wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 07:03 pm GMT

PDB ID	:	5OPT
EMDB ID	:	EMD-3844
Title	:	Structure of KSRP in context of Trypanosoma cruzi 40S
Authors	:	Brito Querido, J.; Mancera-Martinez, E.; Vicens, Q.; Bochler, A.; Chicher, J.; Simonetti, A.; Hashem, Y.
Deposited on	:	2017-08-10
Resolution	:	4.00 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:

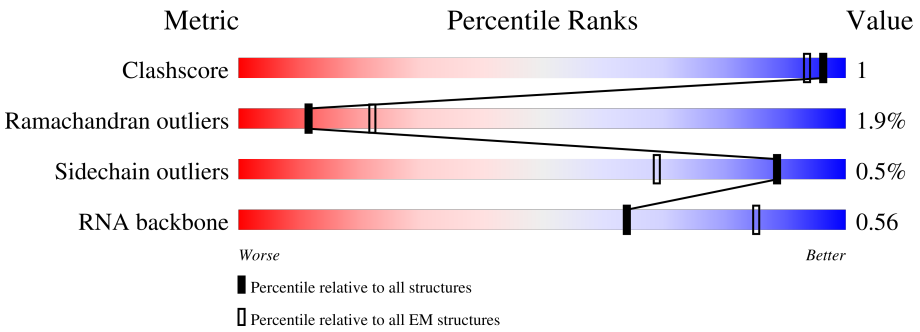
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	p	318	85% / 95%
2	q	57	37% / 63% / 33%
3	r	149	50% / 84% / 9% / 6%
4	t	152	55% / 74% / 22%
5	u	153	51% / 74% / 22%
6	L	273	26% / 94% / 5%
7	M	143	22% / 99%

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Mol	Chain	Length	Quality of chain
8	O	190	58% 95% 5%
9	Q	211	22% 91% • 5%
10	R	151	25% 92% •• 7%
11	S	86	37% 93% •• 5%
12	T	112	32% 93% 7%
13	U	112	43% 60% • 39%
14	V	144	33% 92% •• 6%
15	W	261	21% 81% • 17%
16	X	173	27% 84% • 14%
17	Y	137	13% 90% 10%
18	Z	221	15% 77% • 21%
19	b	190	17% 85% • 14%
20	f	245	23% 82% • 16%
21	d	263	24% 84% • 15%
22	e	130	19% 98% •••
23	g	236	11% 35% 65%
24	a	110	40% 56% 7% 36%
25	i	141	79% 82% • 14%
26	j	150	35% 38% • • 57%
27	P	250	27% 99% •
28	k	196	32% 59% • 40%
29	l	117	57% 85% 15%
30	m	214	67% 88% 5% 7%
31	n	161	41% 55% • 42%
32	o	167	44% 79% • • 16%

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Mol	Chain	Length	Quality of chain
33	c	66	33% 86% 5% 9%
34	h	257	47% 53% 10% • 33%
35	E	2319	12% • 62% 20% • 13%

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 82219 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Activated protein kinase C receptor, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	p	310	2405	1505	424	463	13	0	0

- Molecule 2 is a protein called Ribosomal protein S29, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	q	38	311	191	64	52	4	0	0

- Molecule 3 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	r	140	1113	706	212	192	3	0	0

- Molecule 4 is a protein called 40S ribosomal protein S15, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	t	119	969	615	185	165	4	0	0

- Molecule 5 is a protein called 40S ribosomal protein S18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	u	120	981	614	194	169	4	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	258	2038	1290	383	354	11	0	0

- Molecule 7 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	M	142	1116	706	220	188	2	0	0

- Molecule 8 is a protein called 40S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	O	190	1493	932	286	269	6	0	0

- Molecule 9 is a protein called Ribosomal protein S7, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Q	200	1670	1063	324	277	6	0	0

- Molecule 10 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	R	141	1143	724	221	190	8	0	0

- Molecule 11 is a protein called 40S ribosomal protein S27, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	S	82	630	384	121	116	9	0	0

- Molecule 12 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	T	104	829	510	177	132	10	0	0

- Molecule 13 is a protein called 40S ribosomal protein S33, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	U	68	526	315	107	100	4	0	0

- Molecule 14 is a protein called 40S ribosomal protein S14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	V	135	1011	620	195	187	9	0	0

- Molecule 15 is a protein called 40S ribosomal protein S3a-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	W	217	1781	1124	337	313	7	0	0

- Molecule 16 is a protein called 40S ribosomal protein S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	X	148	1212	760	239	207	6	0	0

- Molecule 17 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Y	123	989	628	194	165	2	0	0

