wwPDB EM Validation Summary Report (i)

Oct 24, 2026 – 10:47 am BST

PDB ID	:	9TRV / pdb_00009trv
EMDB ID	:	EMD-56198
Title	:	Structure of the Plant mitochondrial pre-initiation complex 1, (SSU,mtIF3)
Authors	:	Skaltsogiannis, V.; Giege, P.; Soufari, H.
Deposited on	:	2025-12-28
Resolution	:	2.28 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 (i) 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 (i)) were used in the production of this report:

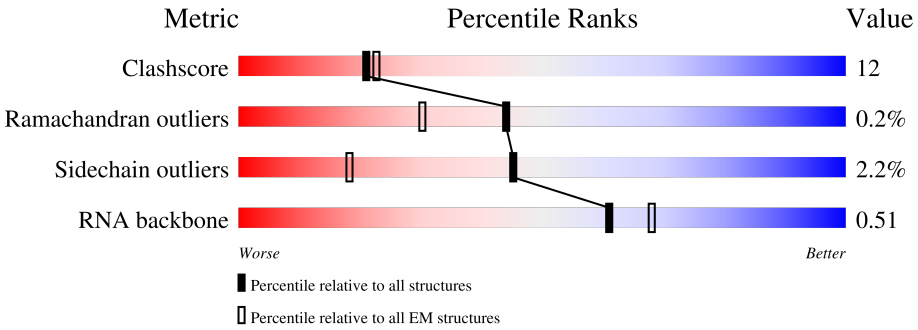
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

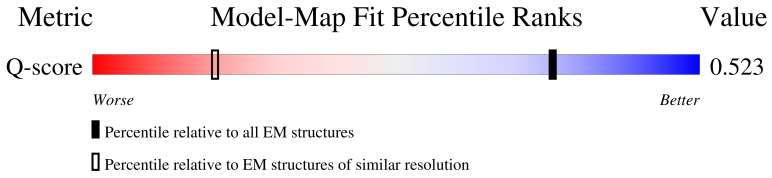
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.28 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	3643 (1.78 - 2.78)

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	1611	7% 55% 35% 9%
2	8	520	11% 14% 5% 79%
3	A	212	79% 17%

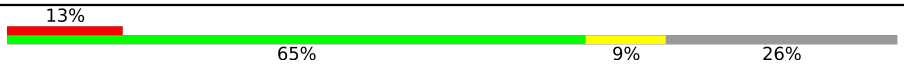
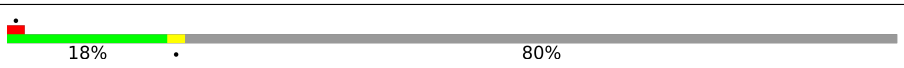
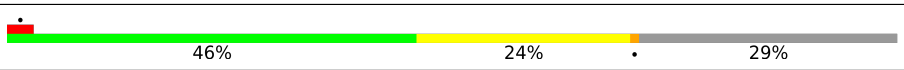
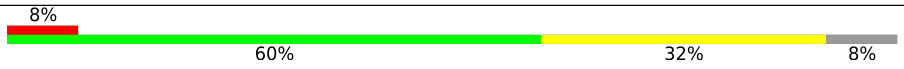
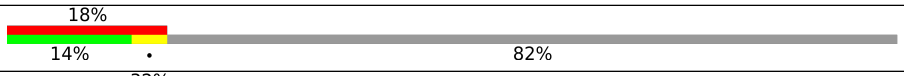
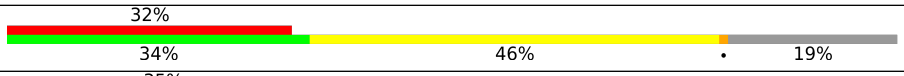
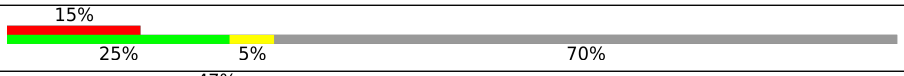
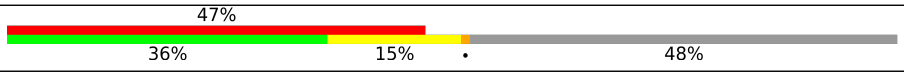
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Mol	Chain	Length	Quality of chain
4	B	554	12% 69% 14% 16%
5	C	362	6% 68% 24% 8%
6	D	501	15% 61% 22% 18%
7	E	138	59% 14% 27%
8	F	157	15% 86% 13%
9	G	129	81% 18%
10	H	383	10% 43% 12% 45%
11	I	228	46% 50%
12	J	304	6% 29% 12% 58%
13	K	125	78% 20%
14	L	154	61% 10% 29%
15	M	155	61% 35%
16	N	414	24% 72%
17	O	136	71% 10% 19%
18	P	110	7% 70% 13% 17%
19	Q	237	33% 62%
20	R	212	43% 66% 12% 22%
21	S	100	11% 55% 20% 25%
22	T	94	49% 47%
23	U	192	32% 41% 24% 34%
24	V	193	64% 20% 15%
25	W	483	73% 5% 21%
26	X	496	5% 36% 5% 59%
27	Y	102	6% 87% 9%
28	Z	153	30% 20% 48%

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Mol	Chain	Length	Quality of chain
29	a	424	
30	b	80	
31	c	128	
32	d	110	
33	e	383	
34	f	410	
35	g	668	
36	h	384	
37	i	725	
38	k	155	
39	l	576	

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 89547 atoms, of which 927 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	1610	34484	15405	6287	11182	1610	0	0

- Molecule 2 is a protein called Translation initiation factor IF3-1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	8	109	1801	566	927	151	153	4	0	0

- Molecule 3 is a protein called Ribosomal protein S2.

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

- Molecule 4 is a protein called Small ribosomal subunit protein uS3m.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	TRP	ARG	conflict	UNP A0A068BCX1
B	62	ILE	LEU	conflict	UNP A0A068BCX1
B	172	LEU	SER	conflict	UNP A0A068BCX1
B	202	LYS	ARG	conflict	UNP A0A068BCX1
B	296	LEU	SER	conflict	UNP A0A068BCX1
B	512	CYS	ARG	conflict	UNP A0A068BCX1
B	524	VAL	ALA	conflict	UNP A0A068BCX1
B	533	LEU	SER	conflict	UNP A0A068BCX1

- Molecule 5 is a protein called Ribosomal protein S4.

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

- Molecule 6 is a protein called S5 DRBM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	413	Total	C	N	O	S	0	0
			3389	2125	596	656	12		

- Molecule 7 is a protein called bS6m.

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

- Molecule 8 is a protein called uS7m,Small ribosomal subunit protein uS7m.

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

- Molecule 9 is a protein called 40S ribosomal protein S15a.

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

- Molecule 10 is a protein called 30S ribosomal protein S9.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	50	SER	PRO	conflict	UNP A0A3P6FWE0
H	94	SER	ASN	conflict	UNP A0A3P6FWE0

- Molecule 11 is a protein called Small ribosomal subunit protein uS10 domain-containing

protein.

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

- Molecule 12 is a protein called Ribosomal protein S11.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS12m.

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

- Molecule 14 is a protein called uS13m.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS14m.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS15c.

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

- Molecule 17 is a protein called 30S ribosomal protein S16.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS17c.

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

- Molecule 19 is a protein called Small ribosomal subunit protein bS18c.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	250	ILE	VAL	conflict	UNP A0A078FCZ9

- Molecule 20 is a protein called Small ribosomal subunit protein uS19m.

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

- Molecule 21 is a protein called Ribosomal protein S21.

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

- Molecule 22 is a protein called 30S ribosomal protein S31, mitochondrial.

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

- Molecule 23 is a protein called mS23.

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

- Molecule 24 is a protein called mS26.

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

- Molecule 25 is a protein called Small ribosomal subunit protein mS29.

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

- Molecule 26 is a protein called BnaC06g06470D protein.

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

- Molecule 27 is a protein called MOSC domain-containing protein.

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

- Molecule 28 is a protein called Mitochondrial 28S ribosomal protein S34.

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

- Molecule 29 is a protein called Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein.

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

- Molecule 30 is a protein called IMS import disulfide relay-system CHCH-CHCH-like Cx9C domain-containing protein.

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

- Molecule 31 is a protein called Small ribosomal subunit protein mS38.

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

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

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

- Molecule 33 is a protein called mS45.

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

- Molecule 34 is a protein called mS47.

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

- Molecule 35 is a protein called Small ribosomal subunit protein mS81 (rPPR8).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	119	Total	C	N	O	S	0	0
			946	608	157	174	7		

- Molecule 36 is a protein called (rape) hypothetical protein.

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

- Molecule 37 is a protein called PROP1-like PPR domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	370	Total	C	N	O	S	0	0
			2993	1890	503	582	18		

- Molecule 38 is a protein called Small ribosomal subunit protein mS86.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	47	Total	C	N	O	S	0	0
			313	194	61	54	4		

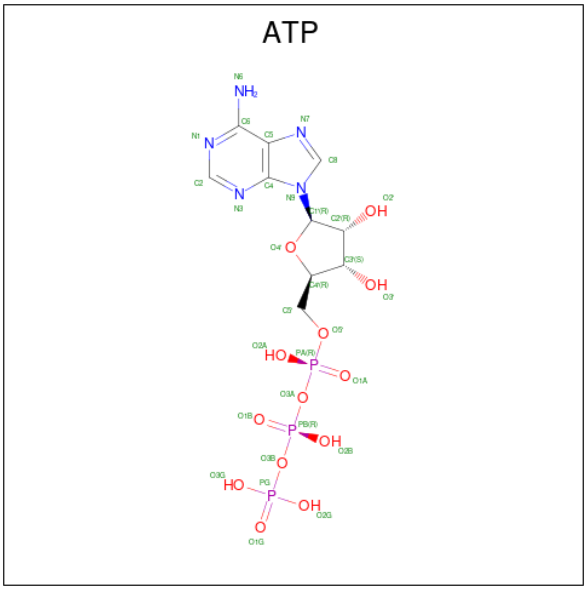
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	9	LYS	ARG	conflict	UNP Q9FZ84
k	20	MET	LEU	conflict	UNP Q9FZ84

- Molecule 39 is a protein called Small ribosomal subunit protein mS80 (rPPR6).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	302	Total	C	N	O	S	0	0
			2371	1506	397	447	21		

- Molecule 40 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
40	W	1	Total	C	N	O	P	0
			31	10	5	13	3	

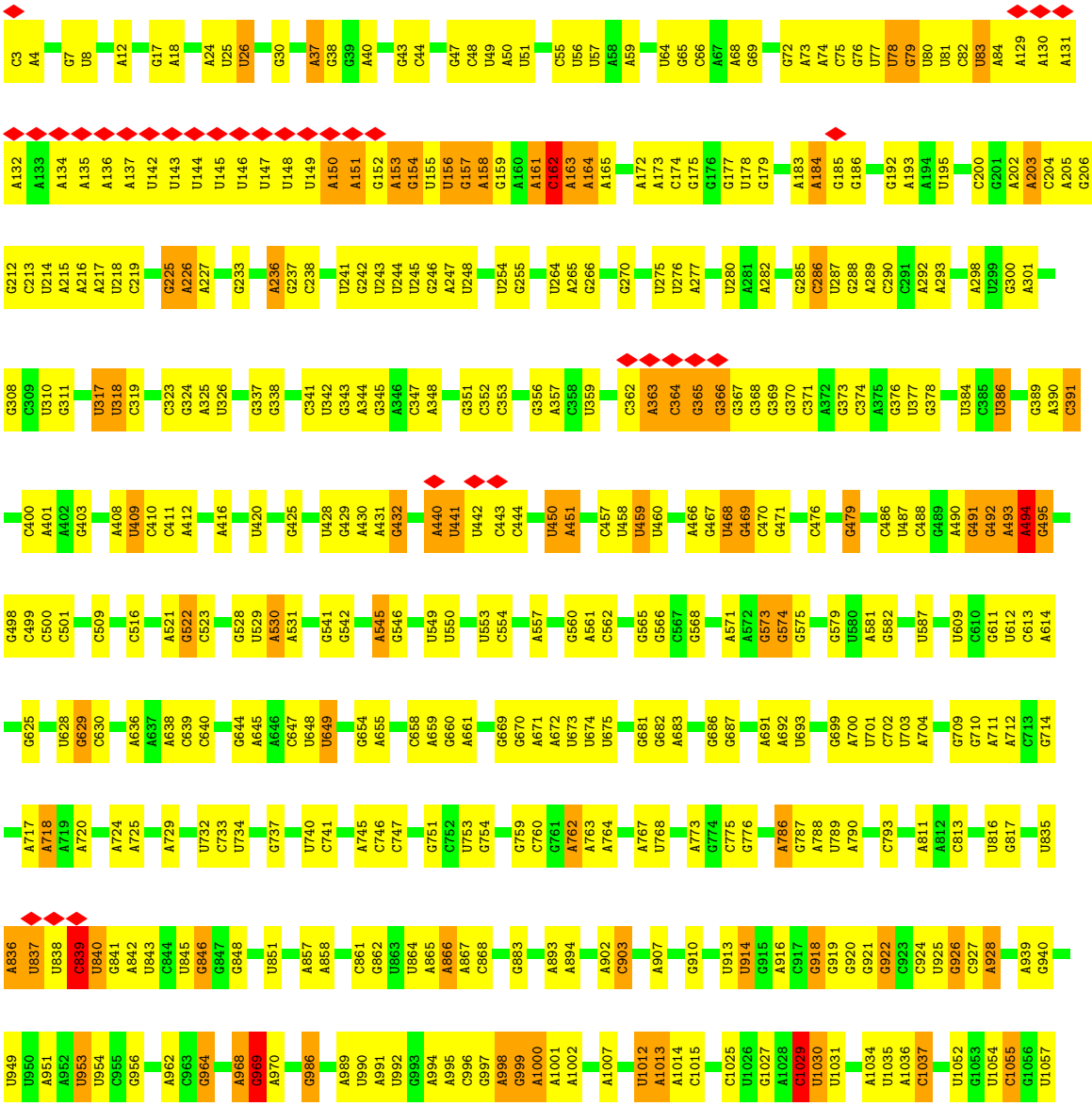
3 Residue-property plots (i)

