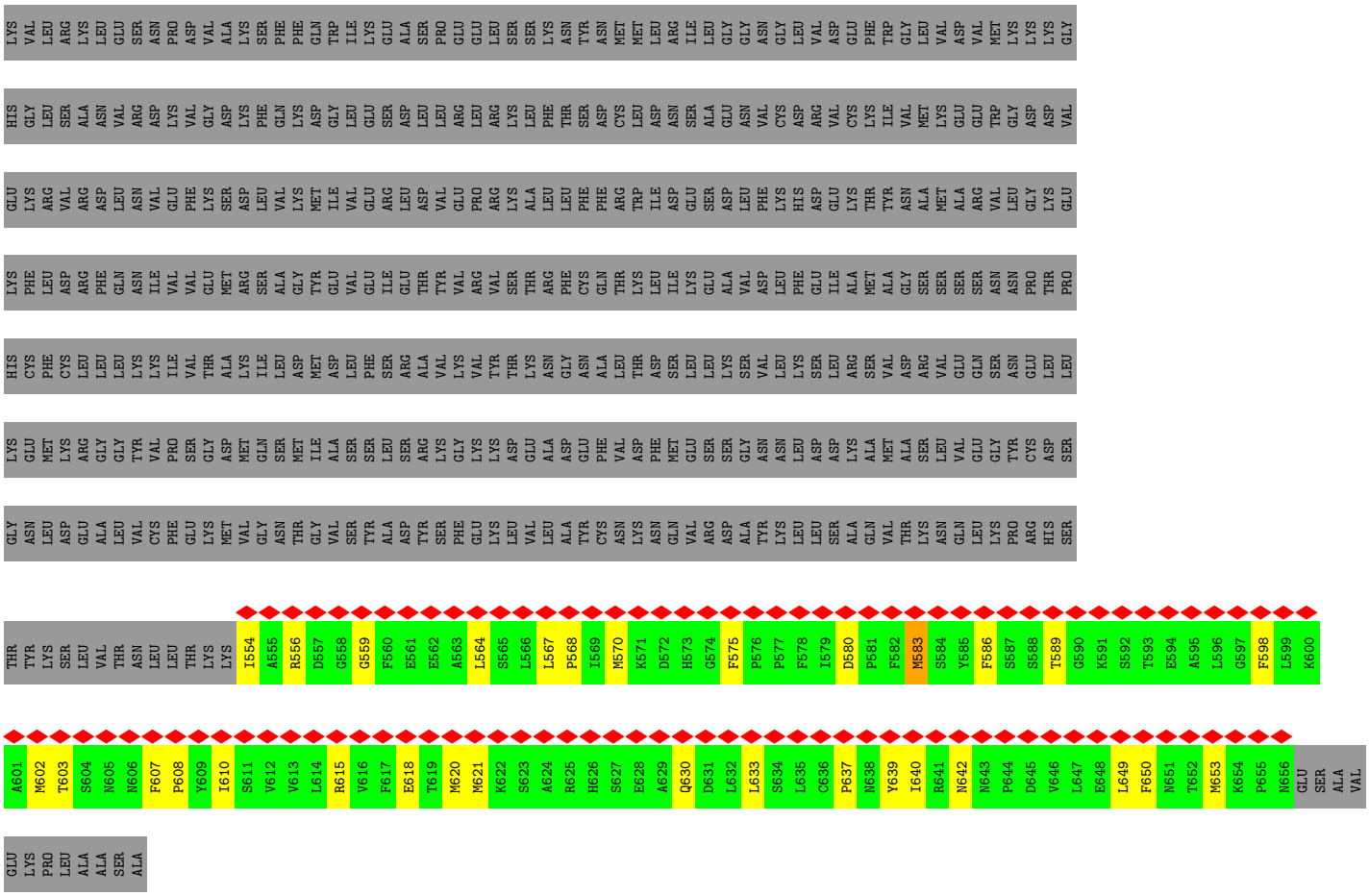
• Molecule 37: Small ribosomal subunit protein mS81 (rPPR8)

Chain g:





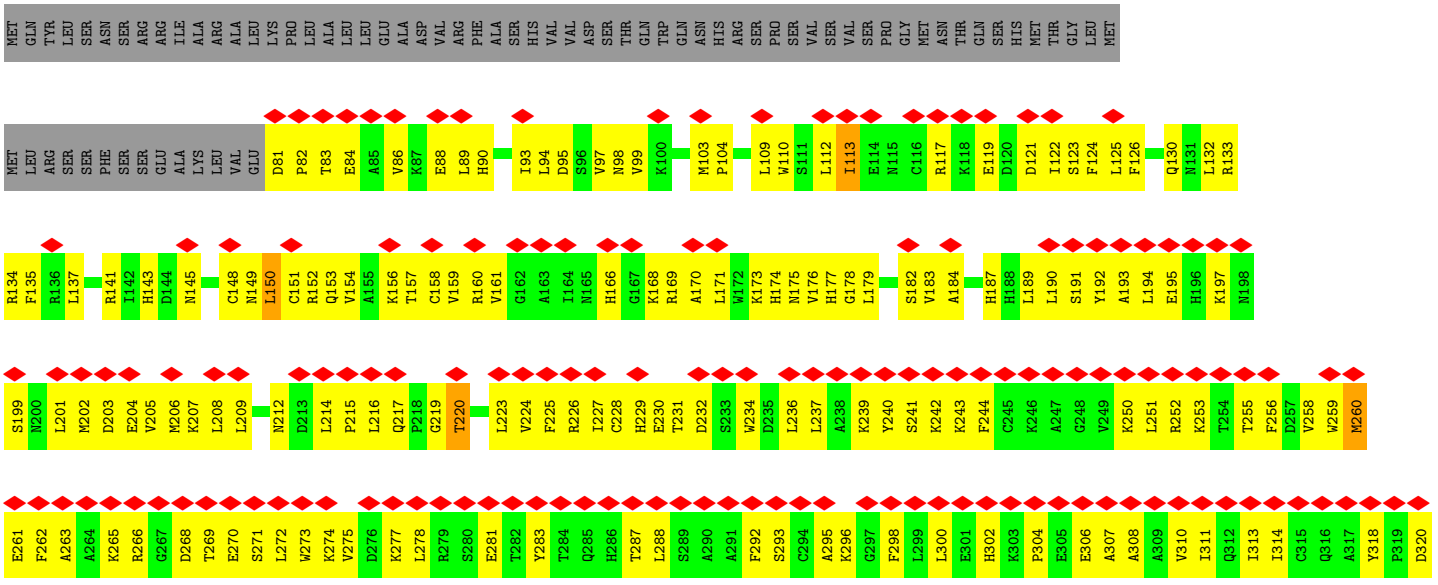


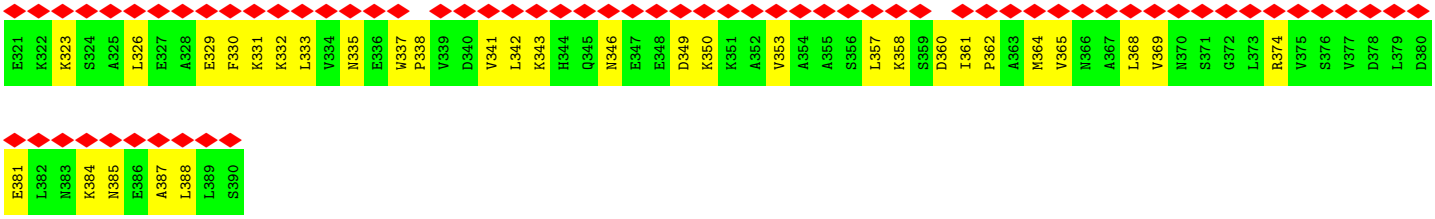


• Molecule 38: Adenylyl cyclase

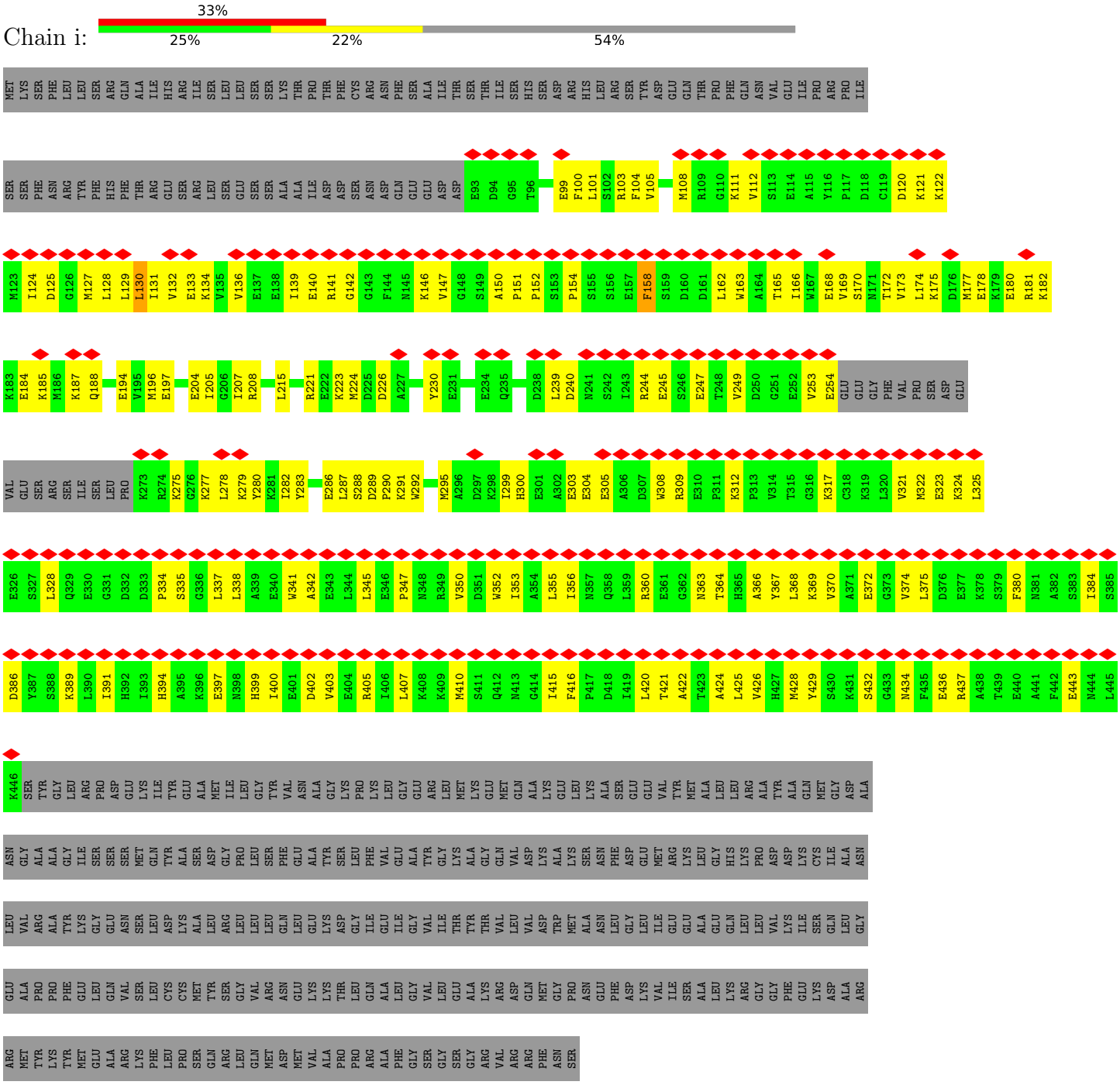
Chain h:







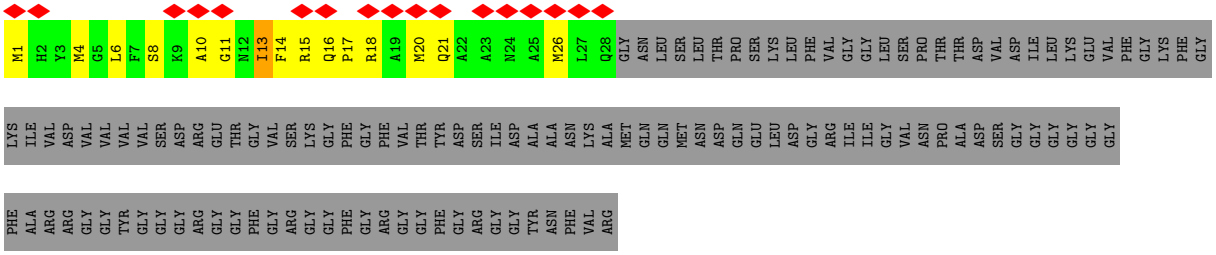
• Molecule 39: PROP1-like PPR domain-containing protein



• Molecule 40: RRM domain-containing protein

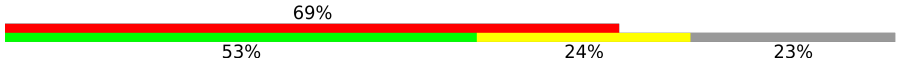
Chain k:

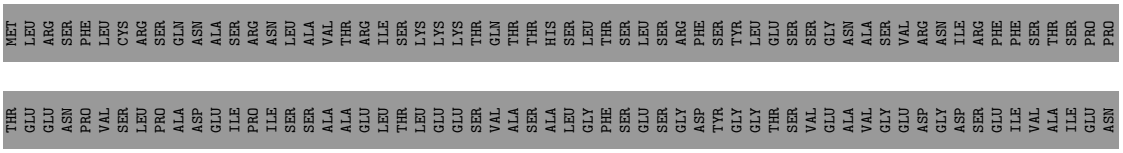


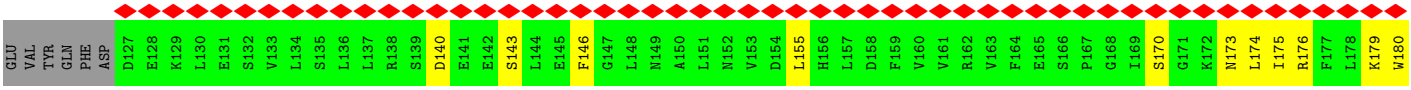


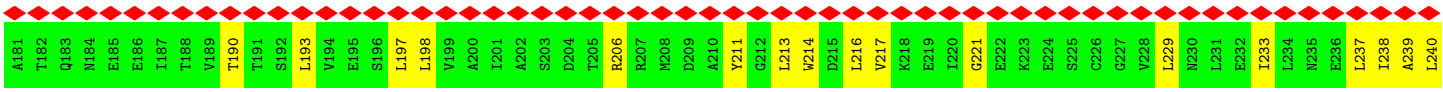
• Molecule 41: Small ribosomal subunit protein mS80 (rPPR6)

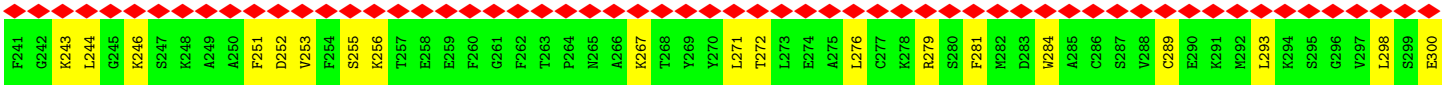
Chain l:

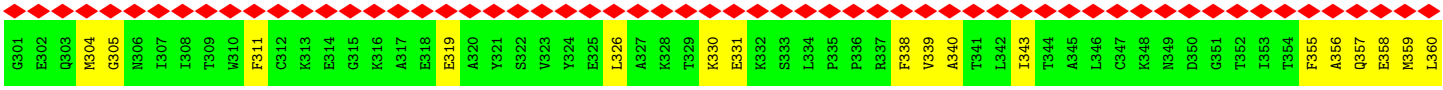


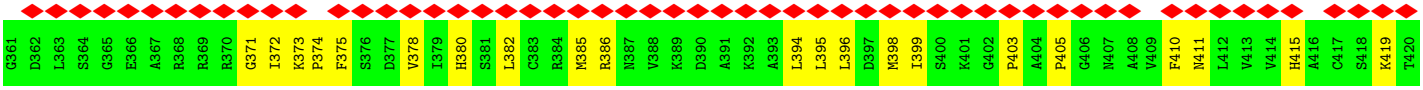


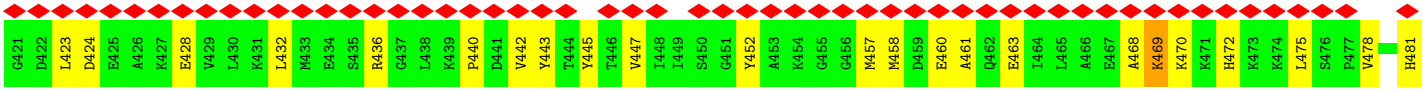


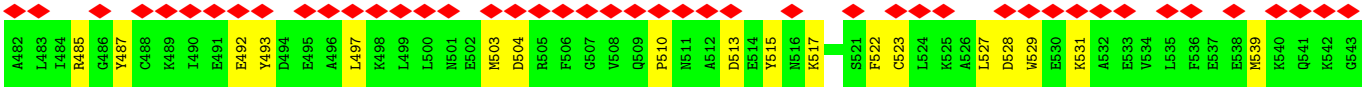


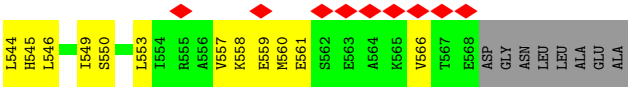












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18894	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.654	Depositor
Minimum map value	-0.281	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.24	Depositor
Map size (Å)	676.2, 676.2, 676.2	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.966, 0.966, 0.966	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, UR3, 4OC, ATP, MA6, G7M

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	2	0.55	0/38185	0.78	19/59524 (0.0%)
2	5	0.56	0/1834	0.88	2/2854 (0.1%)
3	6	0.85	0/119	1.00	0/183
4	8	0.23	0/1539	0.45	0/2055
5	A	0.29	0/1647	0.43	1/2227 (0.0%)
6	B	0.34	0/3969	0.49	0/5320
7	C	0.13	0/2859	0.30	0/3828
8	D	0.23	0/3474	0.36	0/4647
9	E	0.12	0/838	0.27	0/1121
10	F	0.21	0/1225	0.44	0/1641
11	G	0.12	0/1054	0.22	0/1418
12	H	0.34	0/1696	0.47	0/2273
13	I	0.41	0/964	0.43	0/1293
14	J	0.13	0/1000	0.32	0/1340
15	K	0.22	0/1010	0.44	0/1345
16	L	0.31	0/883	0.43	0/1176
17	M	0.41	0/856	0.38	0/1134
18	N	0.13	0/958	0.33	2/1280 (0.2%)
19	O	0.14	0/890	0.29	0/1196
20	P	0.12	0/730	0.25	0/984
21	Q	0.12	0/733	0.28	0/978
22	R	0.28	0/1323	0.43	0/1772
23	S	0.35	0/614	0.47	0/809
24	T	0.40	0/416	0.40	0/547
25	U	0.11	0/1036	0.29	0/1395
26	V	0.22	0/1423	0.34	0/1895
27	W	0.34	0/3139	0.44	0/4250
28	X	0.34	0/1644	0.49	0/2216
29	Y	0.36	0/807	0.46	0/1077
30	Z	0.11	0/669	0.32	0/900
31	a	0.34	0/2523	0.50	0/3386
32	b	0.64	0/618	0.93	0/822

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	c	0.40	0/233	0.55	0/296
34	d	0.13	0/628	0.30	0/840
35	e	0.19	0/2118	0.34	0/2828
36	f	0.11	0/2981	0.31	0/4033
37	g	0.17	0/835	0.43	0/1129
38	h	0.09	0/2511	0.28	0/3391
39	i	0.13	0/2772	0.34	0/3725
40	k	0.11	0/224	0.33	0/297
41	l	0.20	0/3523	0.43	0/4739
All	All	0.41	0/96500	0.61	24/138164 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	0	1
8	D	0	1
15	K	0	2
32	b	0	3
All	All	0	7

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1387	C	N1-C2-O2	9.32	124.49	118.90
1	2	1387	C	C2-N1-C1'	7.83	127.41	118.80
2	5	44	A	C3'-C2'-C1'	-7.60	95.98	101.30
1	2	1387	C	N3-C2-O2	-7.20	116.86	121.90
1	2	1542	A	N7-C8-N9	6.85	117.23	113.80

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	119	ARG	Sidechain
8	D	344	ARG	Sidechain
15	K	12	ARG	Sidechain
15	K	16	ARG	Sidechain

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Mol	Chain	Res	Type	Group
32	b	14	ARG	Sidechain

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	2	34252	0	17267	646	0
2	5	1641	0	831	132	0
3	6	107	0	54	10	0
4	8	1517	1558	1609	35	0
5	A	1611	0	1633	91	0
6	B	3877	0	4008	74	0
7	C	2806	0	2971	160	0
8	D	3425	0	3453	170	0
9	E	823	0	879	32	0
10	F	1254	0	1268	22	0
11	G	1037	0	1058	23	0
12	H	1671	0	1713	85	0
13	I	941	0	970	8	0
14	J	988	0	1022	71	0
15	K	993	0	1052	23	0
16	L	873	0	904	6	0
17	M	843	0	884	3	0
18	N	941	0	978	22	0
19	O	869	0	898	29	0
20	P	717	0	755	20	0
21	Q	724	0	744	31	0
22	R	1299	0	1307	19	0
23	S	611	0	687	40	0
24	T	408	0	444	1	0
25	U	1014	0	1061	91	0
26	V	1399	0	1427	45	0
27	W	3062	0	3030	39	0
28	X	1613	0	1559	37	0
29	Y	793	0	834	7	0
30	Z	649	0	662	46	0
31	a	2486	0	2376	48	0
32	b	610	0	626	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	c	232	0	278	5	0
34	d	616	0	674	25	0
35	e	2074	0	2074	86	0
36	f	2922	0	2870	192	0
37	g	814	0	801	19	0
38	h	2463	0	2488	259	0
39	i	2722	0	2680	207	0
40	k	220	0	223	36	0
41	l	3468	0	3524	98	0
42	W	31	0	12	0	0
All	All	91416	1558	74588	2684	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 16.

The worst 5 of 2684 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)
7:C:175:LEU:HD11	7:C:198:TRP:HB3	1.26	1.16
8:D:181:LEU:HD23	8:D:193:TRP:HB2	1.28	1.16
7:C:182:LYS:HA	7:C:182:LYS:HE2	1.31	1.12
38:h:193:ALA:HB2	38:h:201:LEU:HD23	1.30	1.10
39:i:403:VAL:HG11	39:i:428:MET:HE1	1.25	1.10