- Molecule 18 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Z	175	1404	885	283	233	3	0	0

- Molecule 19 is a protein called 40S ribosomal protein S9, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	b	164	1365	864	266	227	8	0	0

- Molecule 20 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	f	207	1658	1060	299	288	11	0	0

- Molecule 21 is a protein called 40S ribosomal protein S2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	d	223	1726	1098	304	314	10	0	0

- Molecule 22 is a protein called 40S ribosomal protein S15a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	e	129	1019	647	188	176	8	0	0

- Molecule 23 is a protein called 40S ribosomal protein S21, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	g	83	635	395	116	122	2	0	0

- Molecule 24 is a protein called Ribosomal protein S25, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	a	70	553	356	97	97	3	0	0

- Molecule 25 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	i	121	958	594	174	185	5	0	0

- Molecule 26 is a protein called Ubiquitin/ribosomal protein S27a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	j	64	518	324	98	90	6	0	0

- Molecule 27 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	P	249	1983	1244	402	333	4	0	0

- Molecule 28 is a protein called 40S ribosomal protein S17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	k	118	972	610	187	170	5	0	0

- Molecule 29 is a protein called Ribosomal protein S20, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	l	99	784	497	144	140	3	0	0

- Molecule 30 is a protein called 40S ribosomal protein S3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	m	200	1587	995	302	279	11	0	0

- Molecule 31 is a protein called 40S ribosomal protein S10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	n	93	780	508	136	132	4	0	0

- Molecule 32 is a protein called Ribosomal protein S19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	o	140	1116	702	221	185	8	0	0

- Molecule 33 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	c	60	480	303	98	78	1	0	0

- Molecule 34 is a protein called RNA-binding protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	h	173	1358	862	259	234	3	0	0

- Molecule 35 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
35	E	2022	43106	19268	7710	14111	2017	0	0

There are 5 discrepancies between the modelled and reference sequences:

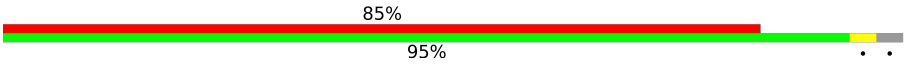
Chain	Residue	Modelled	Actual	Comment	Reference
E	143	C	A	conflict	GB 320364483
E	805	C	U	conflict	GB 320364483
E	2316	U	-	insertion	GB 320364483
E	2317	U	-	insertion	GB 320364483
E	2318	U	-	insertion	GB 320364483

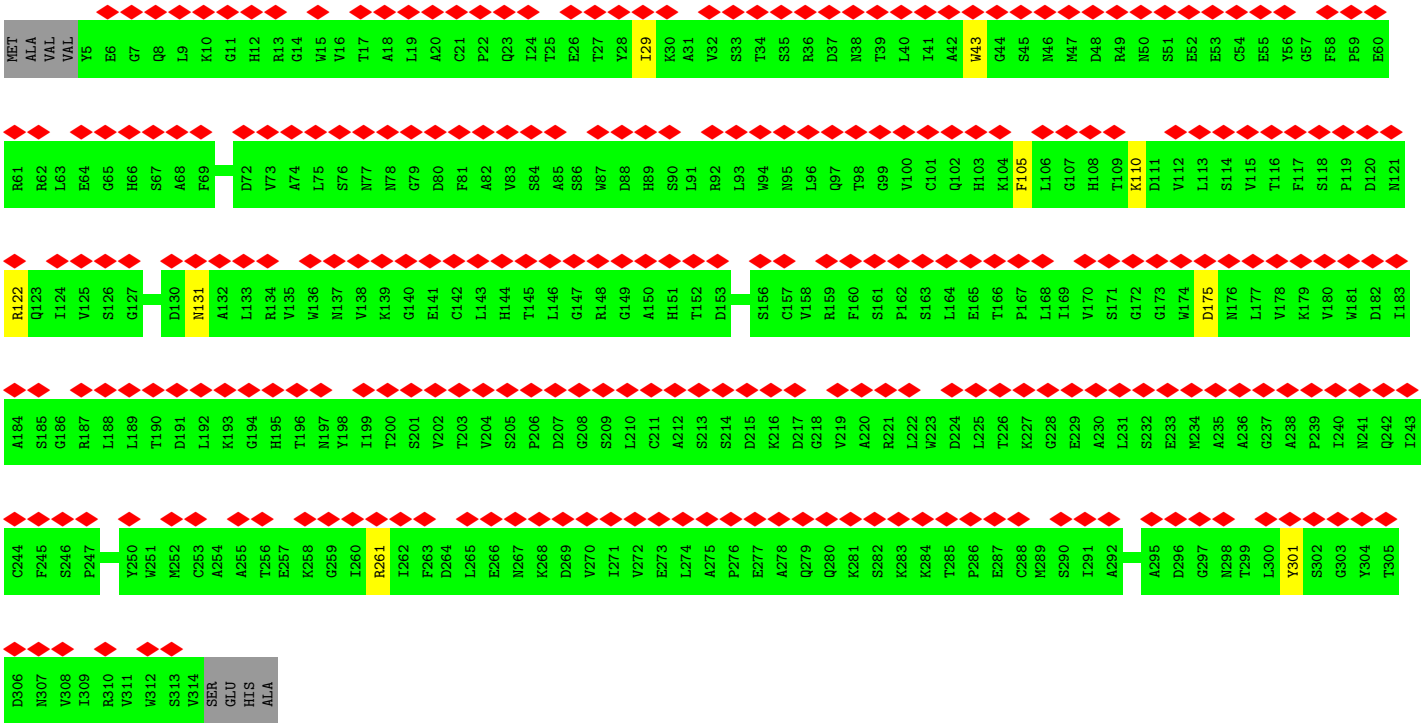
3 Residue-property plots (i)