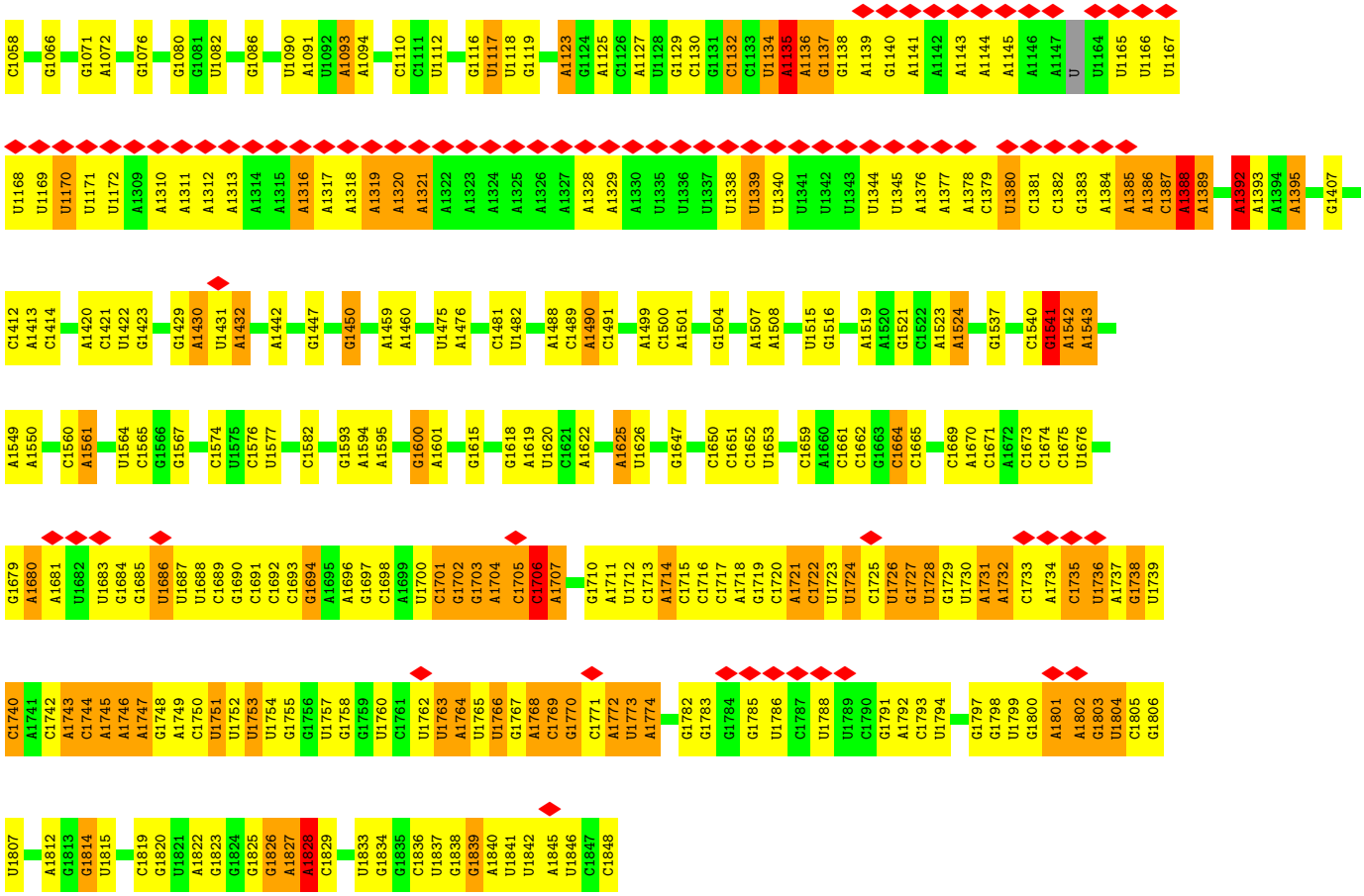
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



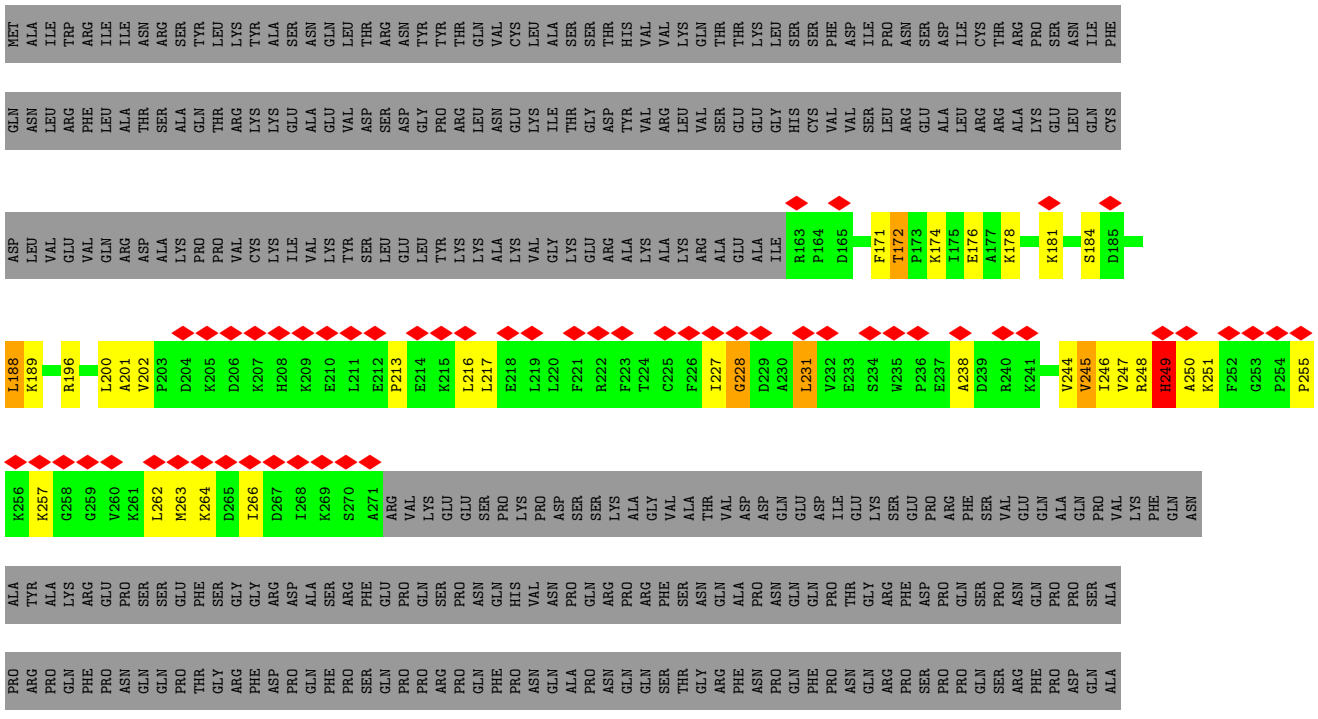


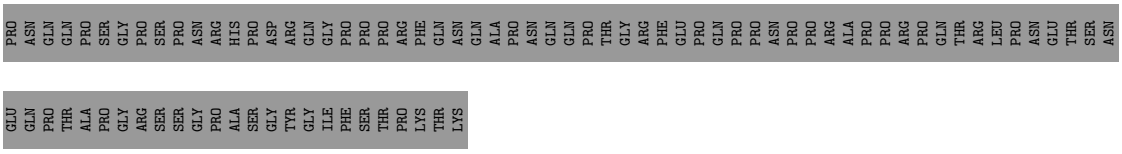


• Molecule 2: Translation initiation factor IF3-1, mitochondrial

Chain 8:



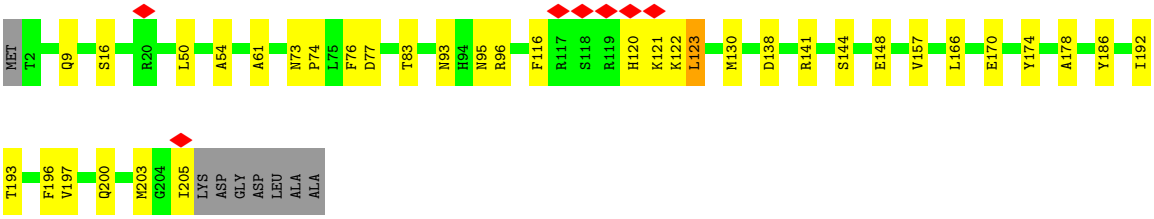




• Molecule 3: Ribosomal protein S2

Chain A:

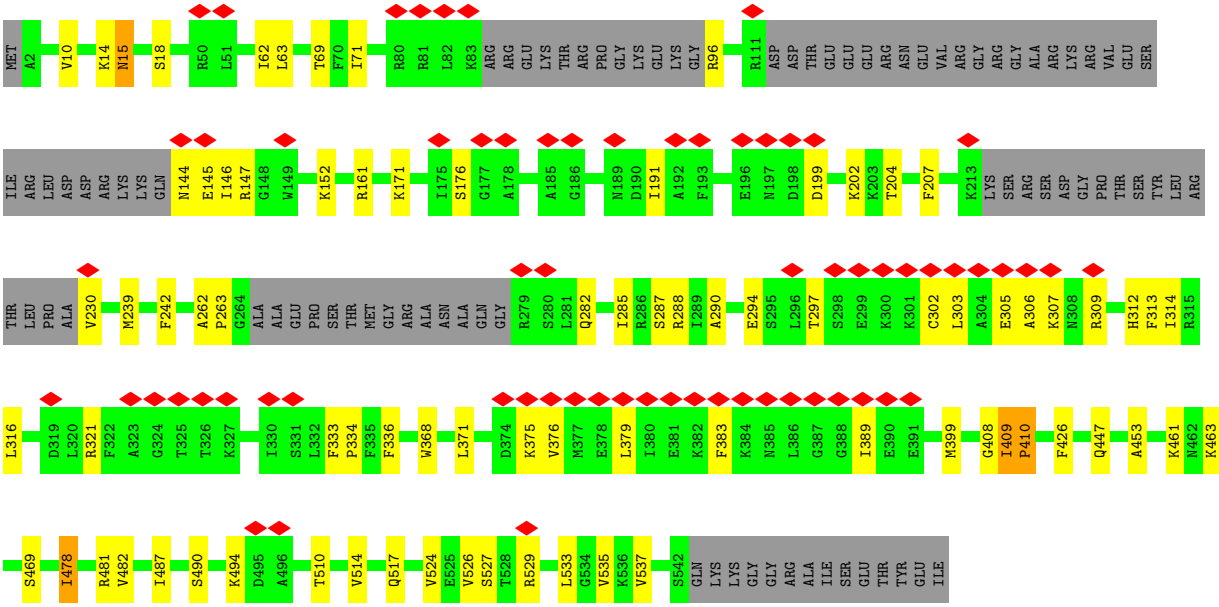




• Molecule 4: Small ribosomal subunit protein uS3m

Chain B:

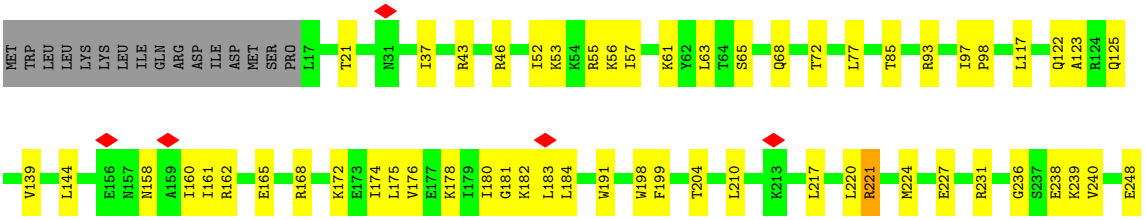


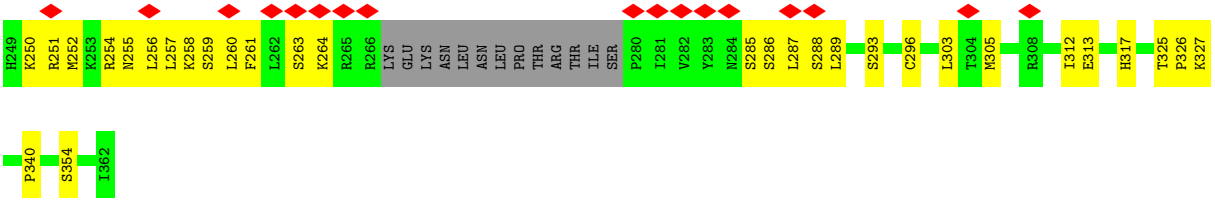


• Molecule 5: Ribosomal protein S4

Chain C:

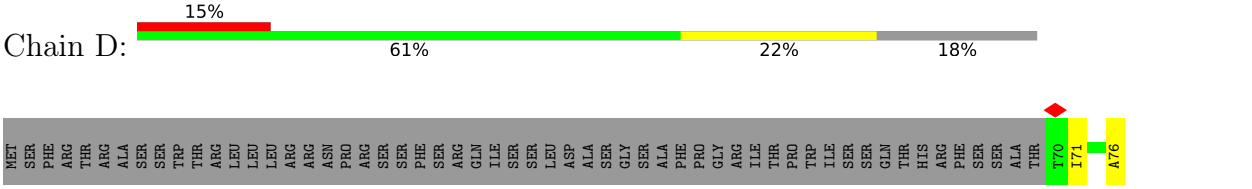


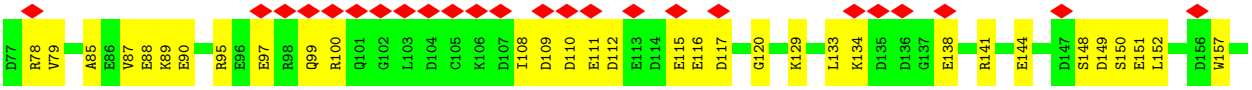


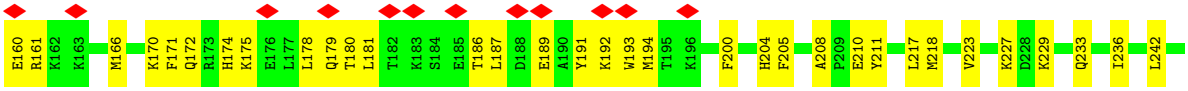


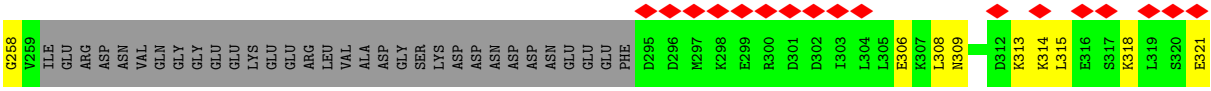
• Molecule 6: S5 DRBM domain-containing protein

Chain D:









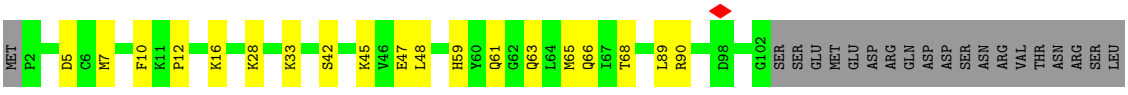


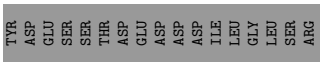


• Molecule 7: bS6m

Chain E:



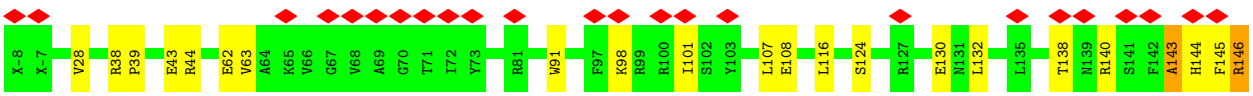




• Molecule 8: uS7m,Small ribosomal subunit protein uS7m

Chain F:







• Molecule 9: 40S ribosomal protein S15a

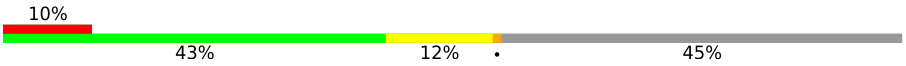
Chain G:

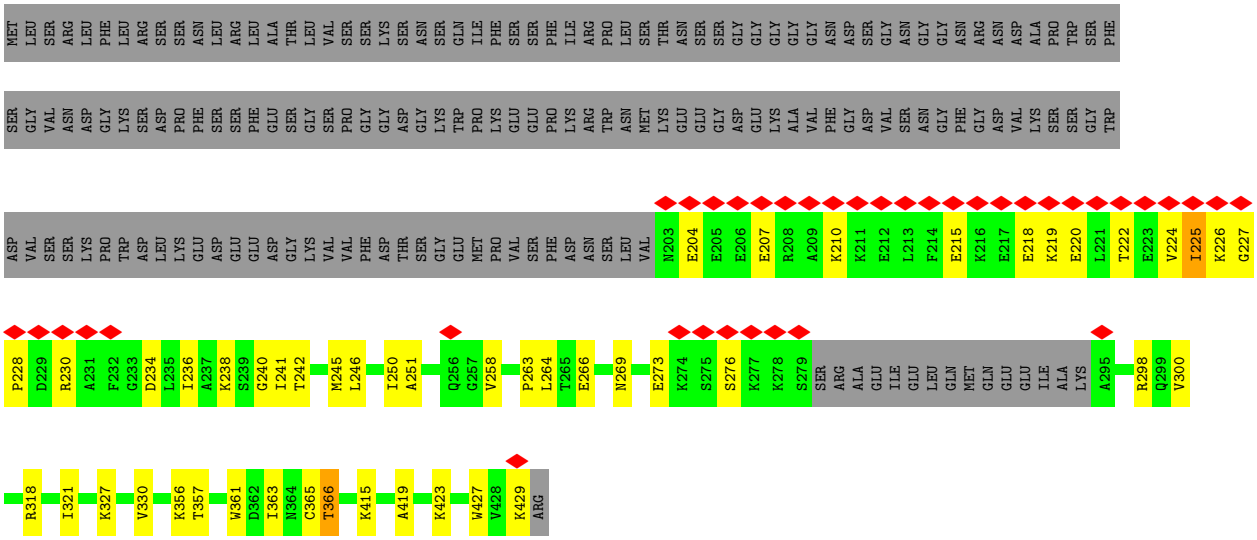




• Molecule 10: 30S ribosomal protein S9

Chain H:

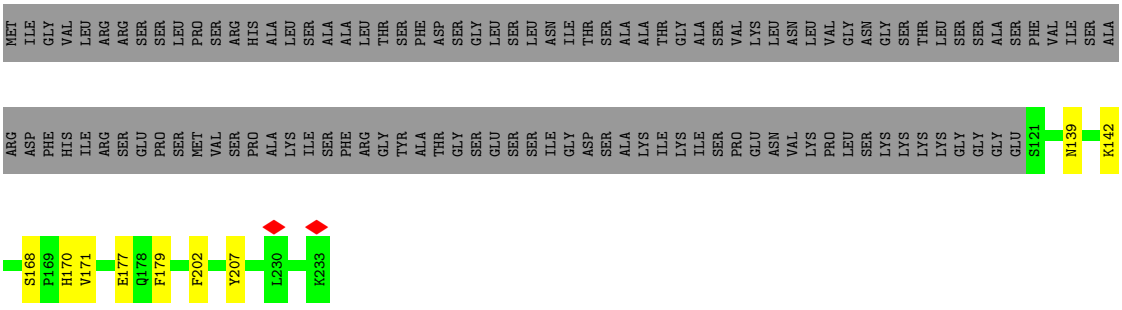




• Molecule 11: Small ribosomal subunit protein uS10 domain-containing protein

Chain I:



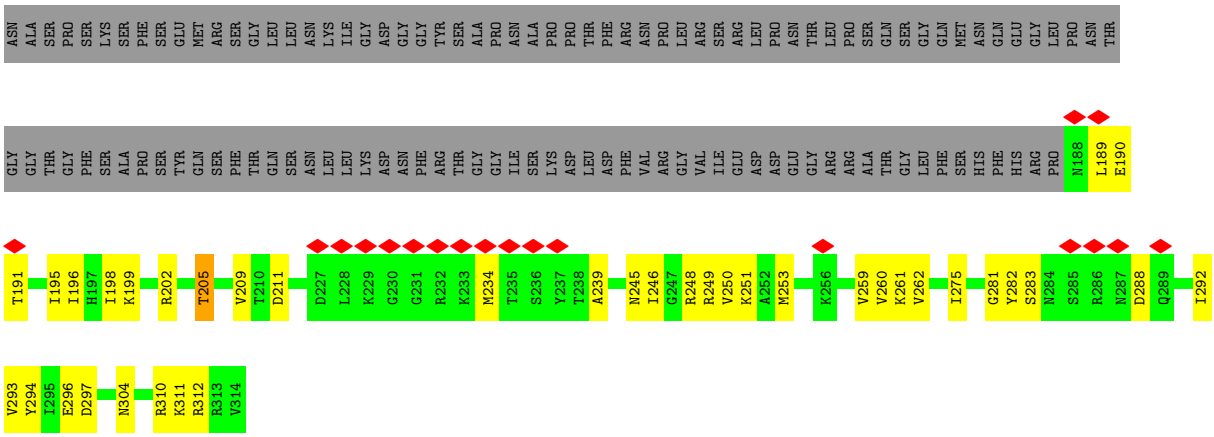


• Molecule 12: Ribosomal protein S11

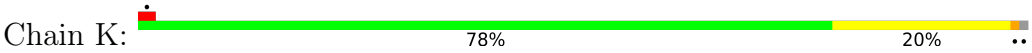
Chain J:







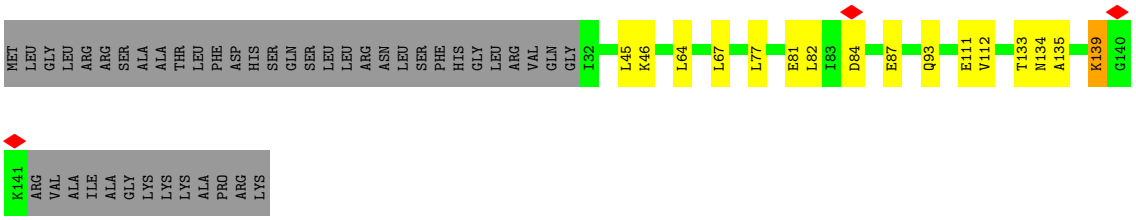
• Molecule 13: Small ribosomal subunit protein uS12m





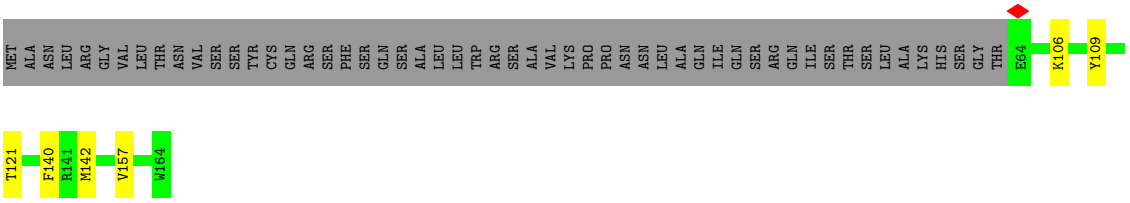
• Molecule 14: uS13m





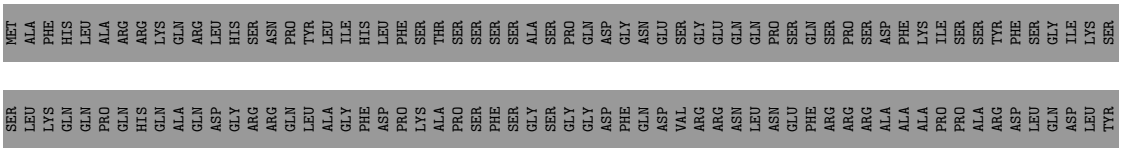
• Molecule 15: Small ribosomal subunit protein uS14m

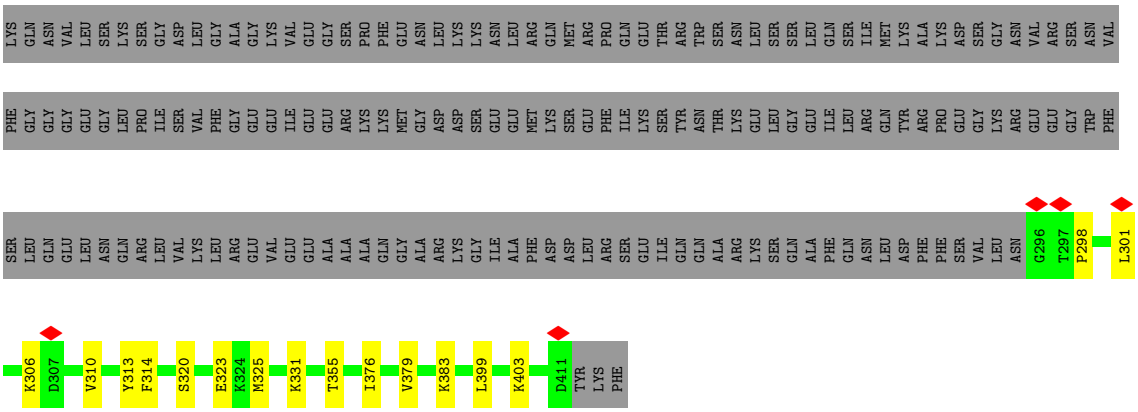




• Molecule 16: Small ribosomal subunit protein uS15c







• Molecule 17: 30S ribosomal protein S16

Chain O:

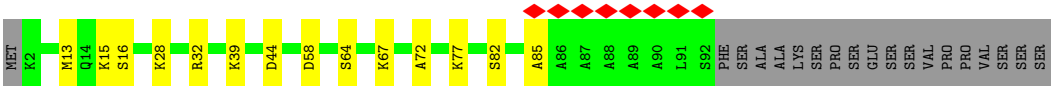




• Molecule 18: Small ribosomal subunit protein uS17c

Chain P:

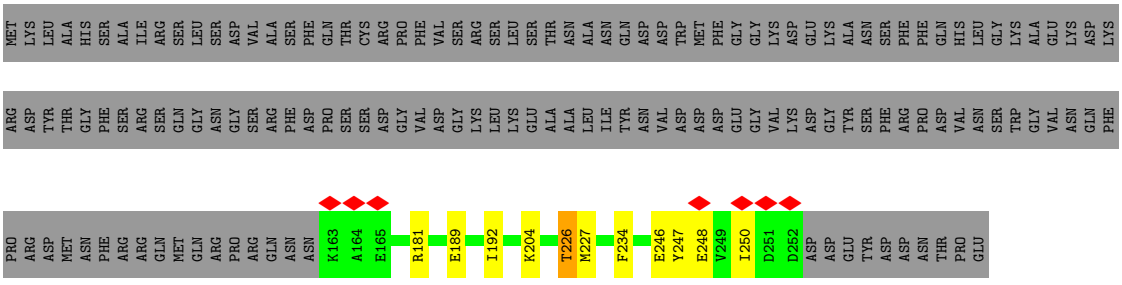




• Molecule 19: Small ribosomal subunit protein bS18c

Chain Q:

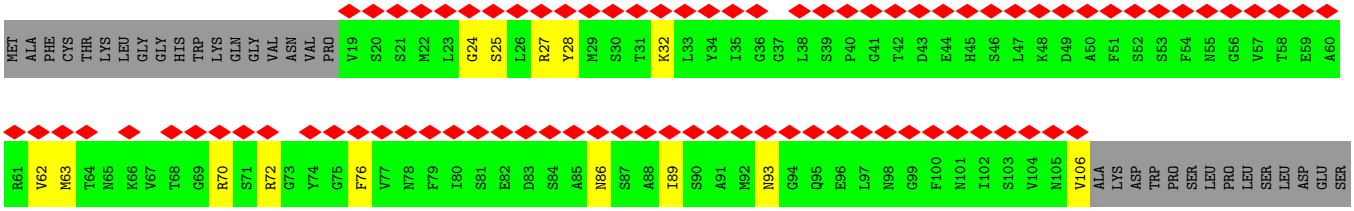


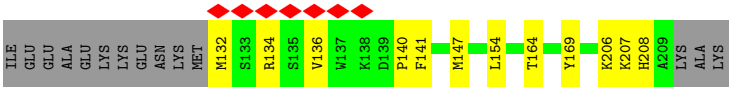


• Molecule 20: Small ribosomal subunit protein uS19m

Chain R:

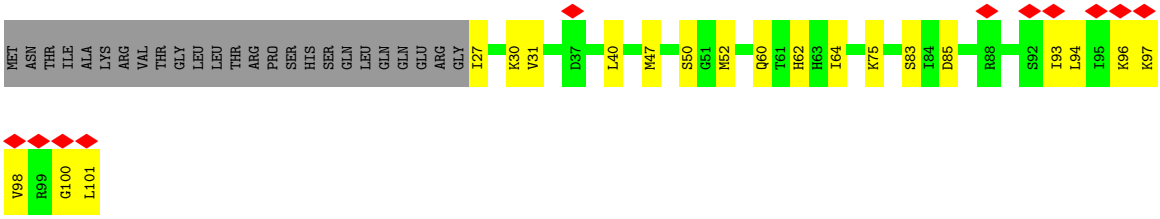




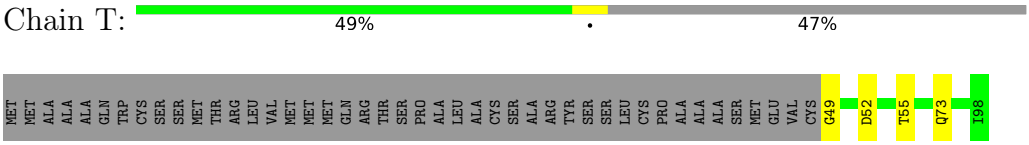


• Molecule 21: Ribosomal protein S21



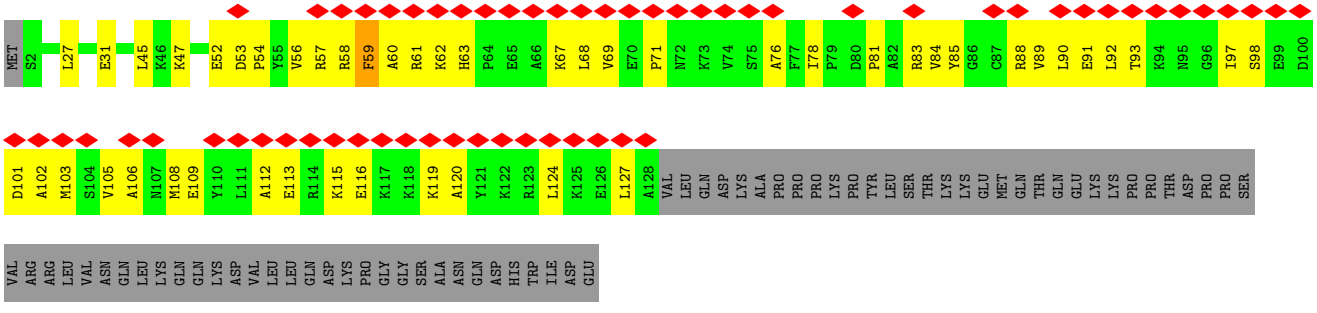


• Molecule 22: 30S ribosomal protein S31, mitochondrial



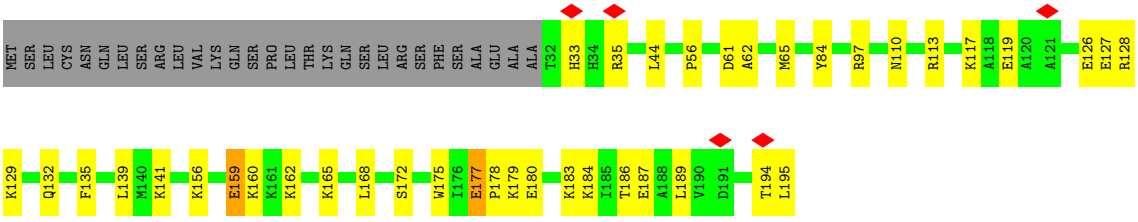
• Molecule 23: mS23





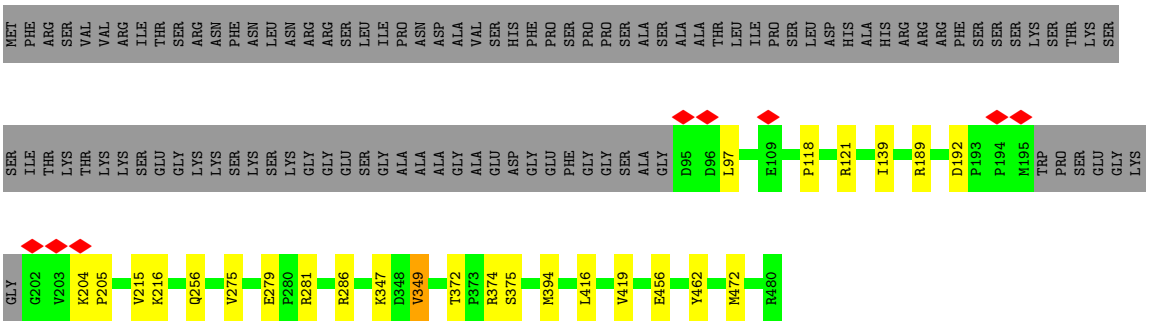
• Molecule 24: mS26





• Molecule 25: Small ribosomal subunit protein mS29

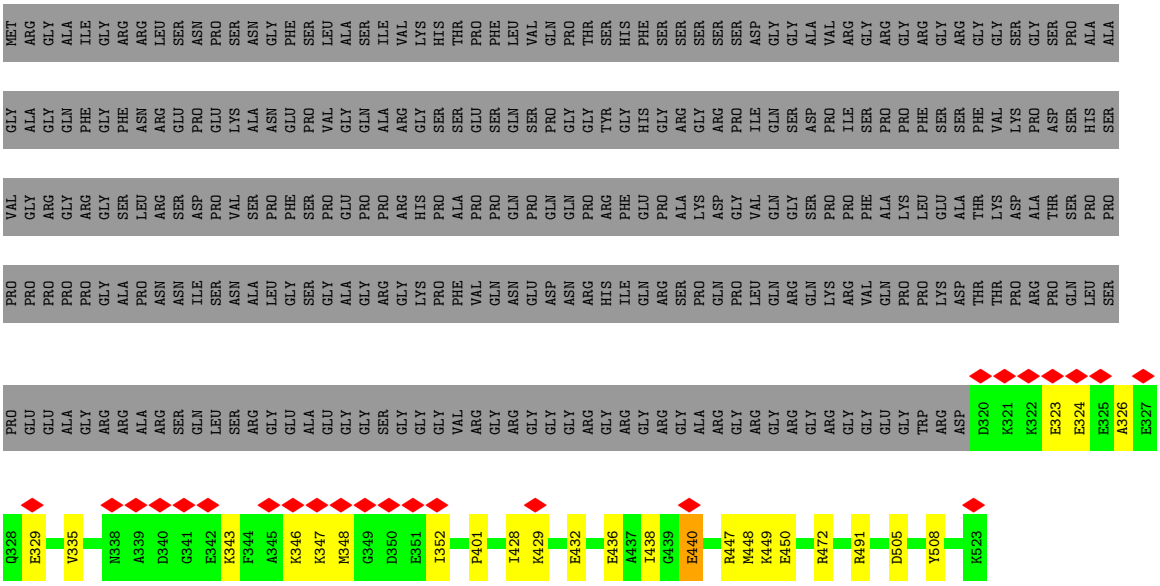




• Molecule 26: BnaC06g06470D protein

Chain X:

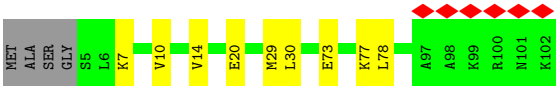




• Molecule 27: MOSC domain-containing protein

Chain Y:

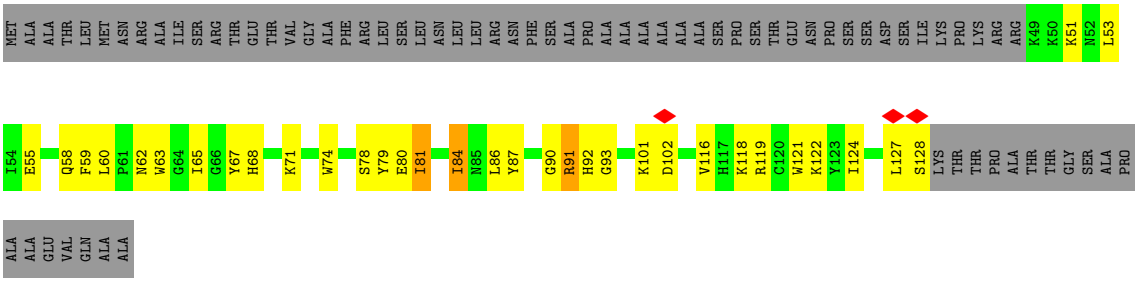




• Molecule 28: Mitochondrial 28S ribosomal protein S34

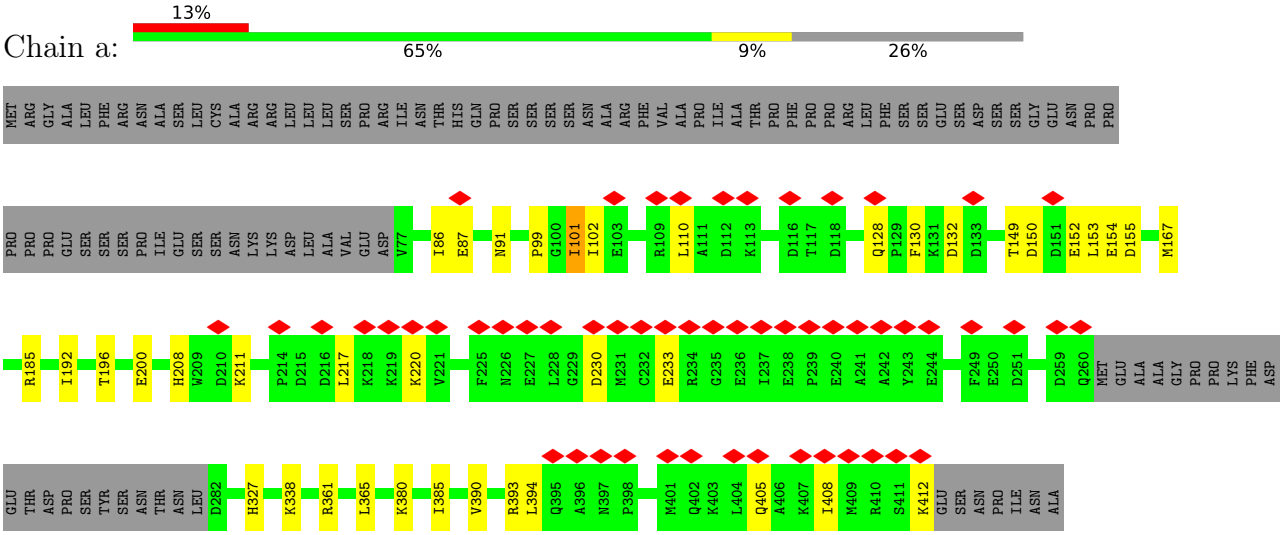
Chain Z:





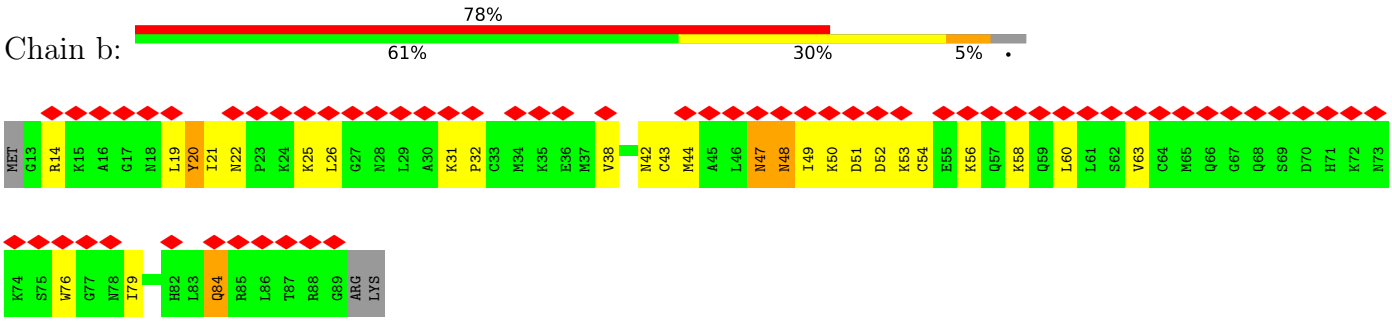
• Molecule 29: Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein

Chain a:



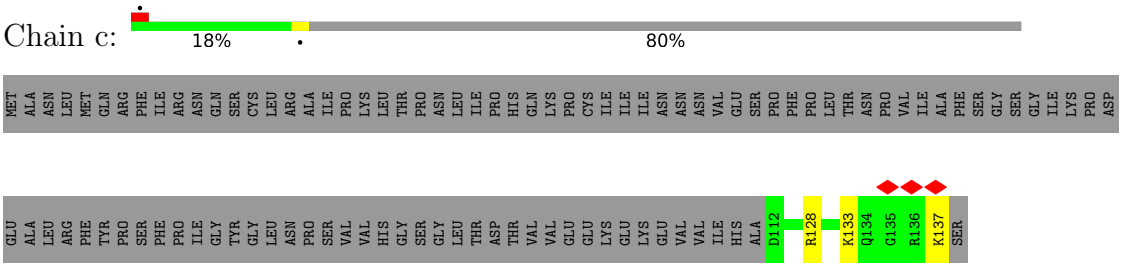
• Molecule 30: IMS import disulfide relay-system CHCH-CHCH-like Cx9C domain-containing protein

Chain b:



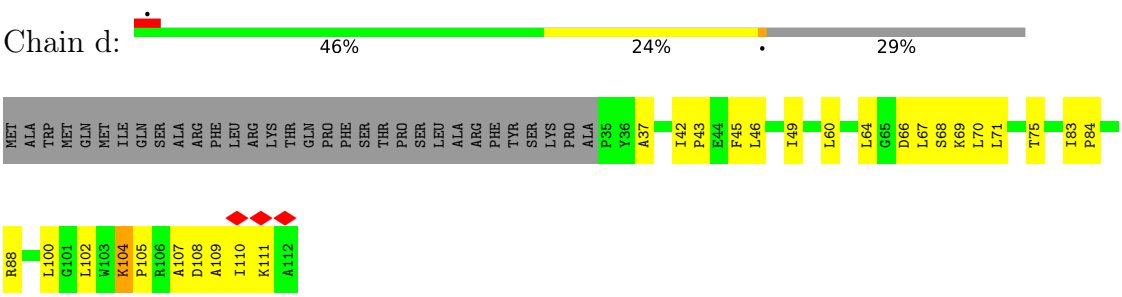
• Molecule 31: Small ribosomal subunit protein mS38

Chain c:



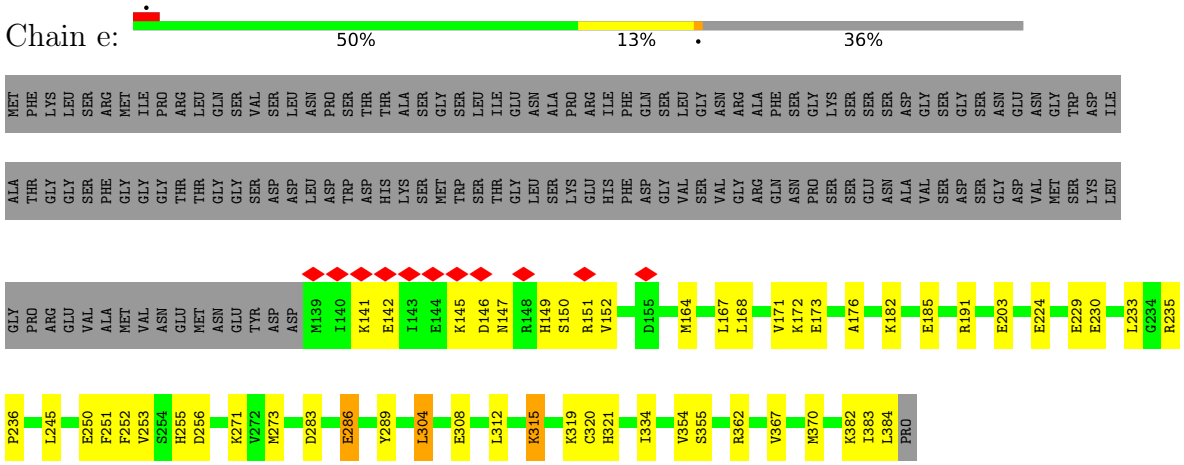
• Molecule 32: IGR domain-containing protein

Chain d:



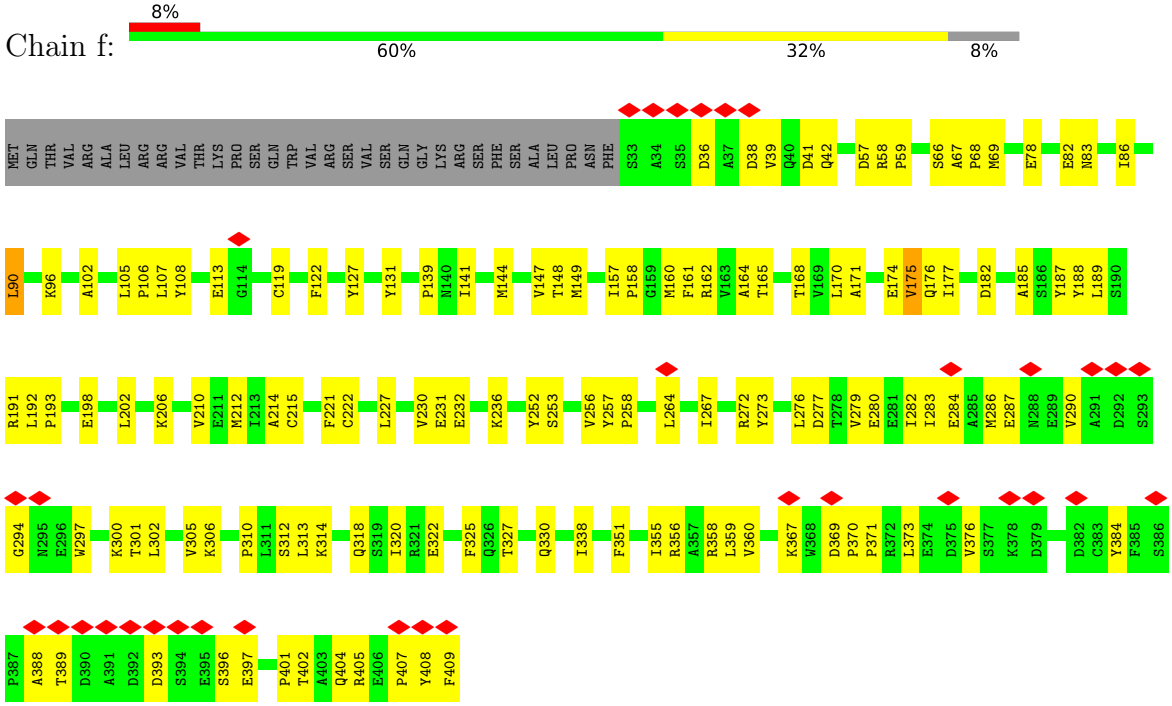
• Molecule 33: mS45

Chain e:



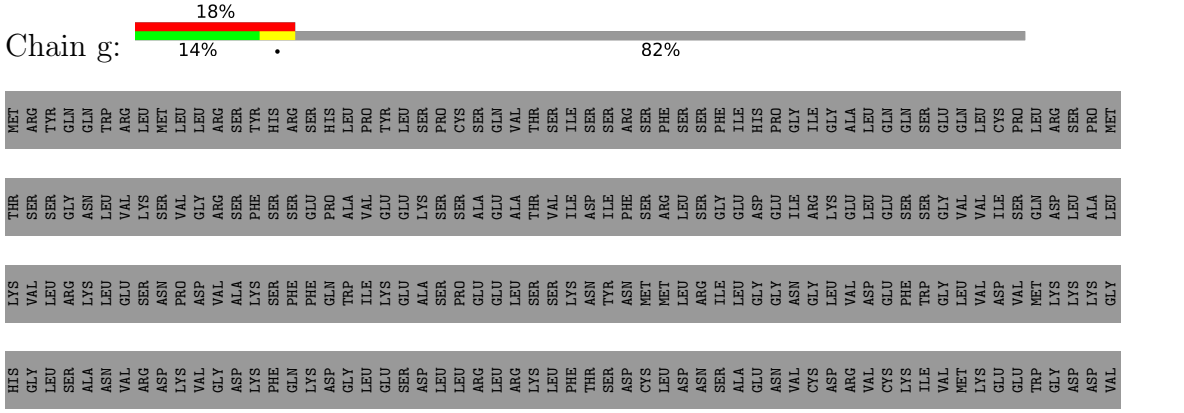
• Molecule 34: mS47

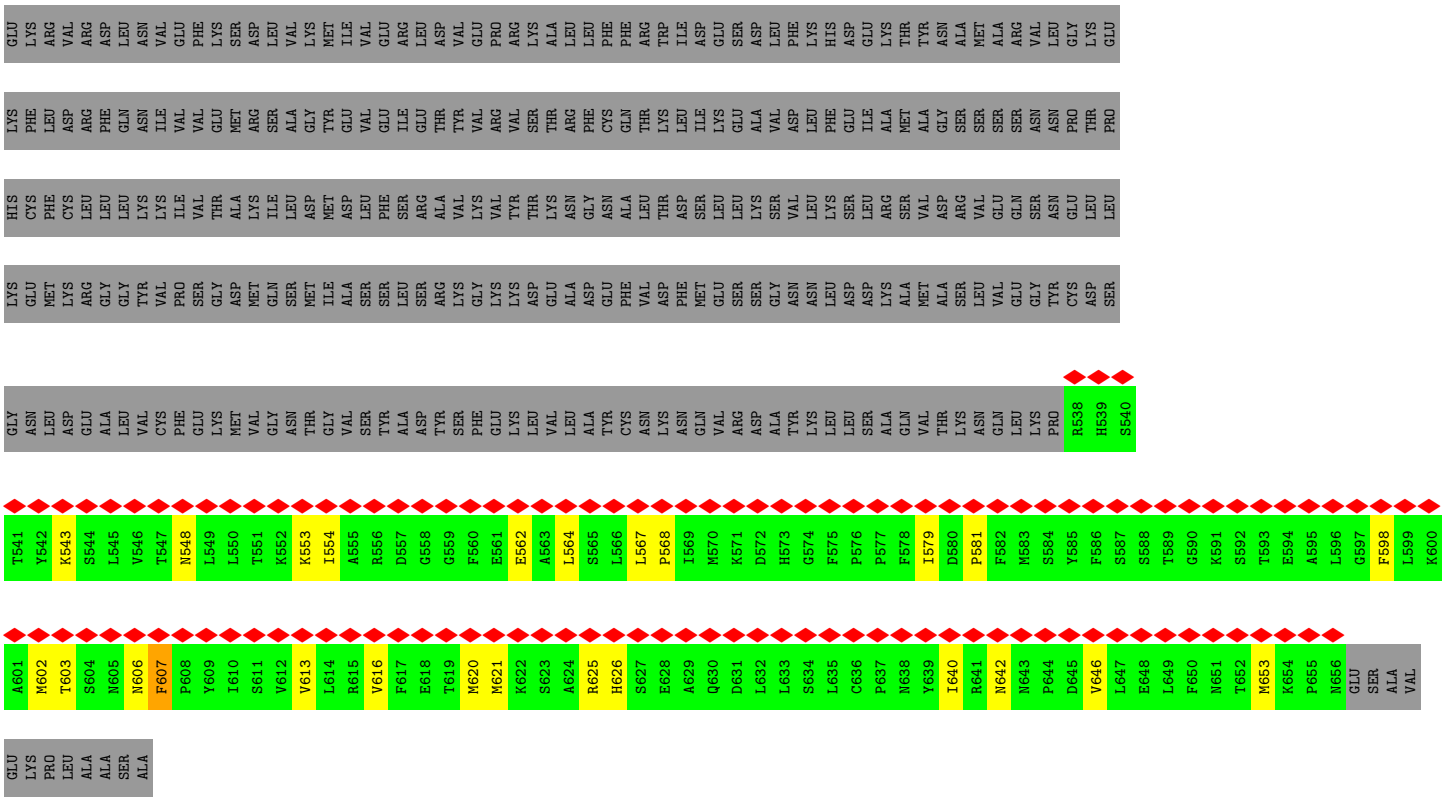
Chain f:



• Molecule 35: Small ribosomal subunit protein mS81 (rPPR8)

Chain g:

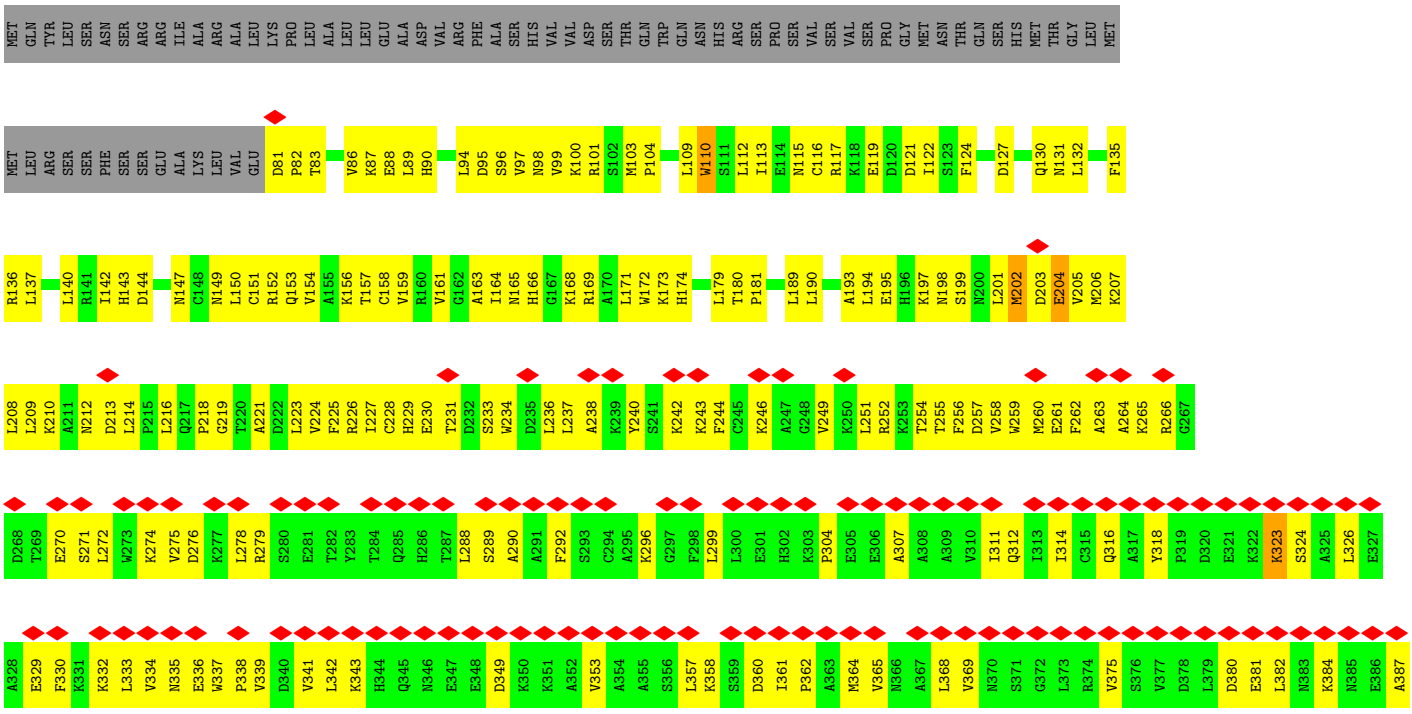




• Molecule 36: (rape) hypothetical protein

Chain h:



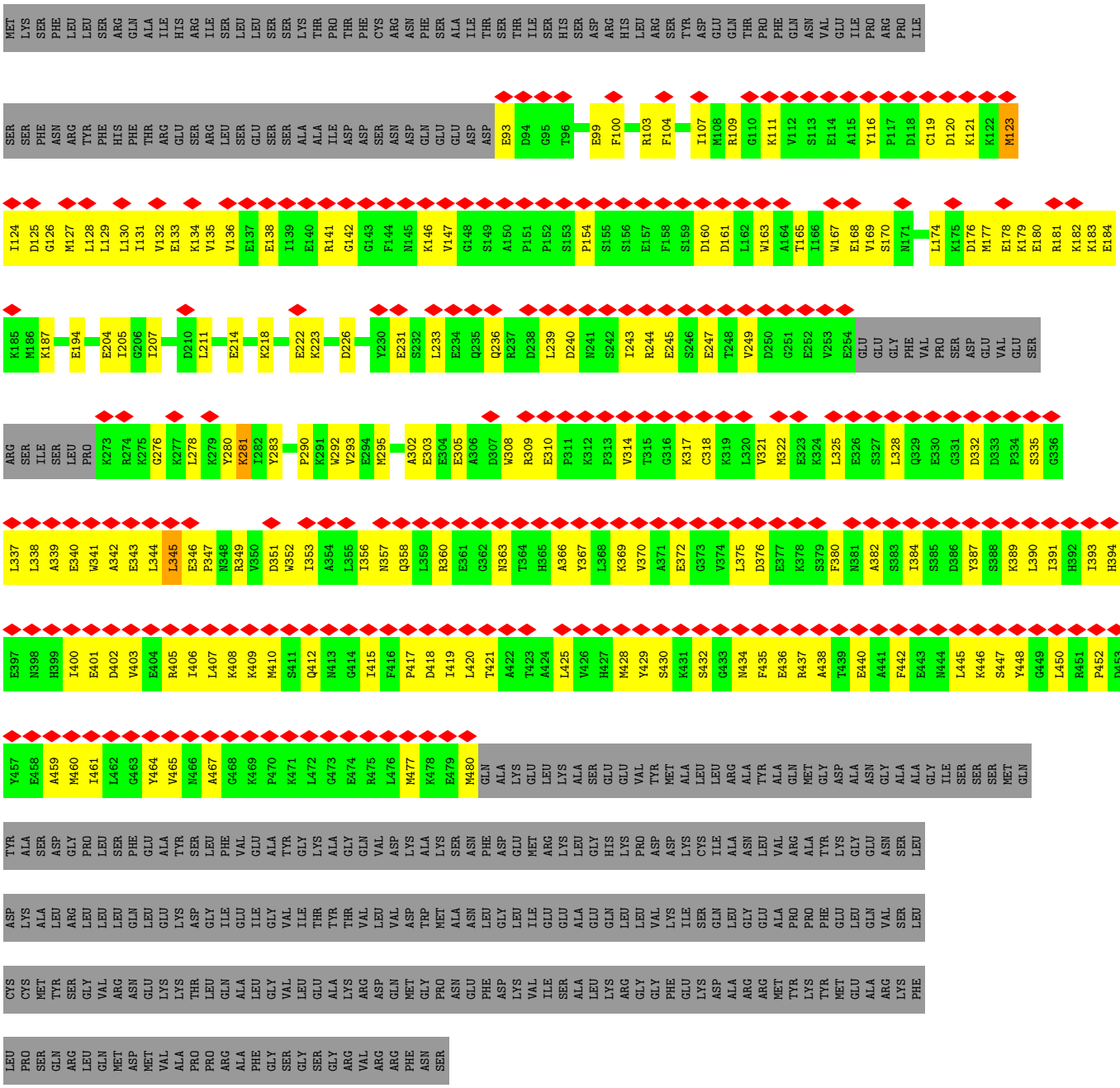




• Molecule 37: PROP1-like PPR domain-containing protein

Chain i:

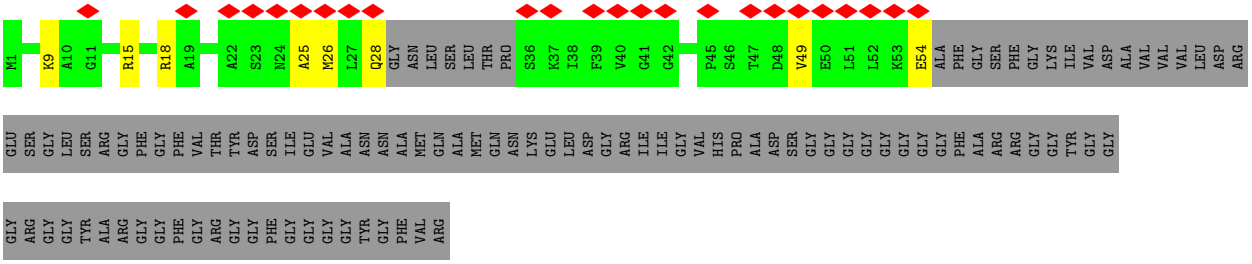




• Molecule 38: Small ribosomal subunit protein mS86

Chain k:

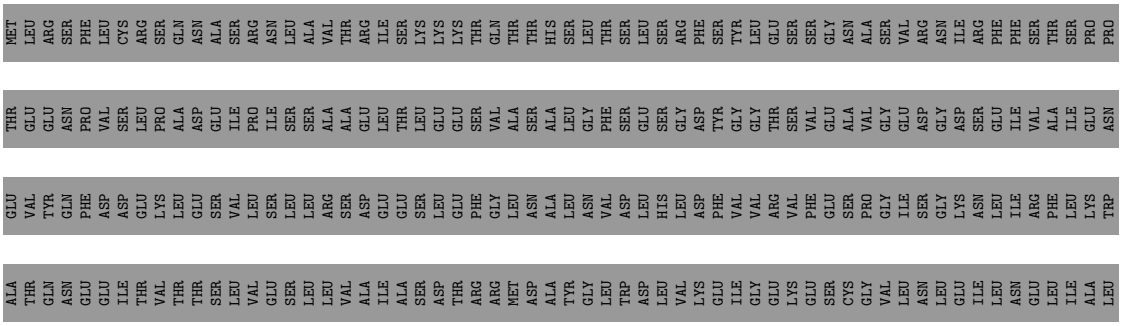


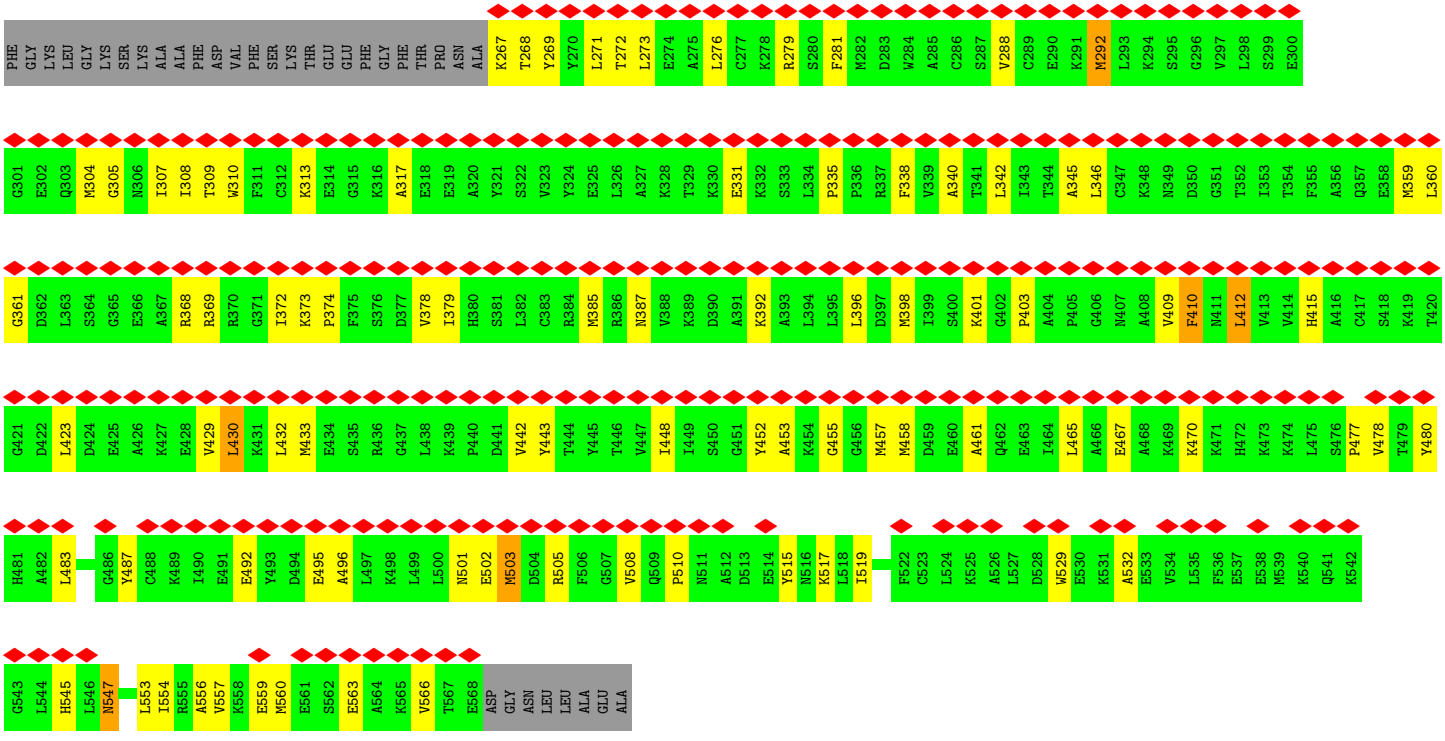


• Molecule 39: Small ribosomal subunit protein mS80 (rPPR6)