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	
4	8	184/520 (35%)	154 (84%)	29 (16%)	1 (0%)	24	52
5	A	202/212 (95%)	193 (96%)	8 (4%)	1 (0%)	24	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	B	457/554 (82%)	428 (94%)	28 (6%)	1 (0%)	43 70
7	C	329/362 (91%)	324 (98%)	5 (2%)	0	100 100
8	D	413/501 (82%)	393 (95%)	18 (4%)	2 (0%)	24 52
9	E	99/138 (72%)	98 (99%)	1 (1%)	0	100 100
10	F	146/157 (93%)	136 (93%)	9 (6%)	1 (1%)	18 45
11	G	126/129 (98%)	124 (98%)	2 (2%)	0	100 100
12	H	208/383 (54%)	197 (95%)	10 (5%)	1 (0%)	24 52
13	I	111/228 (49%)	107 (96%)	4 (4%)	0	100 100
14	J	125/304 (41%)	120 (96%)	5 (4%)	0	100 100
15	K	122/125 (98%)	116 (95%)	6 (5%)	0	100 100
16	L	108/154 (70%)	103 (95%)	5 (5%)	0	100 100
17	M	99/155 (64%)	98 (99%)	1 (1%)	0	100 100
18	N	114/414 (28%)	113 (99%)	1 (1%)	0	100 100
19	O	108/136 (79%)	107 (99%)	1 (1%)	0	100 100
20	P	89/110 (81%)	88 (99%)	1 (1%)	0	100 100
21	Q	88/237 (37%)	87 (99%)	1 (1%)	0	100 100
22	R	162/212 (76%)	155 (96%)	7 (4%)	0	100 100
23	S	73/100 (73%)	73 (100%)	0	0	100 100
24	T	48/94 (51%)	44 (92%)	4 (8%)	0	100 100
25	U	125/192 (65%)	122 (98%)	3 (2%)	0	100 100
26	V	162/193 (84%)	158 (98%)	4 (2%)	0	100 100
27	W	376/483 (78%)	369 (98%)	7 (2%)	0	100 100
28	X	202/496 (41%)	191 (95%)	8 (4%)	3 (2%)	8 28
29	Y	96/102 (94%)	95 (99%)	1 (1%)	0	100 100
30	Z	78/153 (51%)	74 (95%)	4 (5%)	0	100 100
31	a	311/424 (73%)	297 (96%)	14 (4%)	0	100 100
32	b	75/80 (94%)	65 (87%)	7 (9%)	3 (4%)	2 11
33	c	24/128 (19%)	24 (100%)	0	0	100 100
34	d	76/110 (69%)	75 (99%)	1 (1%)	0	100 100
35	e	244/383 (64%)	232 (95%)	11 (4%)	1 (0%)	30 57
36	f	375/410 (92%)	357 (95%)	18 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	g	101/668 (15%)	96 (95%)	5 (5%)	0	100	100
38	h	308/384 (80%)	302 (98%)	6 (2%)	0	100	100
39	i	332/725 (46%)	326 (98%)	6 (2%)	0	100	100
40	k	26/153 (17%)	22 (85%)	4 (15%)	0	100	100
41	l	440/576 (76%)	432 (98%)	8 (2%)	0	100	100
All	All	6762/10885 (62%)	6495 (96%)	253 (4%)	14 (0%)	44	70

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	H	225	ILE
32	b	27	GLY
32	b	87	THR
4	8	266	ILE
32	b	18	ASN

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	
4	8	164/461 (36%)	160 (98%)	4 (2%)	43	66
5	A	177/182 (97%)	173 (98%)	4 (2%)	44	66
6	B	421/492 (86%)	409 (97%)	12 (3%)	37	62
7	C	312/343 (91%)	305 (98%)	7 (2%)	45	67
8	D	370/444 (83%)	364 (98%)	6 (2%)	55	72
9	E	90/126 (71%)	87 (97%)	3 (3%)	33	60
10	F	124/124 (100%)	123 (99%)	1 (1%)	73	79
11	G	112/113 (99%)	110 (98%)	2 (2%)	51	70
12	H	175/320 (55%)	168 (96%)	7 (4%)	28	56
13	I	104/197 (53%)	101 (97%)	3 (3%)	37	62
14	J	108/256 (42%)	101 (94%)	7 (6%)	15	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	K	106/107 (99%)	105 (99%)	1 (1%)	70	78
16	L	93/128 (73%)	89 (96%)	4 (4%)	26	53
17	M	90/137 (66%)	88 (98%)	2 (2%)	45	67
18	N	107/362 (30%)	107 (100%)	0	100	100
19	O	93/117 (80%)	92 (99%)	1 (1%)	65	76
20	P	78/95 (82%)	77 (99%)	1 (1%)	61	74
21	Q	75/203 (37%)	73 (97%)	2 (3%)	39	64
22	R	141/180 (78%)	134 (95%)	7 (5%)	22	49
23	S	68/90 (76%)	67 (98%)	1 (2%)	57	73
24	T	44/79 (56%)	43 (98%)	1 (2%)	44	66
25	U	109/170 (64%)	108 (99%)	1 (1%)	70	78
26	V	147/173 (85%)	143 (97%)	4 (3%)	39	64
27	W	328/410 (80%)	321 (98%)	7 (2%)	47	68
28	X	174/395 (44%)	170 (98%)	4 (2%)	44	66
29	Y	84/86 (98%)	83 (99%)	1 (1%)	63	75
30	Z	65/119 (55%)	64 (98%)	1 (2%)	57	73
31	a	252/375 (67%)	248 (98%)	4 (2%)	55	72
32	b	68/71 (96%)	67 (98%)	1 (2%)	57	73
33	c	25/116 (22%)	25 (100%)	0	100	100
34	d	65/93 (70%)	64 (98%)	1 (2%)	57	73
35	e	226/339 (67%)	224 (99%)	2 (1%)	70	78
36	f	321/351 (92%)	312 (97%)	9 (3%)	38	63
37	g	92/597 (15%)	89 (97%)	3 (3%)	33	60
38	h	271/337 (80%)	265 (98%)	6 (2%)	45	67
39	i	297/629 (47%)	293 (99%)	4 (1%)	61	74
40	k	21/109 (19%)	20 (95%)	1 (5%)	23	50
41	l	378/492 (77%)	371 (98%)	7 (2%)	50	69
All	All	5975/9418 (63%)	5843 (98%)	132 (2%)	45	67

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	h	150	LEU

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Mol	Chain	Res	Type
38	h	374	ARG
41	l	549	ILE
13	I	226	MET
13	I	194	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
38	h	143	HIS
40	k	21	GLN
38	h	177	HIS
38	h	344	HIS
41	l	545	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1592/1601 (99%)	275 (17%)	19 (1%)
2	5	76/77 (98%)	39 (51%)	6 (7%)
3	6	4/5 (80%)	4 (100%)	0
All	All	1672/1683 (99%)	318 (19%)	25 (1%)

5 of 318 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	6	A
1	2	12	A
1	2	17	G
1	2	30	G
1	2	37	A

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1706	C
1	2	1802	A
2	5	41	C
1	2	1769	C
1	2	1845	A

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

6 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
1	MA6	2	1827	1	23,26,27	0.27	0	34,38,41	0.75	1 (2%)
1	G7M	2	525	1	23,26,27	0.70	1 (4%)	35,39,42	0.54	0
1	2MG	2	1825	1	23,26,27	0.50	0	32,38,41	0.52	0
1	UR3	2	1807	1	19,22,23	0.30	0	26,32,35	0.67	0
1	4OC	2	1664	1	20,23,24	0.35	0	26,32,35	0.44	0
1	MA6	2	1828	1	23,26,27	0.29	0	34,38,41	0.68	1 (2%)

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
1	MA6	2	1827	1	-	0/11/29/30	0/3/3/3
1	G7M	2	525	1	-	2/7/25/26	0/3/3/3
1	2MG	2	1825	1	-	0/9/27/28	0/3/3/3
1	UR3	2	1807	1	-	0/7/25/26	0/2/2/2
1	4OC	2	1664	1	-	0/9/29/30	0/2/2/2
1	MA6	2	1828	1	-	2/11/29/30	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	525	G7M	C8-N7	2.45	1.37	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1827	MA6	C2-N1-C6	2.85	118.47	111.75
1	2	1828	MA6	C2-N1-C6	2.78	118.32	111.75

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	525	G7M	C3'-C4'-C5'-O5'
1	2	525	G7M	O4'-C4'-C5'-O5'
1	2	1828	MA6	C4'-C5'-O5'-P
1	2	1828	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1827	MA6	1	0
1	2	1825	2MG	1	0
1	2	1828	MA6	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand 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	$\#\|Z\| > 2$
42	ATP	W	501	-	29,33,33	0.49	0	44,52,52	0.54	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
42	ATP	W	501	-	-	3/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