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: Activated protein kinase C receptor, putative

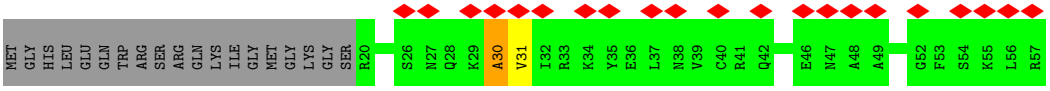
Chain p:





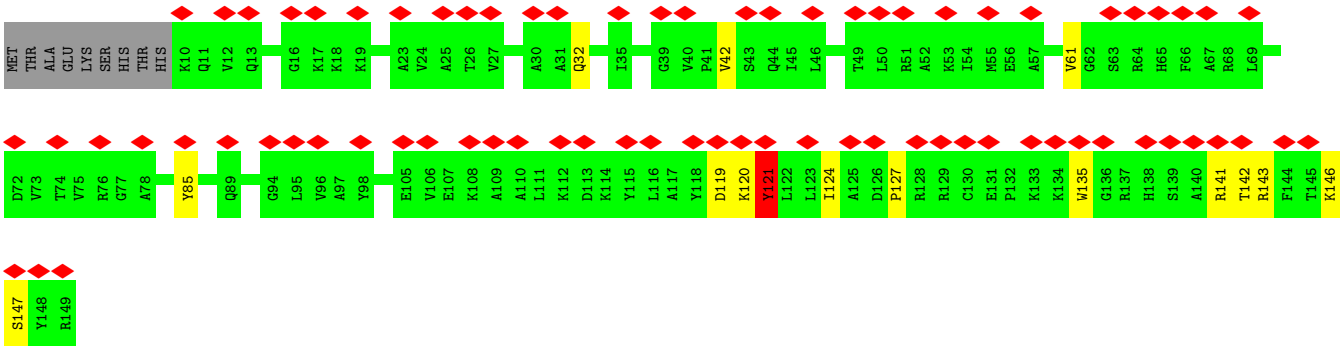
- Molecule 2: Ribosomal protein S29, putative

Chain q:



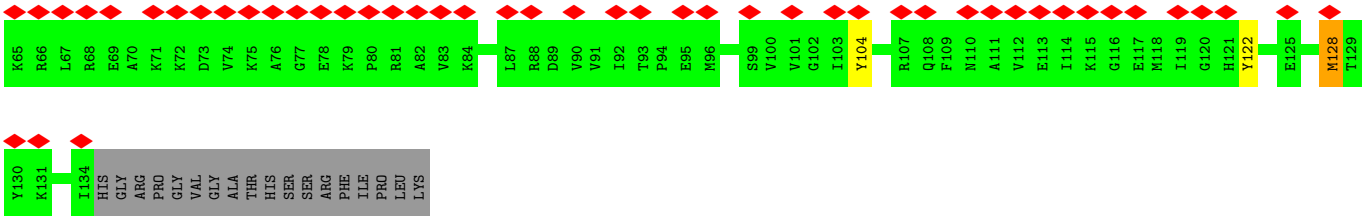
- Molecule 3: 40S ribosomal protein S16, putative

Chain r:



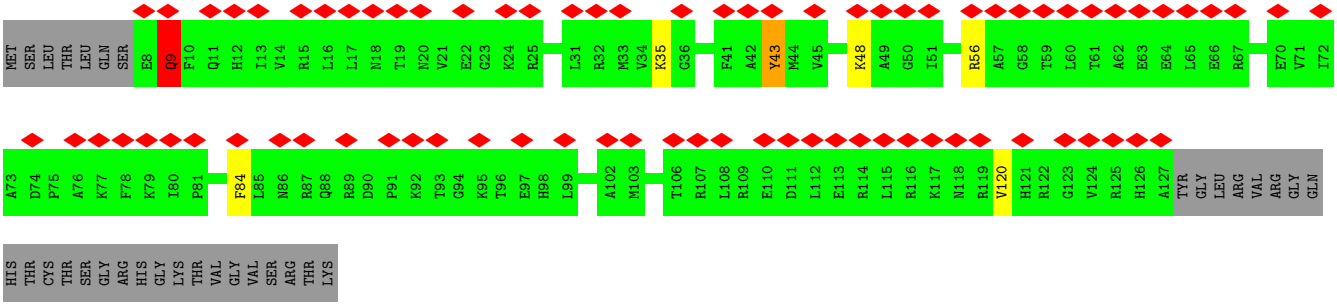
- Molecule 4: 40S ribosomal protein S15, putative

Chain t:



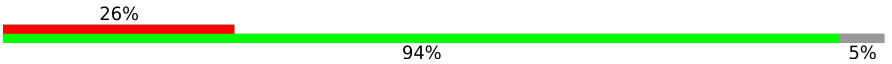
- Molecule 5: 40S ribosomal protein S18, putative

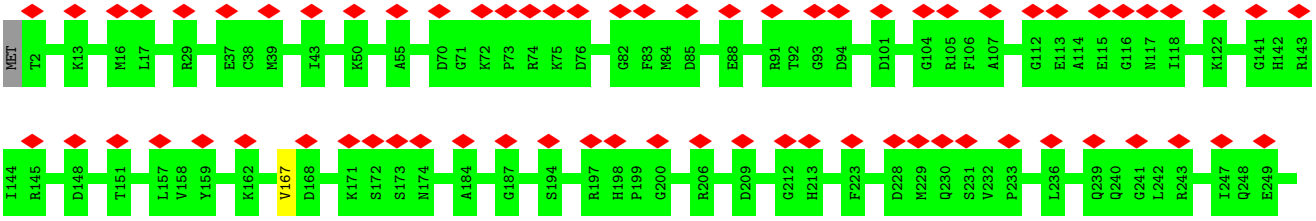
Chain u:

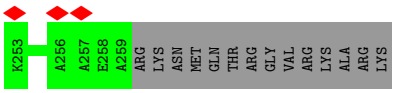


- Molecule 6: 40S ribosomal protein S4

Chain L:

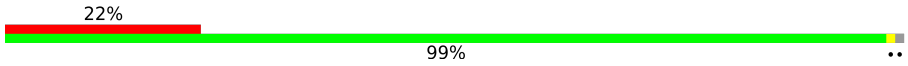


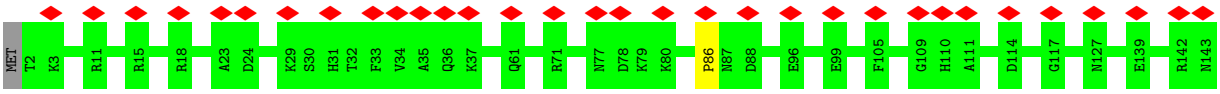




- Molecule 7: 40S ribosomal protein S23, putative

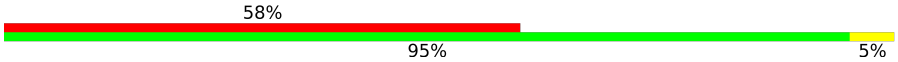
Chain M:

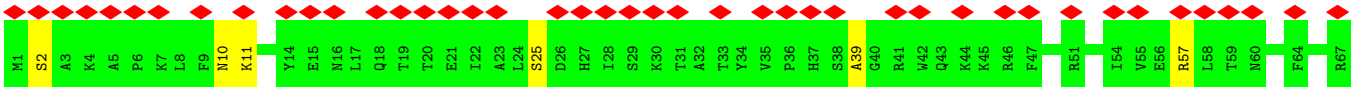


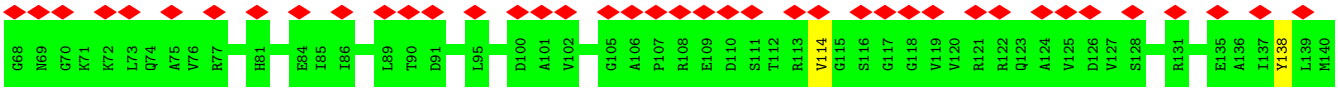


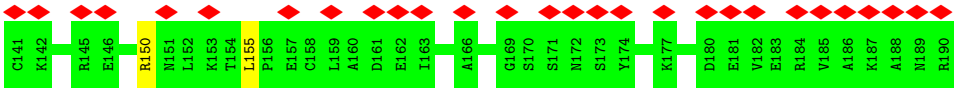
- Molecule 8: 40S ribosomal protein S5, putative