Chain l:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	141355	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	3.786	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.3	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: UR3, 4OC, G7M, MA6, 2MG, ATP

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	0.67	2/38445 (0.0%)	0.90	57/59928 (0.1%)
2	8	0.69	1/891 (0.1%)	0.95	2/1191 (0.2%)
3	A	0.15	0/1647	0.29	0/2227
4	B	0.42	0/3969	0.60	1/5320 (0.0%)
5	C	0.13	0/2859	0.32	0/3828
6	D	0.23	0/3438	0.38	0/4599
7	E	0.12	0/838	0.29	0/1121
8	F	0.34	0/1225	0.51	0/1641
9	G	0.13	0/1054	0.26	0/1418
10	H	0.35	0/1696	0.46	0/2273
11	I	0.41	0/964	0.52	0/1293
12	J	0.35	0/1000	0.47	0/1340
13	K	0.20	0/1010	0.42	0/1345
14	L	0.38	0/883	0.66	5/1176 (0.4%)
15	M	0.41	0/856	0.43	0/1134
16	N	0.12	0/958	0.25	0/1280
17	O	0.14	0/890	0.32	0/1196
18	P	0.12	0/730	0.28	0/984
19	Q	0.11	0/733	0.27	0/978
20	R	0.30	0/1323	0.42	0/1772
21	S	0.18	0/614	0.37	0/809
22	T	0.45	0/416	0.44	0/547
23	U	0.12	0/1036	0.34	0/1395
24	V	0.10	0/1423	0.24	0/1895
25	W	0.34	0/3139	0.44	0/4250
26	X	0.36	0/1644	0.54	0/2216
27	Y	0.36	0/807	0.43	0/1077
28	Z	0.11	0/669	0.34	0/900
29	a	0.39	0/2523	0.55	0/3386
30	b	0.60	0/618	0.94	1/822 (0.1%)
31	c	0.35	0/233	0.58	0/296
32	d	0.26	0/628	0.47	1/840 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.25	0/2118	0.45	1/2828 (0.0%)
34	f	0.11	0/2981	0.34	0/4033
35	g	0.16	0/969	0.44	0/1309
36	h	0.11	0/2511	0.34	0/3391
37	i	0.10	0/3048	0.31	0/4093
38	k	0.12	0/316	0.34	0/423
39	l	0.21	0/2409	0.44	0/3233
All	All	0.48	3/93511 (0.0%)	0.69	68/133787 (0.1%)

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
2	8	0	3
8	F	0	2
31	c	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	8	249	HIS	C-O	-8.69	1.12	1.24
1	2	1524	A	N9-C4	-6.50	1.33	1.37
1	2	1524	A	N3-C4	-5.75	1.31	1.34

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	8	249	HIS	O-C-N	-14.51	104.36	123.23
1	2	1542	A	N7-C8-N9	11.76	119.68	113.80
30	b	20	TYR	CB-CA-C	-11.15	96.81	111.42
1	2	1542	A	C5-N7-C8	-10.12	98.84	103.90
1	2	1387	C	N1-C2-O2	9.58	124.65	118.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	8	196	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	8	248	ARG	Sidechain
2	8	249	HIS	Mainchain
8	F	140	ARG	Sidechain
8	F	146	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	34484	0	17382	553	0
2	8	874	927	926	22	0
3	A	1611	0	1633	32	0
4	B	3877	0	4008	62	0
5	C	2806	0	2971	108	0
6	D	3389	0	3419	109	0
7	E	823	0	879	14	0
8	F	1254	0	1268	14	0
9	G	1037	0	1058	15	0
10	H	1671	0	1713	58	0
11	I	941	0	970	6	0
12	J	988	0	1022	33	0
13	K	993	0	1052	20	0
14	L	873	0	904	5	0
15	M	843	0	884	3	0
16	N	941	0	978	18	0
17	O	869	0	898	9	0
18	P	717	0	755	9	0
19	Q	724	0	744	17	0
20	R	1299	0	1307	19	0
21	S	611	0	687	22	0
22	T	408	0	444	2	0
23	U	1014	0	1061	57	0
24	V	1399	0	1427	38	0
25	W	3062	0	3030	14	0
26	X	1613	0	1559	21	0
27	Y	793	0	834	7	0
28	Z	649	0	662	28	0
29	a	2486	0	2376	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	b	610	0	626	32	0
31	c	232	0	278	1	0
32	d	616	0	674	21	0
33	e	2074	0	2074	50	0
34	f	2922	0	2870	113	0
35	g	946	0	948	17	0
36	h	2463	0	2488	221	0
37	i	2993	0	2962	230	0
38	k	313	0	258	9	0
39	l	2371	0	2420	72	0
40	W	31	0	12	0	0
All	All	88620	927	72461	1908	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 12.

The worst 5 of 1908 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)
36:h:166:HIS:HA	36:h:169:ARG:HD2	1.25	1.14
36:h:234:TRP:HA	36:h:237:LEU:HD12	1.25	1.14
1:2:1750:C:H3'	1:2:1751:U:H5"	1.30	1.14
1:2:1091:A:OP2	3:A:121:LYS:HD2	1.50	1.11
36:h:193:ALA:HB2	36:h:201:LEU:HD22	1.32	1.11

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	8	107/520 (21%)	89 (83%)	14 (13%)	4 (4%)	2 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	202/212 (95%)	191 (95%)	11 (5%)	0	100	100
4	B	457/554 (82%)	427 (93%)	28 (6%)	2 (0%)	30	36
5	C	329/362 (91%)	323 (98%)	6 (2%)	0	100	100
6	D	409/501 (82%)	393 (96%)	16 (4%)	0	100	100
7	E	99/138 (72%)	97 (98%)	2 (2%)	0	100	100
8	F	146/157 (93%)	141 (97%)	4 (3%)	1 (1%)	18	21
9	G	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
10	H	208/383 (54%)	200 (96%)	7 (3%)	1 (0%)	24	29
11	I	111/228 (49%)	107 (96%)	4 (4%)	0	100	100
12	J	125/304 (41%)	119 (95%)	6 (5%)	0	100	100
13	K	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
14	L	108/154 (70%)	105 (97%)	3 (3%)	0	100	100
15	M	99/155 (64%)	98 (99%)	1 (1%)	0	100	100
16	N	114/414 (28%)	114 (100%)	0	0	100	100
17	O	108/136 (79%)	108 (100%)	0	0	100	100
18	P	89/110 (81%)	89 (100%)	0	0	100	100
19	Q	88/237 (37%)	88 (100%)	0	0	100	100
20	R	162/212 (76%)	153 (94%)	9 (6%)	0	100	100
21	S	73/100 (73%)	73 (100%)	0	0	100	100
22	T	48/94 (51%)	45 (94%)	3 (6%)	0	100	100
23	U	125/192 (65%)	122 (98%)	3 (2%)	0	100	100
24	V	162/193 (84%)	158 (98%)	3 (2%)	1 (1%)	21	25
25	W	376/483 (78%)	374 (100%)	2 (0%)	0	100	100
26	X	202/496 (41%)	200 (99%)	1 (0%)	1 (0%)	24	29
27	Y	96/102 (94%)	96 (100%)	0	0	100	100
28	Z	78/153 (51%)	74 (95%)	4 (5%)	0	100	100
29	a	311/424 (73%)	303 (97%)	8 (3%)	0	100	100
30	b	75/80 (94%)	65 (87%)	9 (12%)	1 (1%)	9	9
31	c	24/128 (19%)	23 (96%)	1 (4%)	0	100	100
32	d	76/110 (69%)	74 (97%)	1 (1%)	1 (1%)	9	9
33	e	244/383 (64%)	240 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	f	375/410 (92%)	362 (96%)	13 (4%)	0	100	100
35	g	117/668 (18%)	109 (93%)	8 (7%)	0	100	100
36	h	308/384 (80%)	299 (97%)	9 (3%)	0	100	100
37	i	366/725 (50%)	356 (97%)	10 (3%)	0	100	100
38	k	43/155 (28%)	37 (86%)	6 (14%)	0	100	100
39	l	300/576 (52%)	296 (99%)	4 (1%)	0	100	100
All	All	6608/10887 (61%)	6386 (97%)	210 (3%)	12 (0%)	44	53

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	8	251	LYS
10	H	225	ILE
30	b	48	ASN
2	8	228	GLY
32	d	108	ASP

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	8	95/461 (21%)	87 (92%)	8 (8%)	10	12
3	A	177/182 (97%)	176 (99%)	1 (1%)	78	87
4	B	421/492 (86%)	413 (98%)	8 (2%)	50	66
5	C	312/343 (91%)	307 (98%)	5 (2%)	55	71
6	D	366/444 (82%)	361 (99%)	5 (1%)	59	74
7	E	90/126 (71%)	88 (98%)	2 (2%)	45	62
8	F	124/124 (100%)	117 (94%)	7 (6%)	19	25
9	G	112/113 (99%)	110 (98%)	2 (2%)	51	68
10	H	175/320 (55%)	170 (97%)	5 (3%)	37	52
11	I	104/197 (53%)	103 (99%)	1 (1%)	68	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	J	108/256 (42%)	105 (97%)	3 (3%)	38	53
13	K	106/107 (99%)	104 (98%)	2 (2%)	50	66
14	L	93/128 (73%)	88 (95%)	5 (5%)	20	27
15	M	90/137 (66%)	88 (98%)	2 (2%)	45	62
16	N	107/362 (30%)	107 (100%)	0	100	100
17	O	93/117 (80%)	92 (99%)	1 (1%)	65	79
18	P	78/95 (82%)	76 (97%)	2 (3%)	40	56
19	Q	75/203 (37%)	74 (99%)	1 (1%)	61	76
20	R	141/180 (78%)	140 (99%)	1 (1%)	76	86
21	S	68/90 (76%)	66 (97%)	2 (3%)	37	52
22	T	44/79 (56%)	43 (98%)	1 (2%)	44	60
23	U	109/170 (64%)	107 (98%)	2 (2%)	51	68
24	V	147/173 (85%)	143 (97%)	4 (3%)	39	55
25	W	328/410 (80%)	321 (98%)	7 (2%)	47	63
26	X	174/395 (44%)	170 (98%)	4 (2%)	44	60
27	Y	84/86 (98%)	82 (98%)	2 (2%)	43	59
28	Z	65/119 (55%)	61 (94%)	4 (6%)	16	21
29	a	252/375 (67%)	246 (98%)	6 (2%)	43	59
30	b	68/71 (96%)	65 (96%)	3 (4%)	25	35
31	c	25/116 (22%)	25 (100%)	0	100	100
32	d	65/93 (70%)	65 (100%)	0	100	100
33	e	226/339 (67%)	220 (97%)	6 (3%)	39	55
34	f	321/351 (92%)	317 (99%)	4 (1%)	63	77
35	g	108/597 (18%)	106 (98%)	2 (2%)	50	66
36	h	271/337 (80%)	264 (97%)	7 (3%)	40	56
37	i	325/629 (52%)	319 (98%)	6 (2%)	51	68
38	k	21/106 (20%)	20 (95%)	1 (5%)	23	32
39	l	256/492 (52%)	250 (98%)	6 (2%)	44	60
All	All	5824/9415 (62%)	5696 (98%)	128 (2%)	45	62

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	i	123	MET
37	i	345	LEU
13	K	88	LYS
13	K	25	ASP
38	k	18	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
24	V	96	GLN
28	Z	92	HIS
25	W	248	HIS
26	X	521	ASN
30	b	84	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1602/1611 (99%)	289 (18%)	21 (1%)

5 of 289 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	12	A
1	2	17	G
1	2	26	U
1	2	30	G
1	2	37	A

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1705	C
1	2	1769	C
1	2	1814	G
1	2	1773	U
1	2	1726	U

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	0.32	0	34,38,41	0.68	1 (2%)
1	UR3	2	1807	1	19,22,23	0.34	0	26,32,35	0.83	1 (3%)
1	MA6	2	1828	1	23,26,27	0.33	0	34,38,41	0.66	1 (2%)
1	2MG	2	1825	1	23,26,27	0.31	0	32,38,41	0.57	0
1	G7M	2	525	1	23,26,27	0.64	0	35,39,42	0.57	0
1	4OC	2	1664	1	20,23,24	0.40	0	26,32,35	0.87	2 (7%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1828	MA6	C2-N1-C6	3.00	118.83	111.75
1	2	1827	MA6	C2-N1-C6	2.95	118.72	111.75
1	2	1664	4OC	O2'-C2'-C1'	-2.73	103.75	109.08
1	2	1664	4OC	O3'-C3'-C2'	2.53	118.36	111.17
1	2	1807	UR3	C4-N3-C2	-2.07	122.61	124.56

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	1664	4OC	C3'-C2'-O2'-CM2
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.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1827	MA6	1	0
1	2	1828	MA6	1	0
1	2	1825	2MG	1	0
1	2	1664	4OC	1	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	$\#\|Z\| > 2$
40	ATP	W	501	-	29,33,33	0.65	0	44,52,52	0.50	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
40	ATP	W	501	-	-	0/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

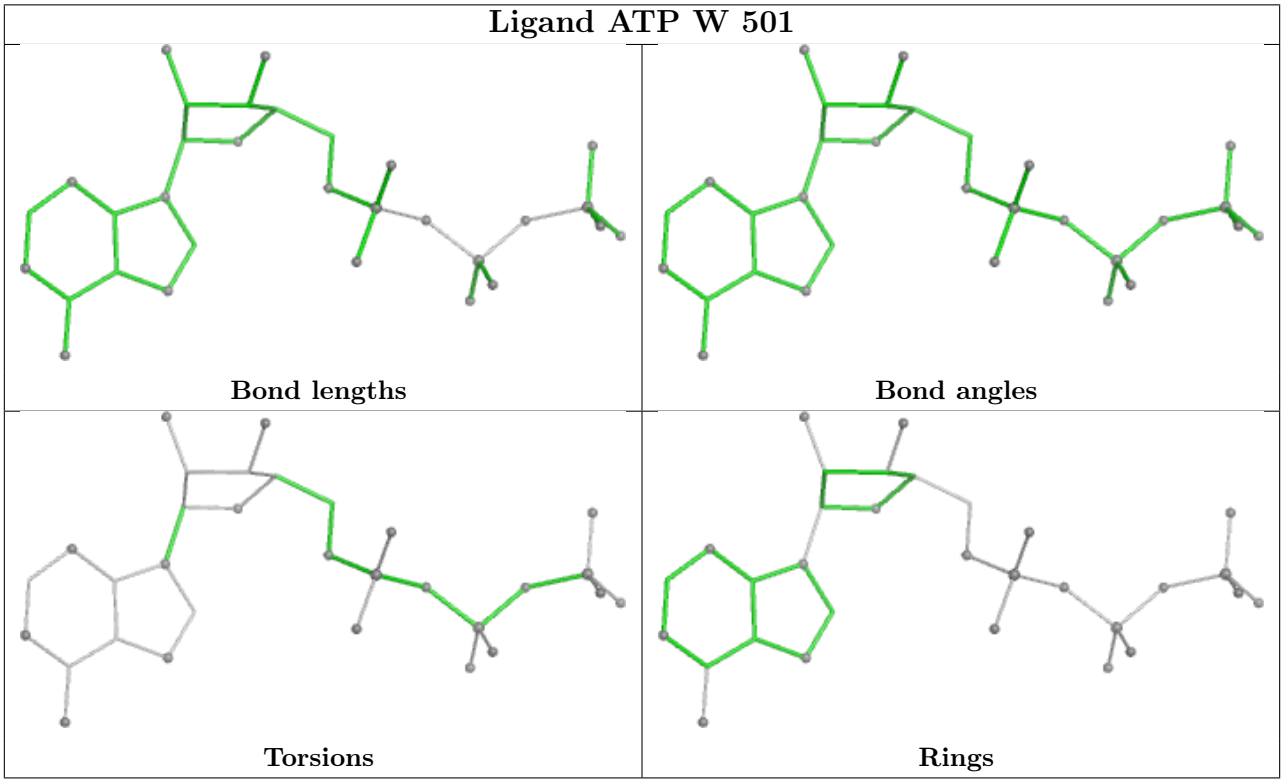
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	6

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1172:U	O3'	1309:A	P	20.56
1	2	1330:A	O3'	1335:U	P	18.93
1	2	137:A	O3'	142:U	P	14.70
1	2	1345:U	O3'	1376:A	P	14.09
1	2	84:A	O3'	129:A	P	13.51

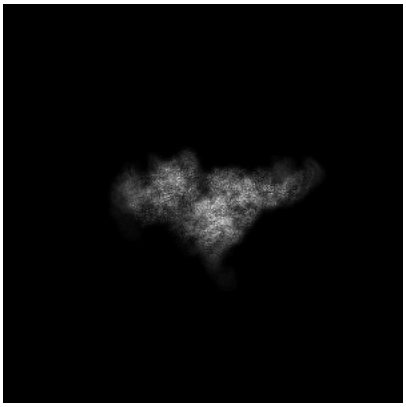
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-56198. These allow visual inspection of the internal detail of the map and identification of artifacts.