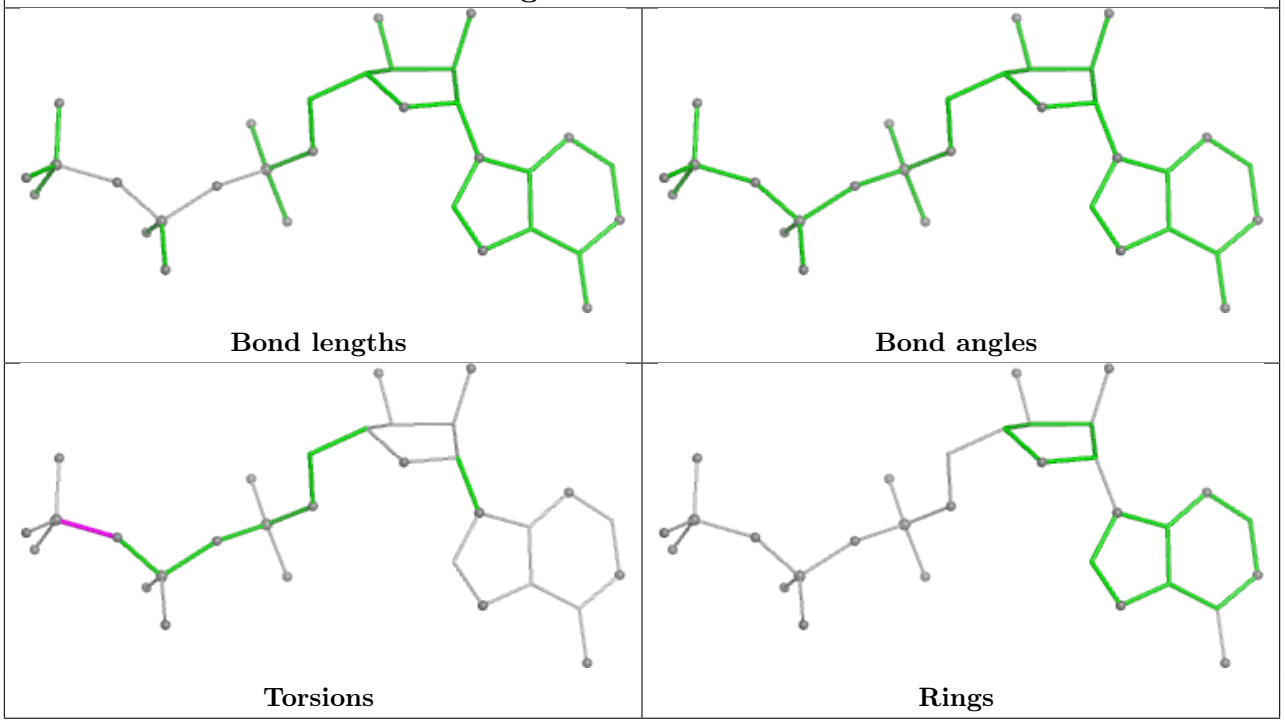
Mol	Chain	Res	Type	Atoms
42	W	501	ATP	PB-O3B-PG-O1G
42	W	501	ATP	PB-O3B-PG-O2G
42	W	501	ATP	PB-O3B-PG-O3G

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand ATP W 501



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
1	2	7
4	8	2

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1147:A	O3'	1164:U	P	23.26
1	2	1330:A	O3'	1335:U	P	18.29
1	2	1167:U	O3'	1314:A	P	18.25
1	2	83:U	O3'	129:A	P	17.64
1	2	137:A	O3'	142:U	P	13.88

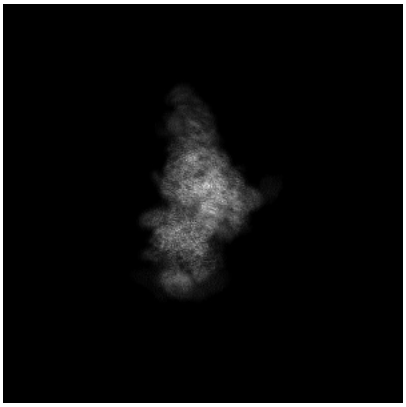
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-56197. These allow visual inspection of the internal detail of the map and identification of artifacts.

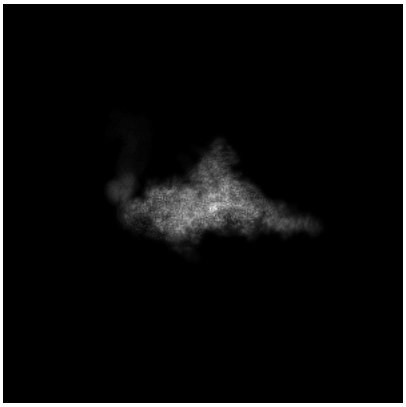
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

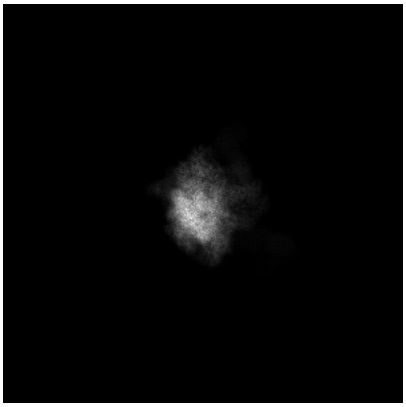
6.1.1 Primary map



X



Y

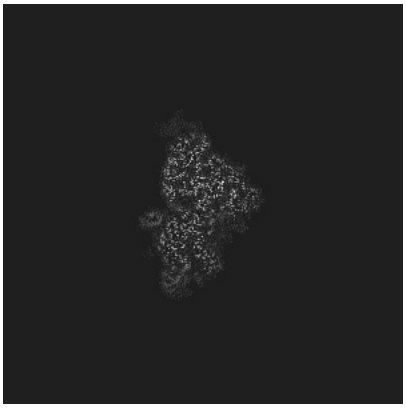


Z

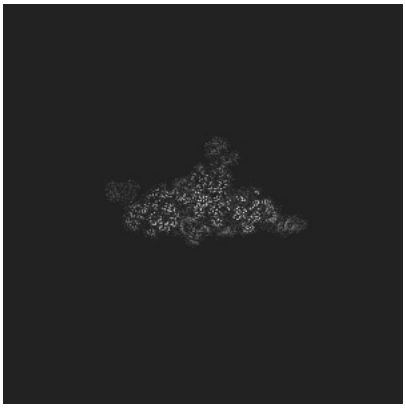
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 350



Y Index: 350

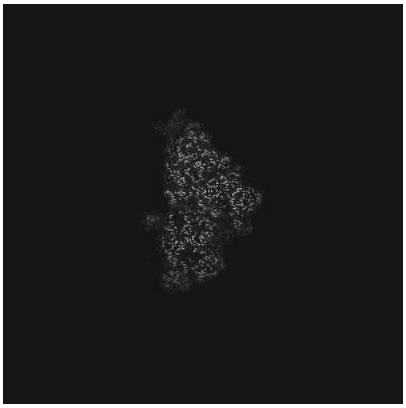


Z Index: 350

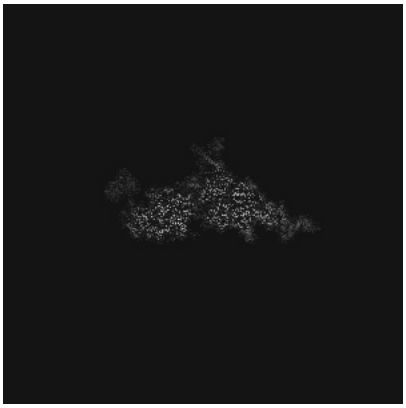
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