Chain O:



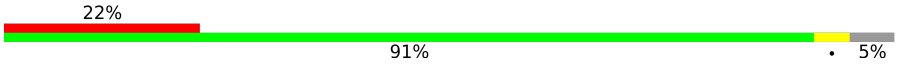


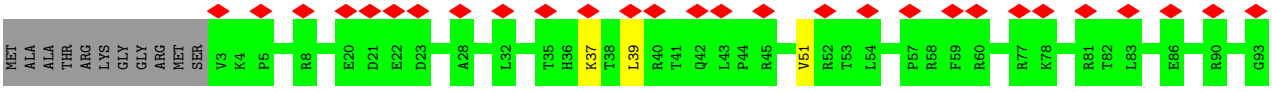


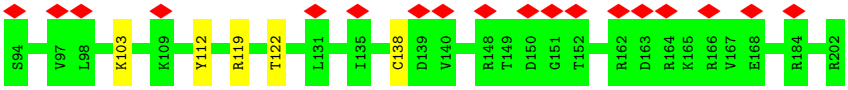


- Molecule 9: Ribosomal protein S7, putative

Chain Q:

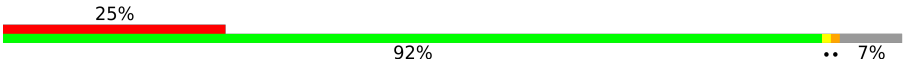


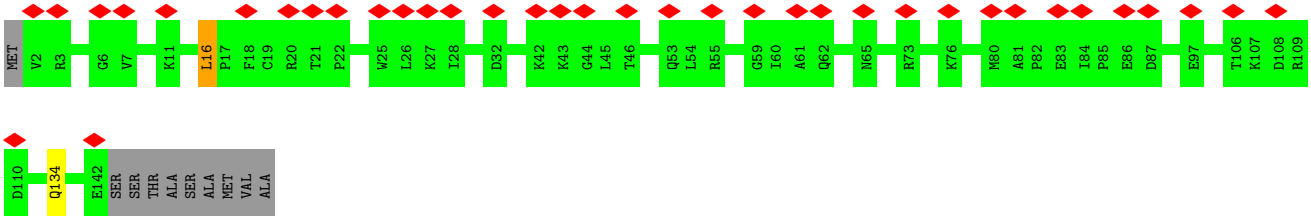




- Molecule 10: 40S ribosomal protein S13, putative

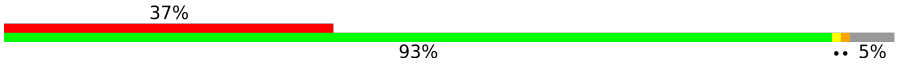
Chain R:

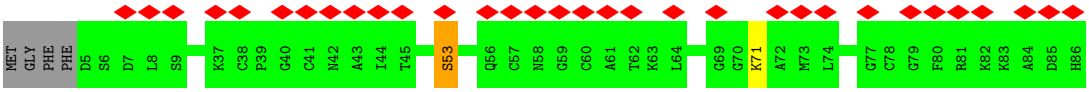




- Molecule 11: 40S ribosomal protein S27, putative

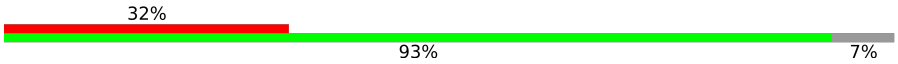
Chain S:

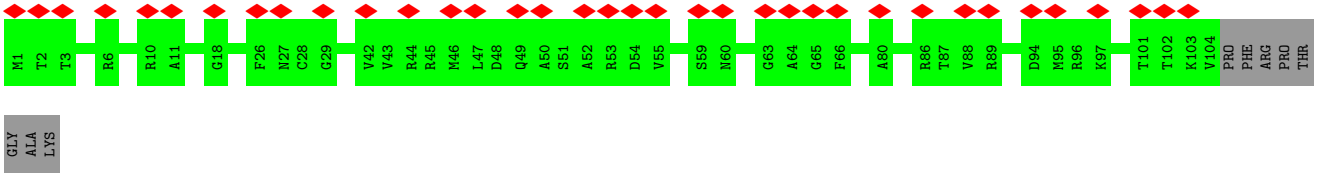




- Molecule 12: 40S ribosomal protein S26

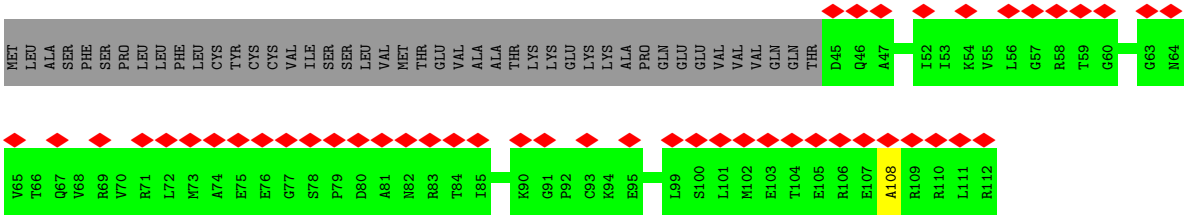
Chain T:





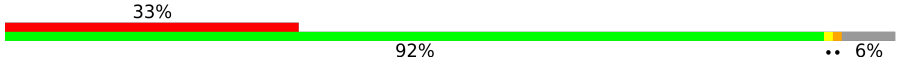
- Molecule 13: 40S ribosomal protein S33, putative

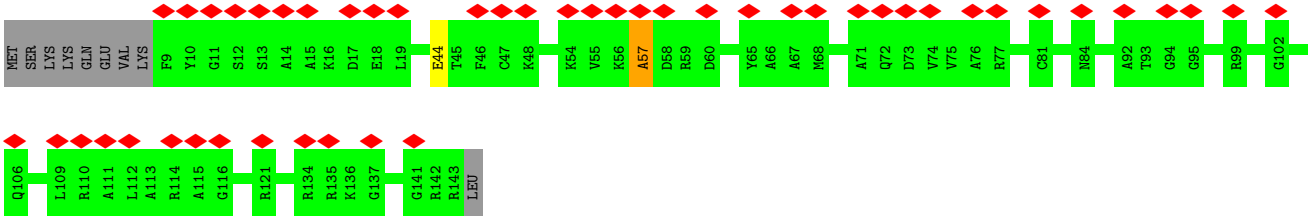
Chain U:



- Molecule 14: 40S ribosomal protein S14, putative

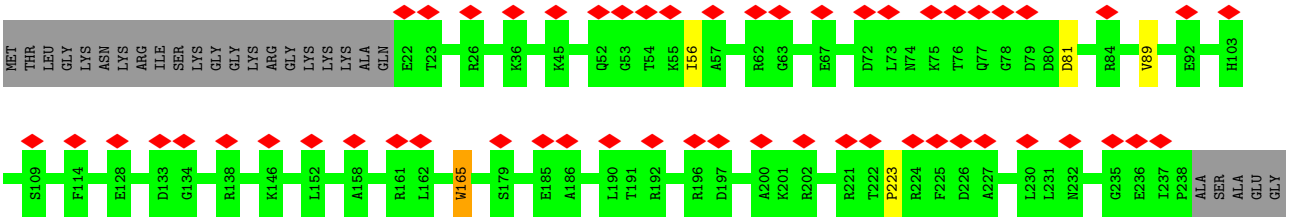
Chain V:





- Molecule 15: 40S ribosomal protein S3a-2

Chain W:



GLU ALA ARG VAL VAL GLU GLU ALA GLN GLU ALA PRO ALA ALA GLU ALA THR ALA

- Molecule 16: 40S ribosomal protein S11, putative

Chain X: 27% 84% • 14%

MET THR ALA PRO GLU GLN TYR ALA ARG VAL H11 S12 V13 D14 L15 H19 E20 K21 Q24 R25 A28 E31 N32 S33 H34 N35 P36 N37 K38 K39 H40 V41 N42 M43 S50 I53 G54 L55 G56 F57 K58 K61 I64 I69 D78 G83 R84 V89

V90 H91 S92 T93 K94 R97 R103 D104 S121 F130 D131 G135 D136 E156 V157 V158 SER LYS SER ALA PRO GLY LYS LEU GLY ARG LYS PHE SER LYS ASN