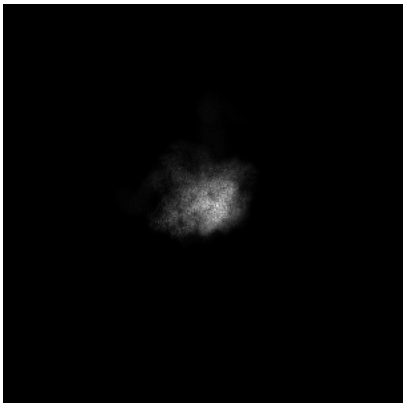
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

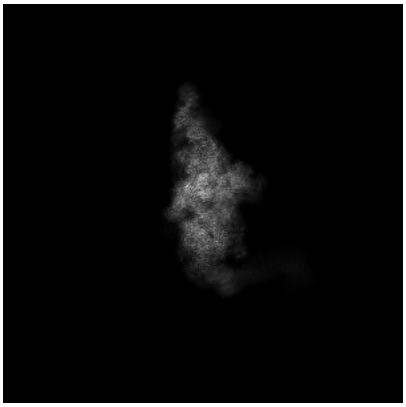
6.1.1 Primary map



X



Y

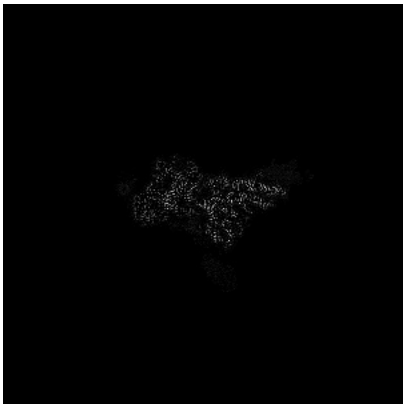


Z

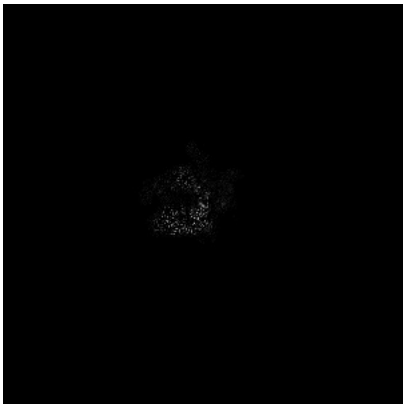
The images above show the map projected in three orthogonal directions.

6.2 Central slices

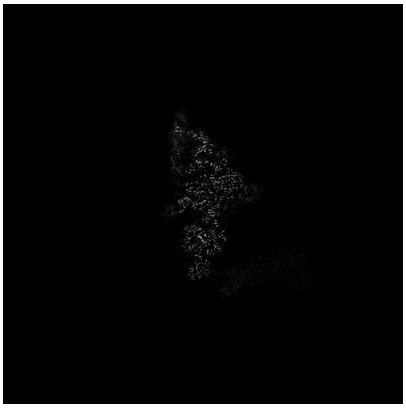
6.2.1 Primary map



X Index: 350



Y Index: 350

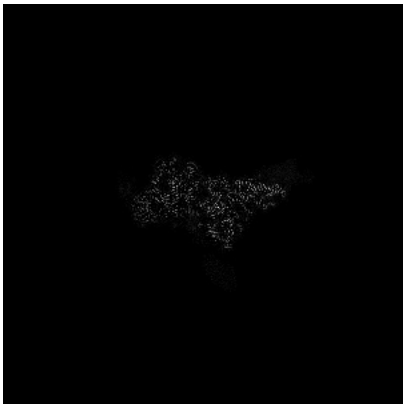


Z Index: 350

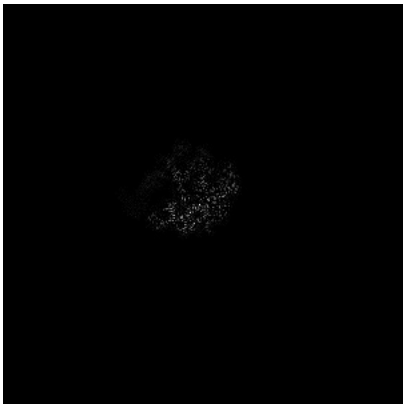
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

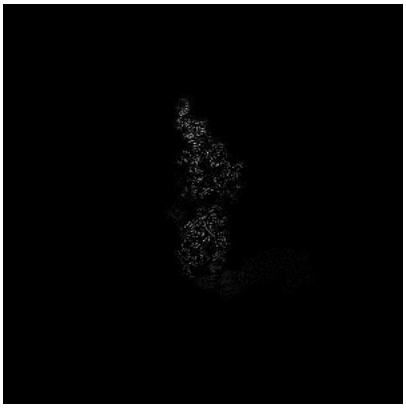
6.3.1 Primary map



X Index: 348



Y Index: 376

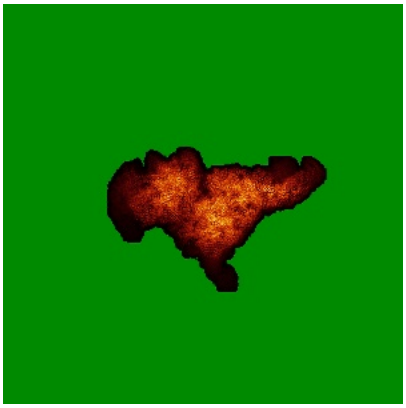


Z Index: 371

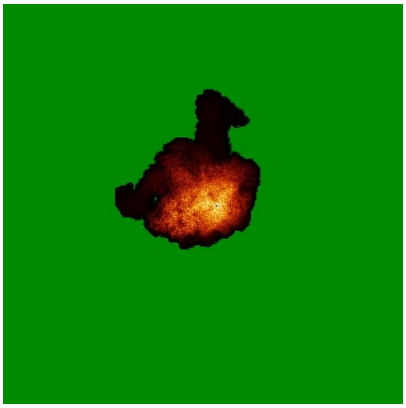
The images above show the largest variance slices of the map in three orthogonal directions.

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

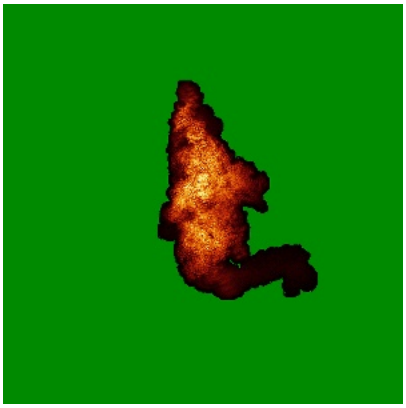
6.4.1 Primary map



X



Y

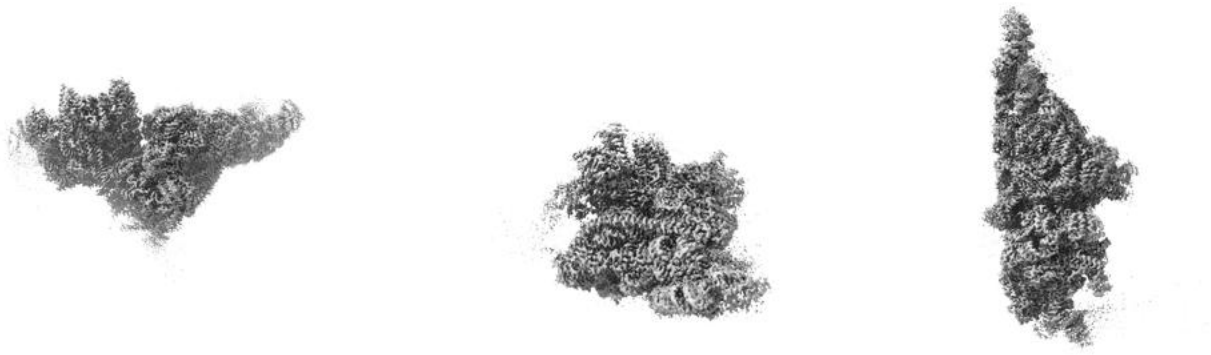


Z

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 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

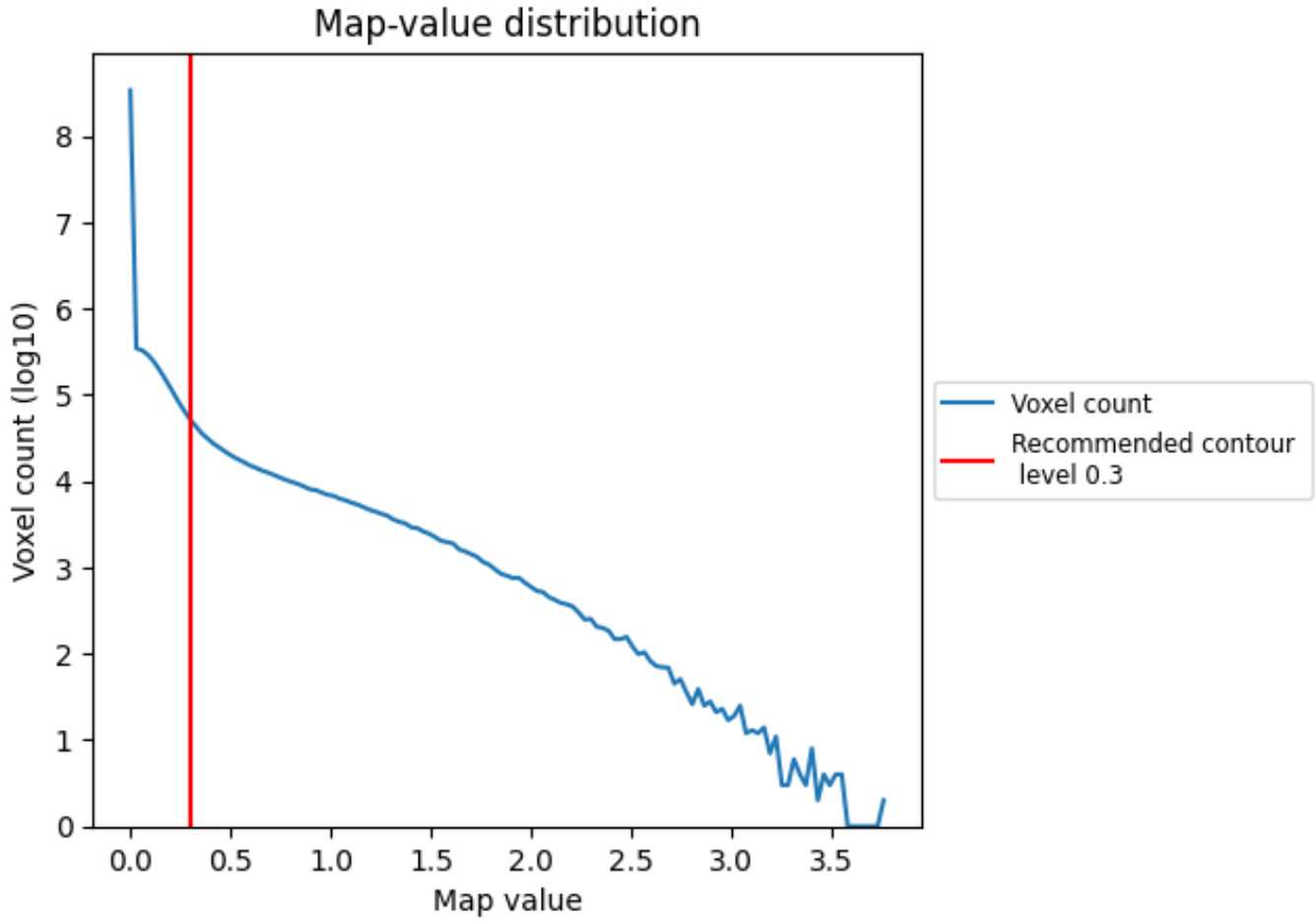
6.6 Mask visualisation (i)

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

7 Map analysis

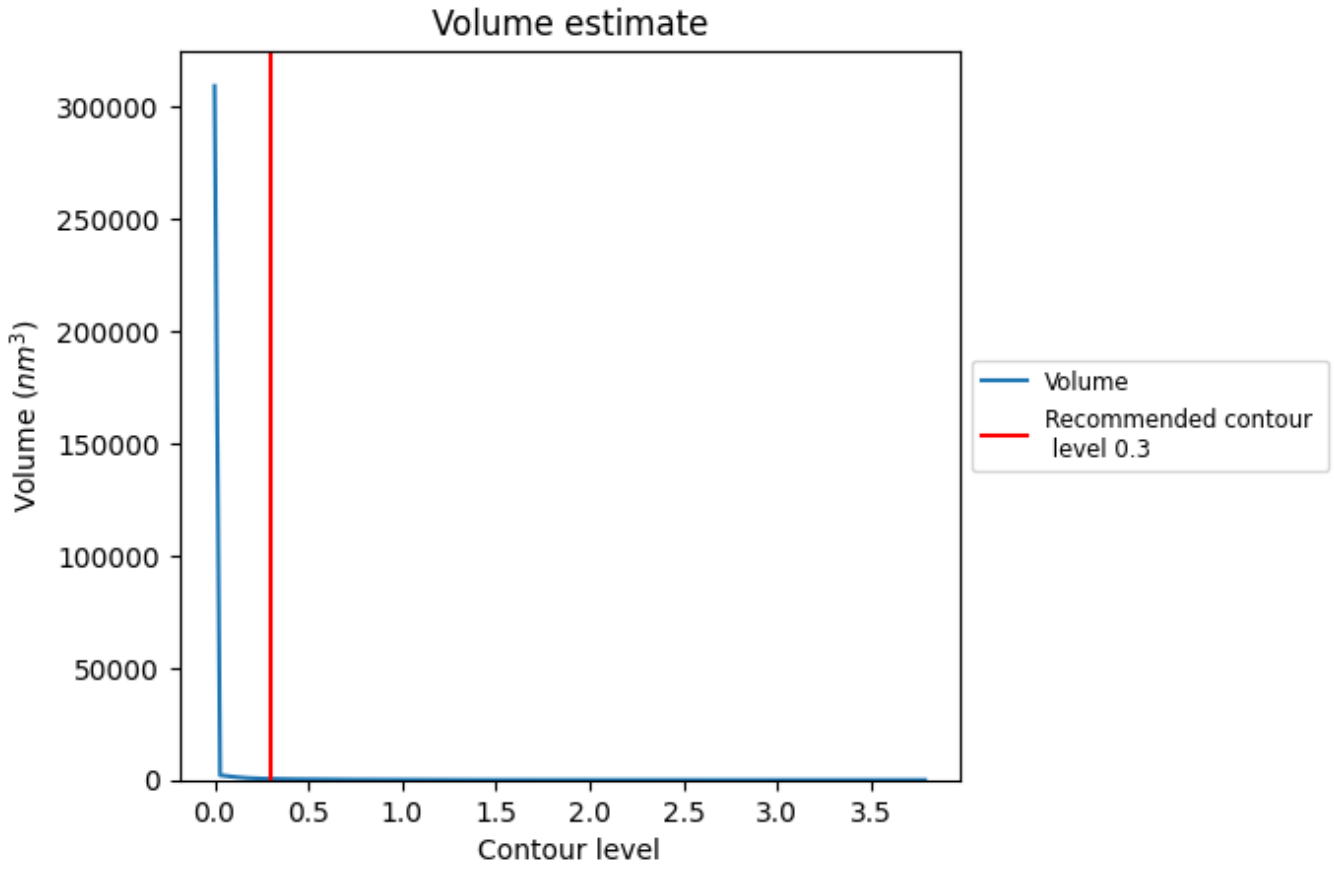
This section contains the results of statistical analysis of the map.