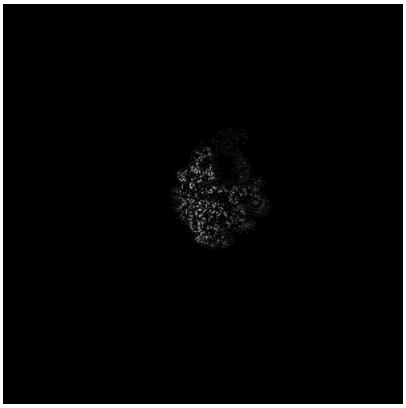
6.3.1 Primary map



X Index: 343



Y Index: 334

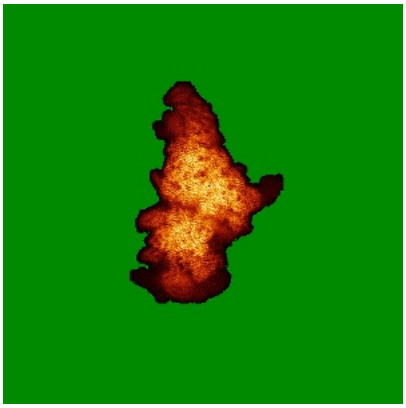


Z Index: 369

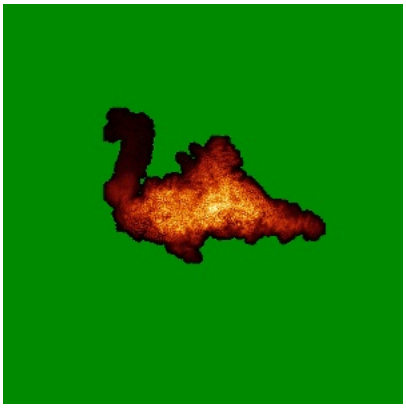
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

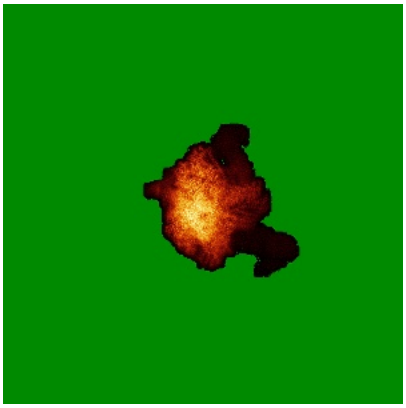
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

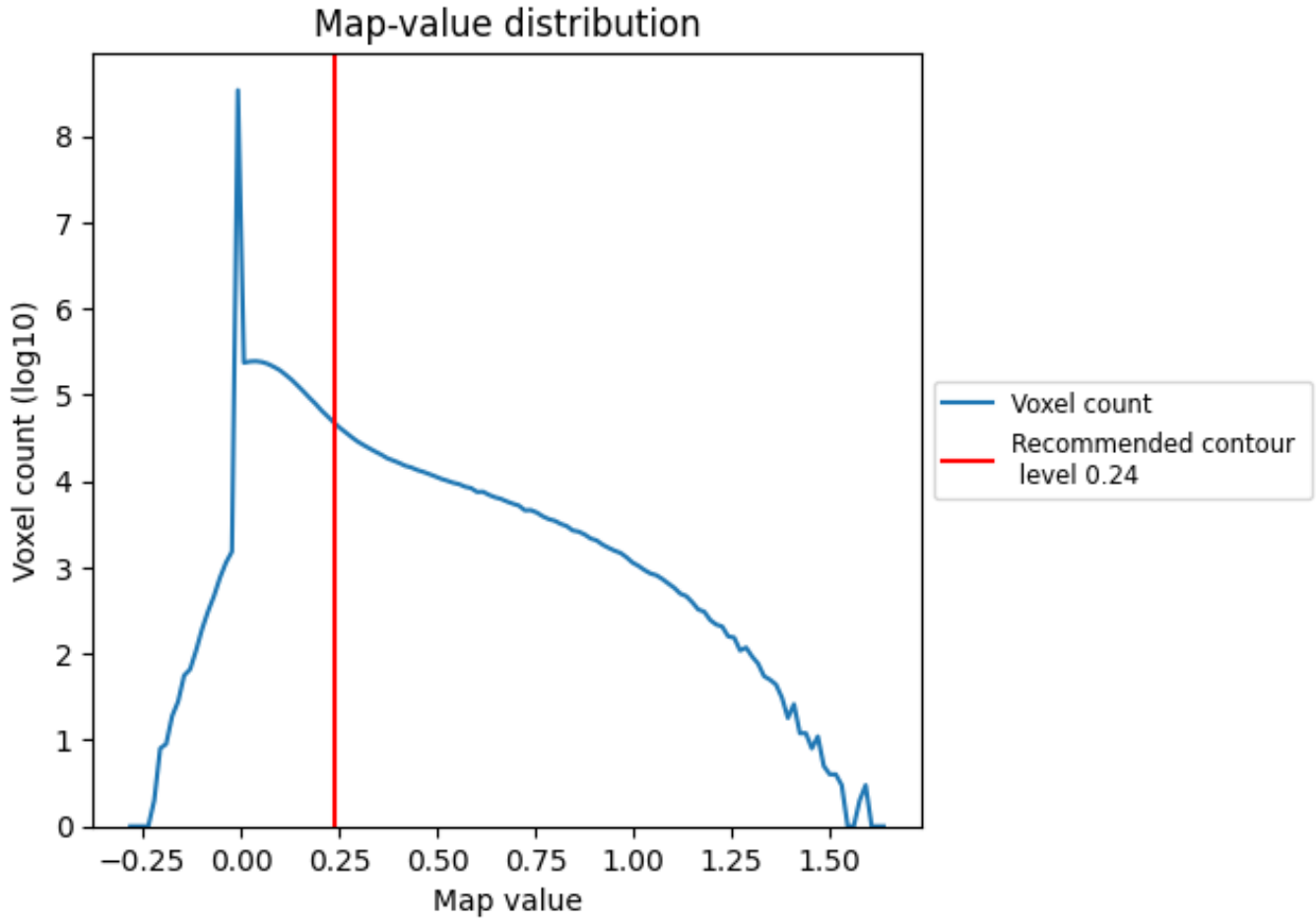
6.6 Mask visualisation (i)

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

7 Map analysis

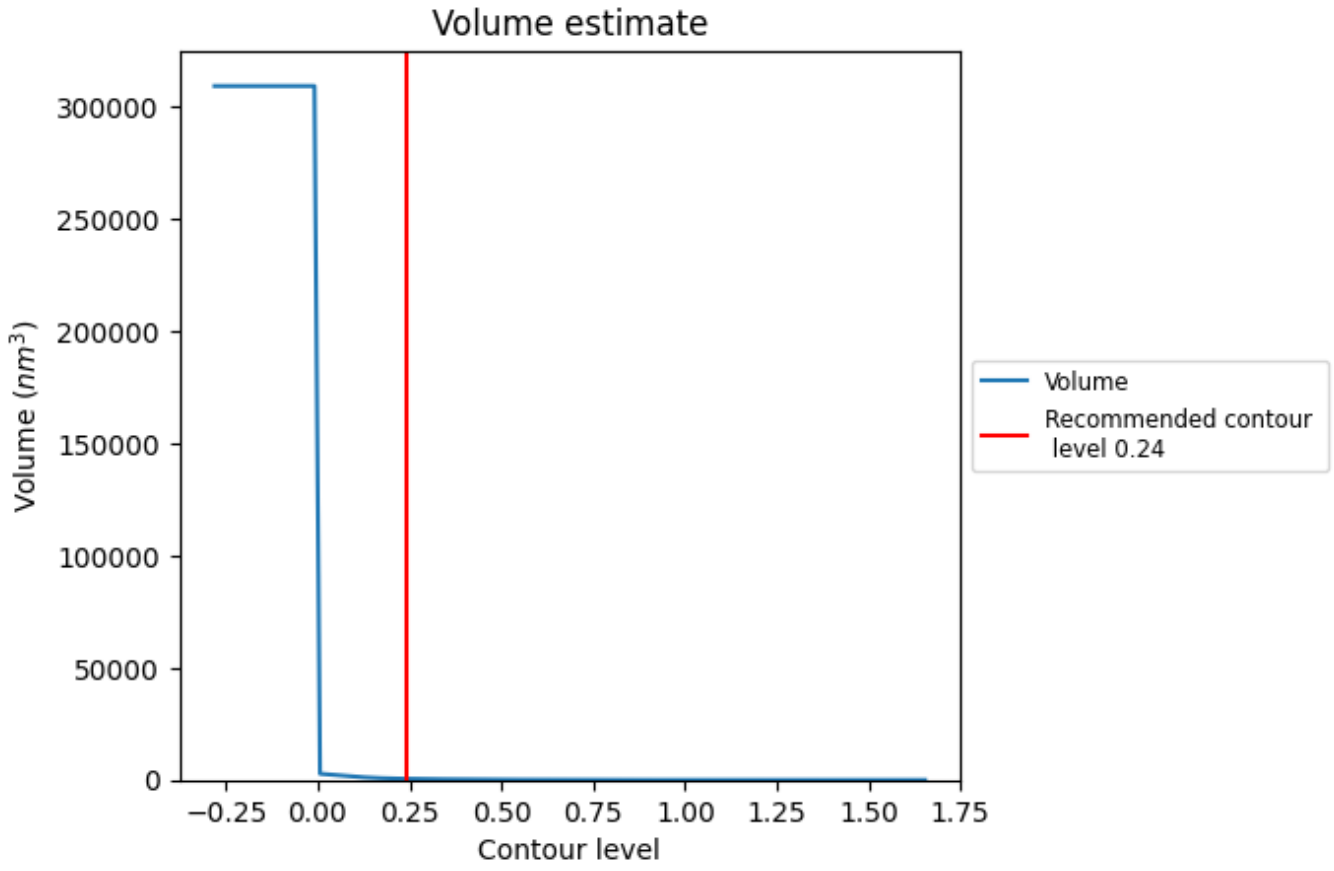
This section contains the results of statistical analysis of the map.