- Molecule 17: 40S ribosomal protein S24

Chain Y: 13% 90% 10%

MET VAL PHE Q4 K5 K6 E9 Q27 E31 K55 E59 K68 G72 D84 R91 L101 G102 M103 G104 Q108 R111 N121 K122 G126 LYS ALA LYS GLY LYS MET GLN THR LYS LYS LYS

- Molecule 18: 40S ribosomal protein S8

Chain Z: 15% 77% • 21%

MET G2 L8 H9 I13 K17 T18 K19 L29 H35 G39 A40 G50 F53 R56 R59 N64 T69 I72 I78 L79 D80 A85 T86 D105 F109 H116 TYR GLY ILE ASP LEU ASP ALA ALA LYS SER LYS LYS THR LEU GLN

SER THR THR GLU LYS LYS LYS SER LYS LYS THR SER HIS ALA MET THR GLU LYS TYR ASP VAL LYS LYS ALA SER D157 R167 E168 N169 H170 K171 I172 E173 K174 A175 D178 G183 R188 D200 E205 K214 K215 L216 GLU LYS LYS LYS ARG

- Molecule 19: 40S ribosomal protein S9, putative

Chain b: 17% 85% • 14%

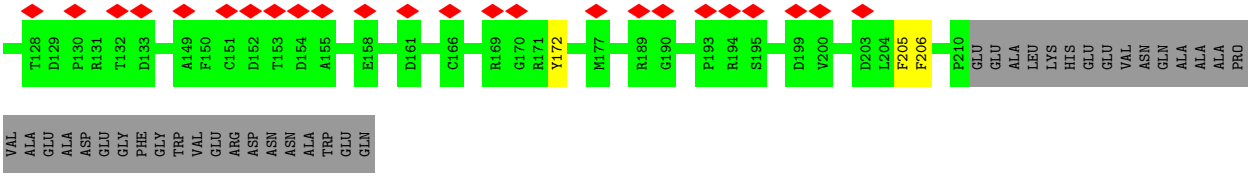
M1 R2 N3 A13 P14 R15 E21 C30 G34 L35 R36 M46 R53 R56 L59 E63 N64 H65 P66 R67 E71 G72 G83 E87 E88 K89 D90 K91 L92 D93 H115 K119 A136 K137 R148 V149 S150 S151 E152 H153 A156 D159

G164 ASN GLY ARG PRO GLY ARG VAL LYS ARG VAL LYS ARG LYS ALA ALA LYS LYS GLY ALA ALA GLY GLY ASP ASP ASP GLU

- Molecule 20: 40S ribosomal protein SA

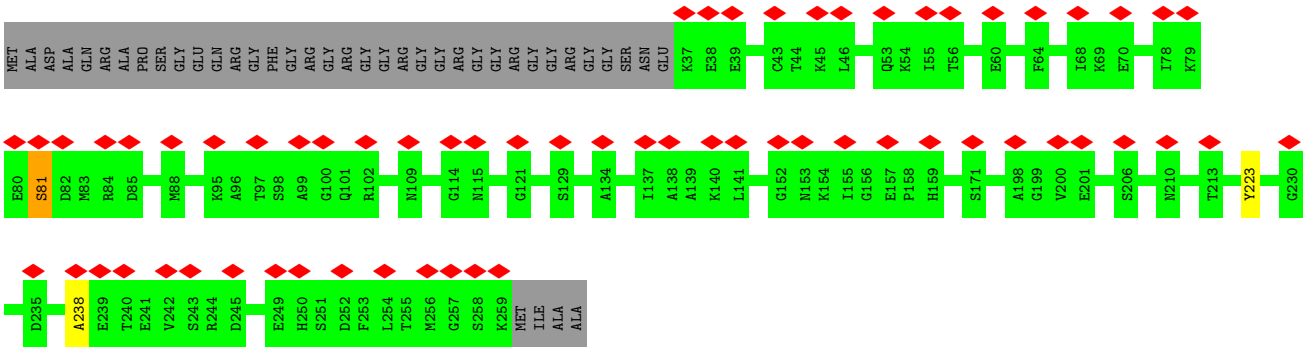
Chain f: 23% 82% • 16%

MET THR SER V4 E5 A8 K9 R12 M13 K14 E15 G16 Q19 M24 H25 C26 H27 L28 G29 T30 R33 S34 N35 A36 I41 H42 S43 R44 T45 K46 E47 I62 A70 V71 E72 D76 Q95 G98 L102 A103 G104 R105 Q114 I115 Q116 K117 K118



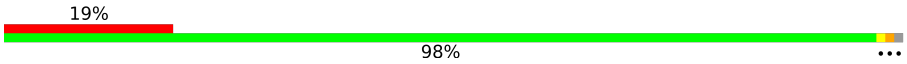
- Molecule 21: 40S ribosomal protein S2, putative