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.

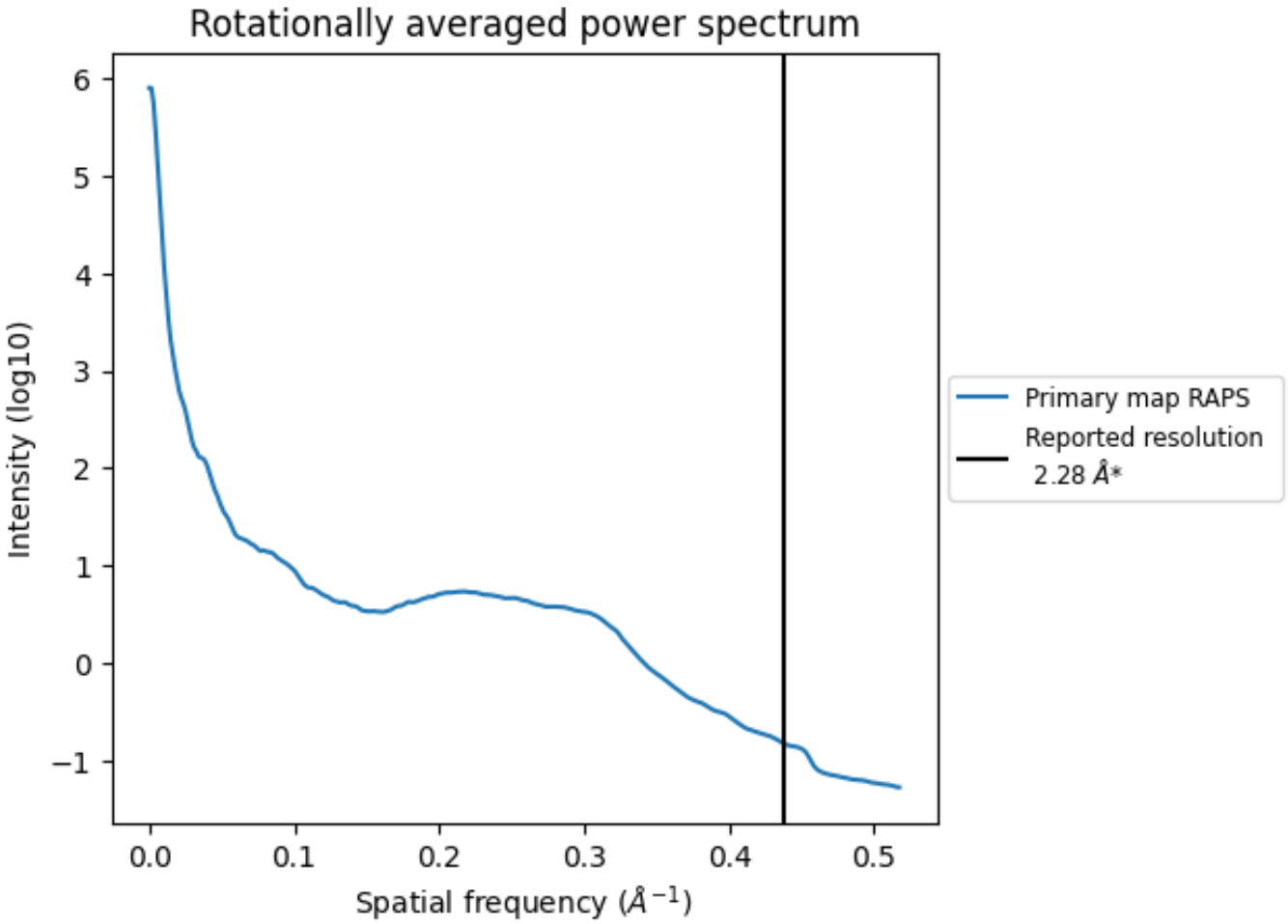
7.2 Volume estimate (i)



The volume at the recommended contour level is 481 nm^3; this corresponds to an approximate mass of 435 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 0.439 Å^{-1}

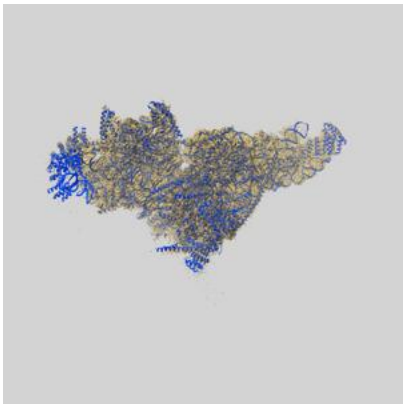
8 Fourier-Shell correlation (i)

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

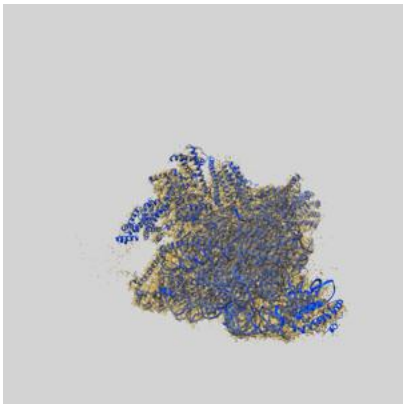
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-56198 and PDB model 9TRV. Per-residue inclusion information can be found in section 3 on page 12.

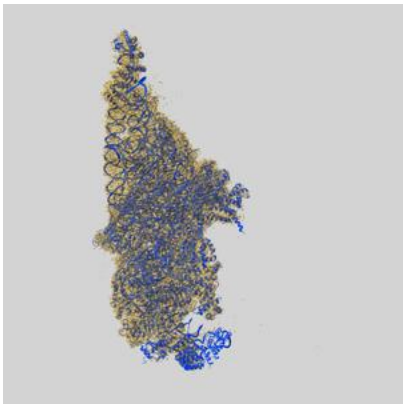
9.1 Map-model overlay



X



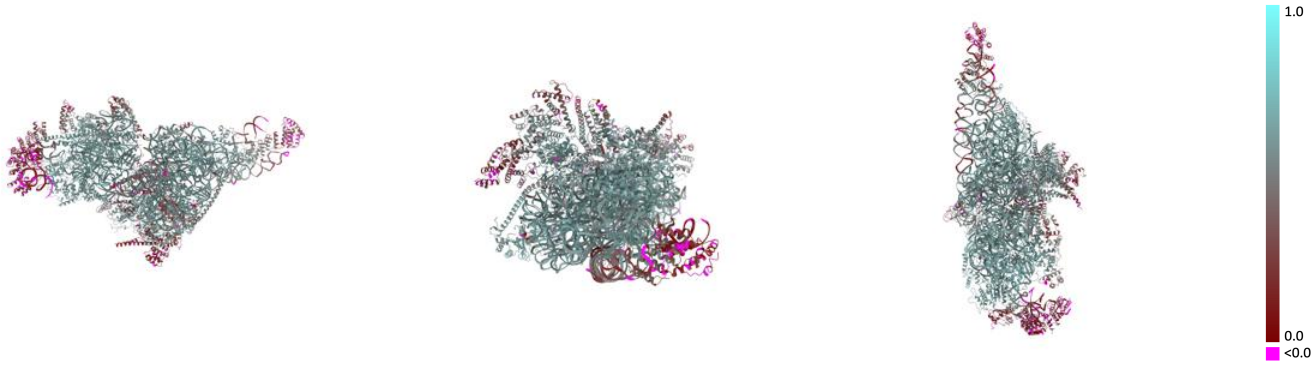
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

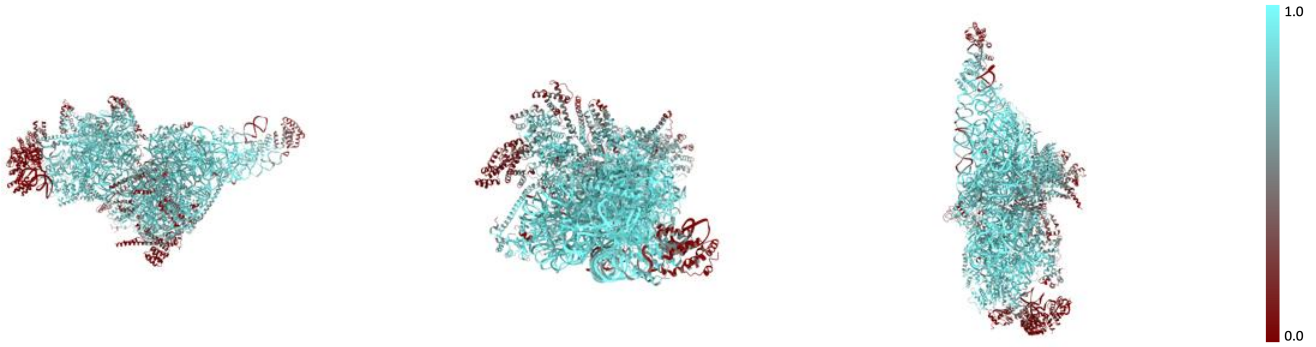
9.2 Q-score mapped to coordinate model (i)



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.

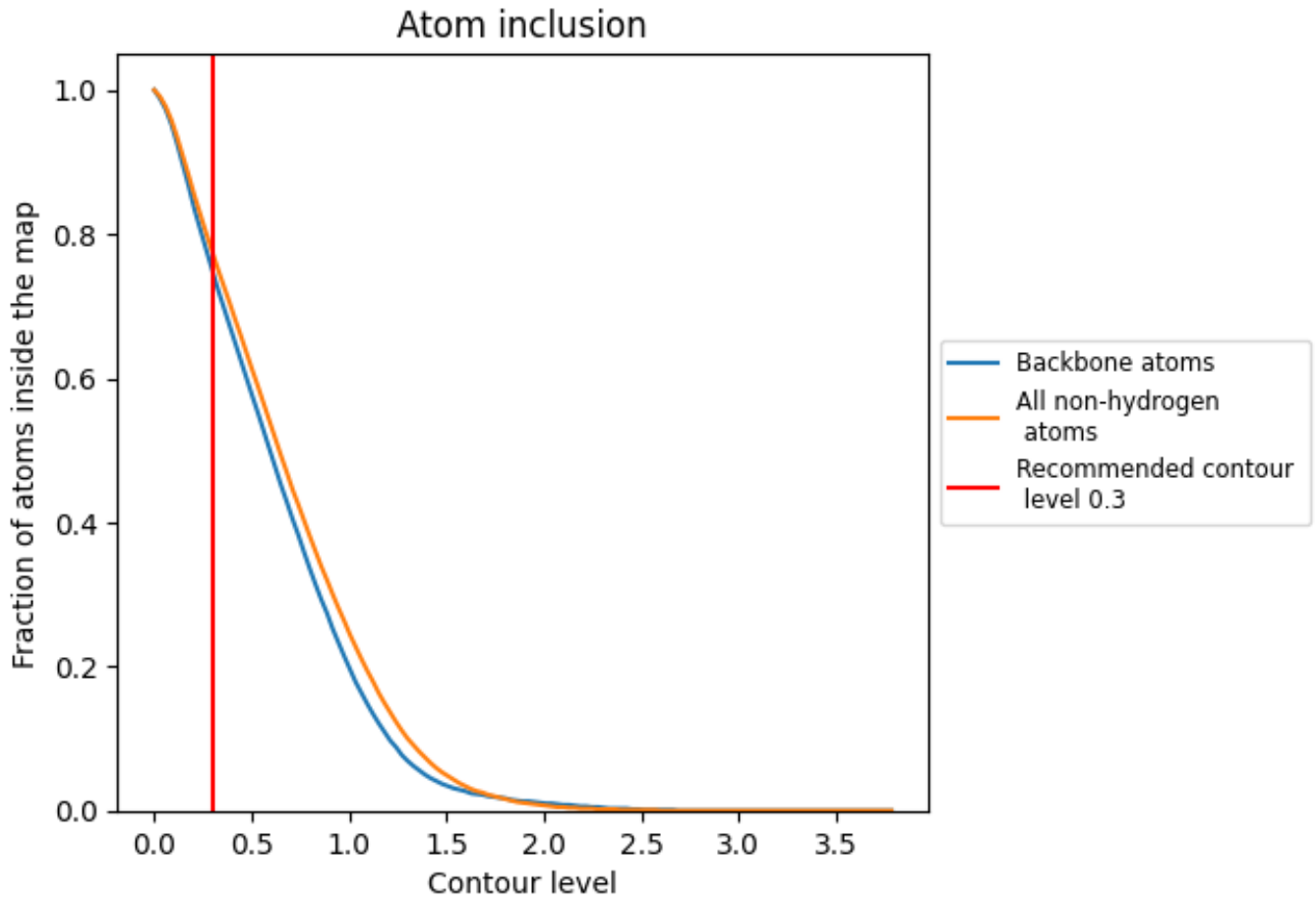
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 77% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7740	0.5230
2	0.8940	0.5540
8	0.3770	0.3240
A	0.8640	0.5960
B	0.7500	0.5360
C	0.8410	0.5680
D	0.7240	0.5220
E	0.9070	0.6270
F	0.7330	0.5760
G	0.9560	0.6400
H	0.7430	0.5480
I	0.9430	0.6440
J	0.7570	0.5260
K	0.9140	0.6130
L	0.8000	0.6110
M	0.9630	0.6610
N	0.8910	0.6160
O	0.9620	0.6240
P	0.8830	0.6050
Q	0.8320	0.5970
R	0.4300	0.3650
S	0.7370	0.5430
T	0.9550	0.6460
U	0.4920	0.3920
V	0.7850	0.5510
W	0.8870	0.6260
X	0.7740	0.5580
Y	0.8310	0.6070
Z	0.9100	0.5280
a	0.7250	0.5410
b	0.2030	0.3040
c	0.8120	0.5560
d	0.8650	0.5560
e	0.8520	0.5750
f	0.7490	0.5380



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Chain	Atom inclusion	Q-score
g	0.0000	0.1080
h	0.5230	0.2660
i	0.2920	0.3180
k	0.4900	0.4280
l	0.1100	0.1910