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.

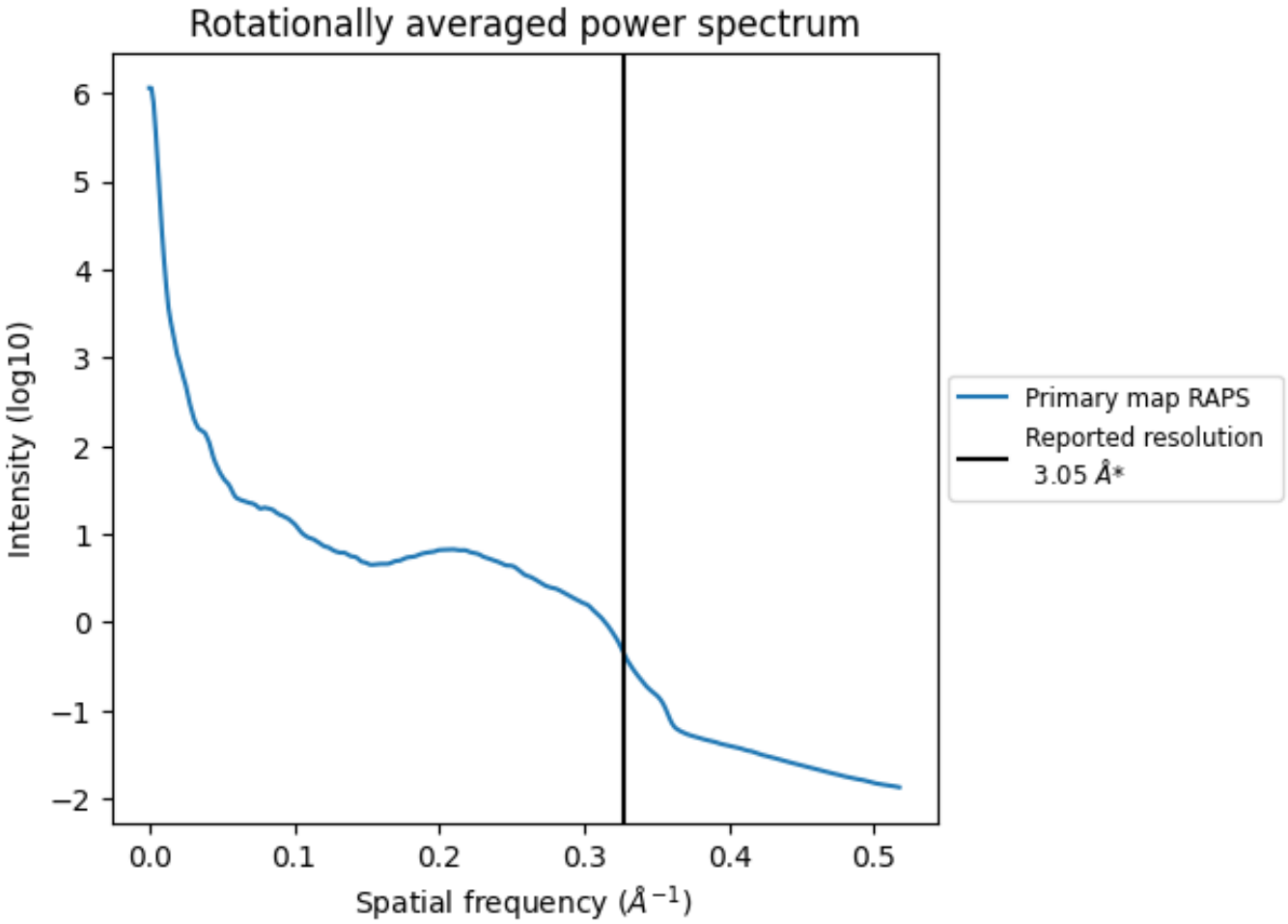
7.2 Volume estimate (i)



The volume at the recommended contour level is 515 nm^3; this corresponds to an approximate mass of 465 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 0.328 Å^{-1}

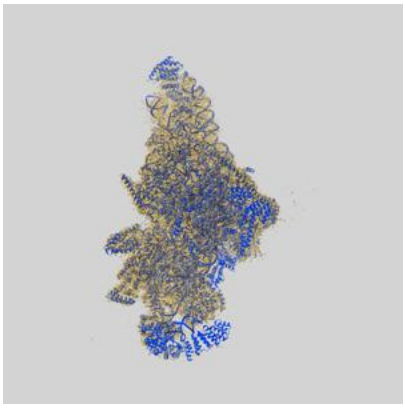
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

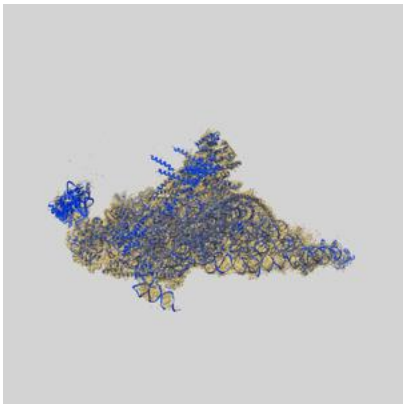
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-56197 and PDB model 9TRT. Per-residue inclusion information can be found in section 3 on page 12.

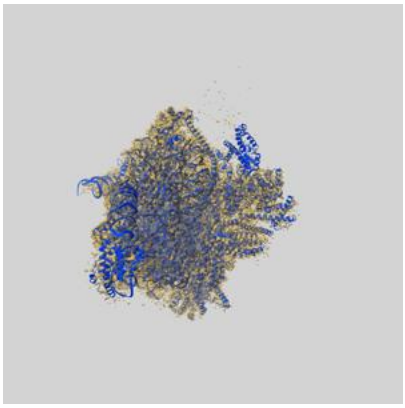
9.1 Map-model overlay



X



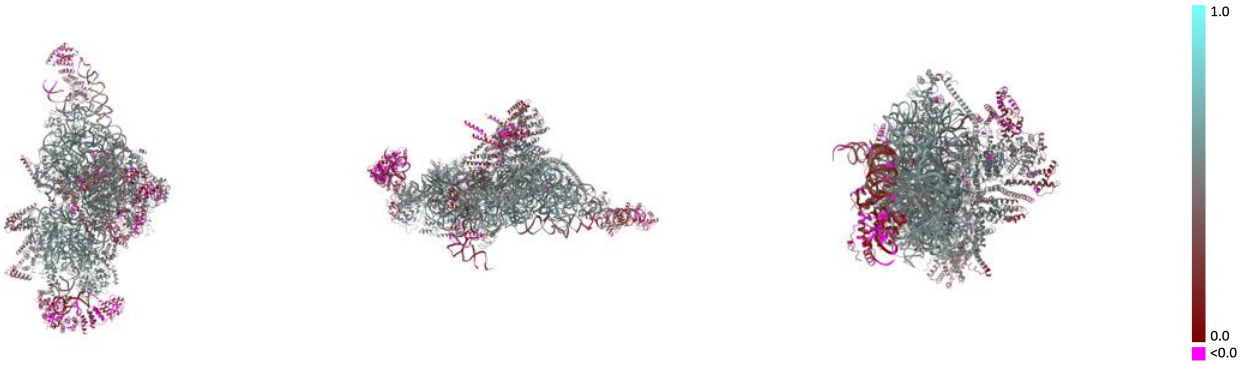
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.24 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.

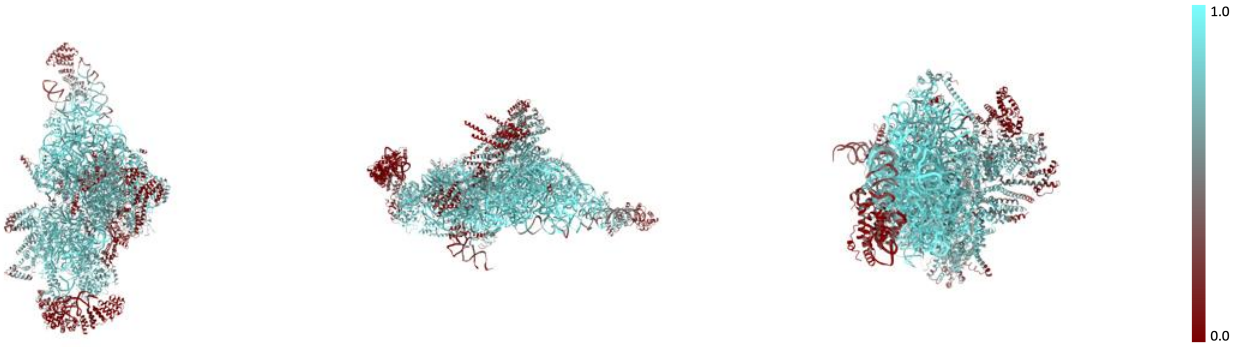
9.2 Q-score mapped to coordinate model (i)



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.

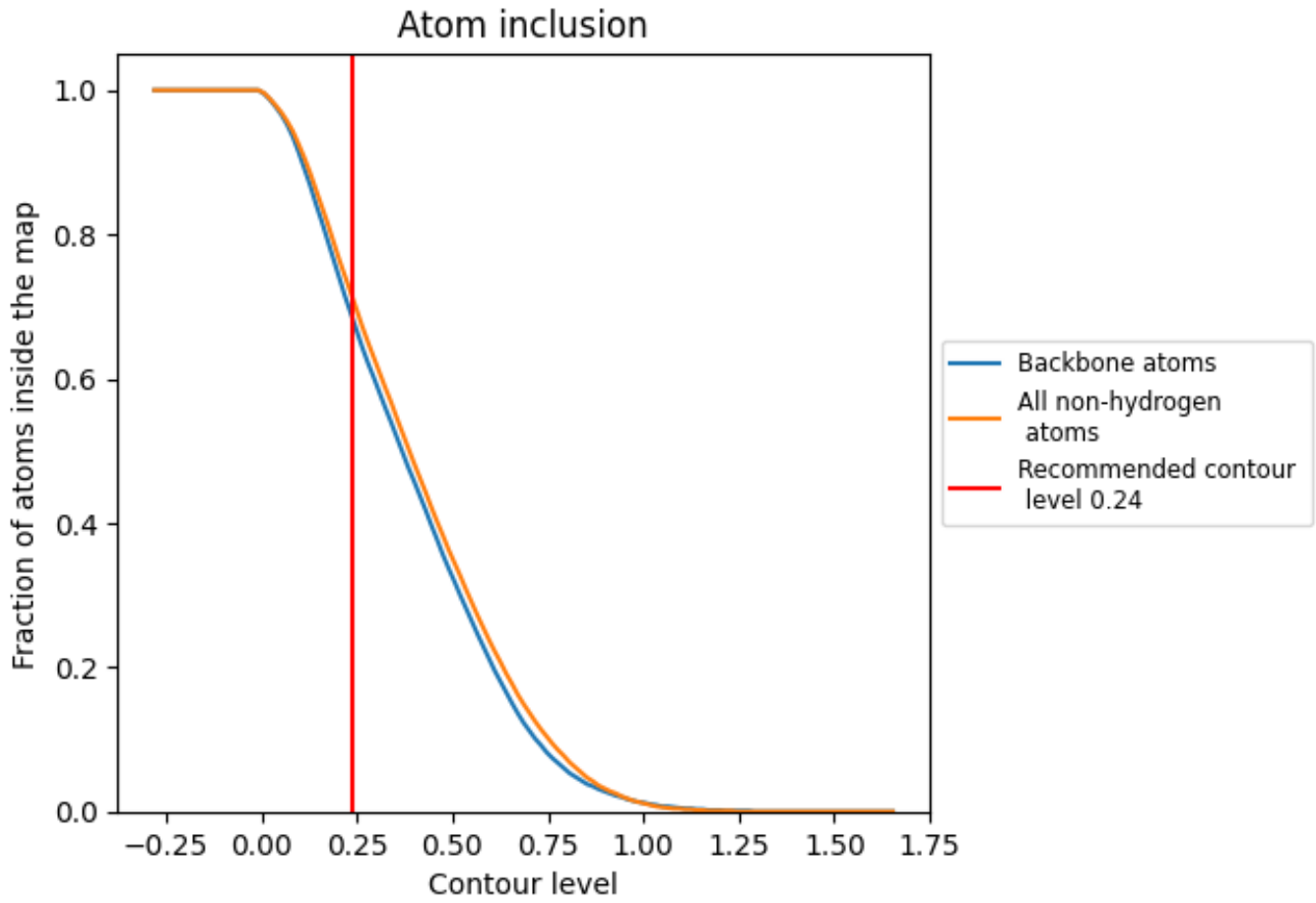
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.24).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 71% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7090	0.4460
2	0.8750	0.4950
5	0.3930	0.1840
6	0.4210	0.3350
8	0.4060	0.2720
A	0.7760	0.5220
B	0.7280	0.4760
C	0.8060	0.5130
D	0.6960	0.4640
E	0.7990	0.5090
F	0.1660	0.3850
G	0.8740	0.5520
H	0.6560	0.4510
I	0.9000	0.5770
J	0.7060	0.4420
K	0.8640	0.5430
L	0.8310	0.5570
M	0.9120	0.5780
N	0.8060	0.5210
O	0.9150	0.5550
P	0.8230	0.5370
Q	0.7570	0.5100
R	0.4650	0.3310
S	0.6160	0.4380
T	0.9190	0.5780
U	0.3270	0.3040
V	0.7190	0.4890
W	0.7980	0.5320
X	0.7480	0.4980
Y	0.7960	0.5330
Z	0.7570	0.4500
a	0.7040	0.4710
b	0.0300	0.1640
c	0.7890	0.5020
d	0.8040	0.5030



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Chain	Atom inclusion	Q-score
e	0.8080	0.5130
f	0.6360	0.4490
g	0.0060	0.0930
h	0.2940	0.1950
i	0.2440	0.2460
k	0.3260	0.3700
l	0.1080	0.1350