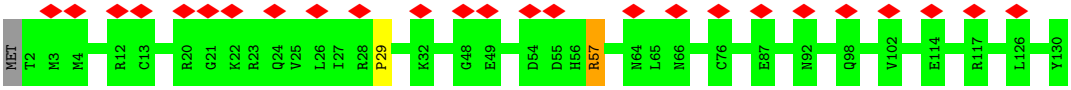
Chain d:



- Molecule 22: 40S ribosomal protein S15a, putative

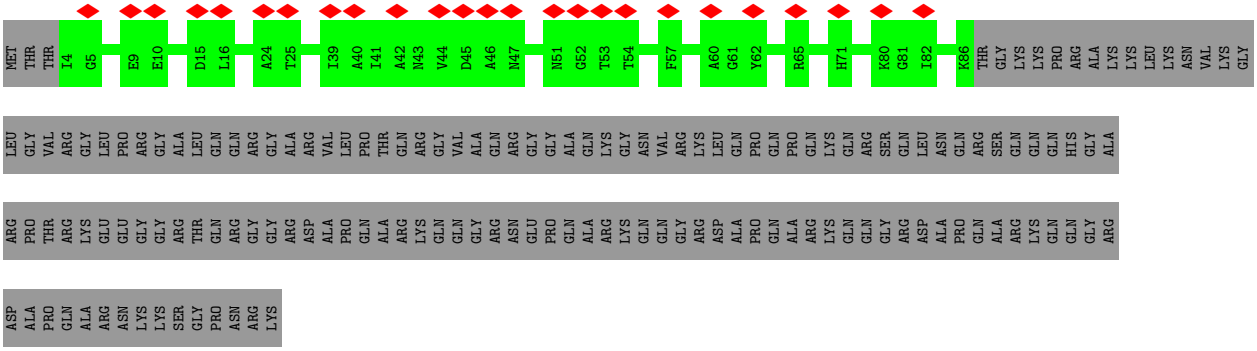
Chain e:





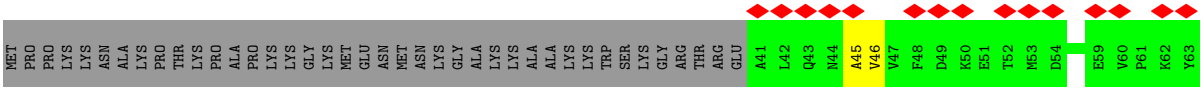
- Molecule 23: 40S ribosomal protein S21, putative

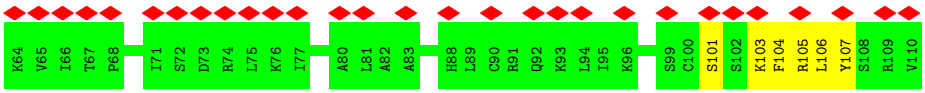
Chain g:



- Molecule 24: Ribosomal protein S25, putative

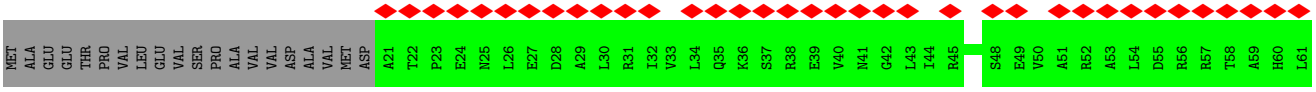
Chain a:

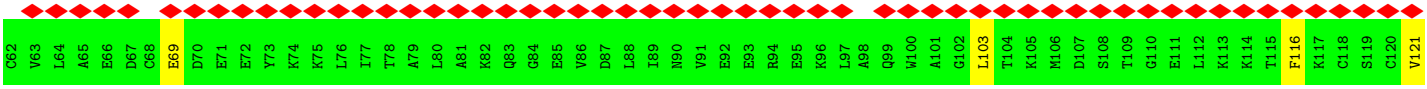


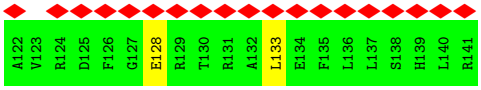


- Molecule 25: 40S ribosomal protein S12

Chain i:

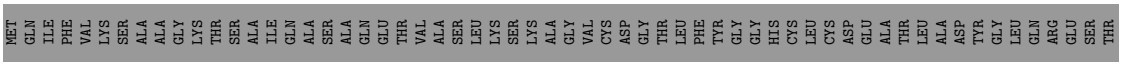


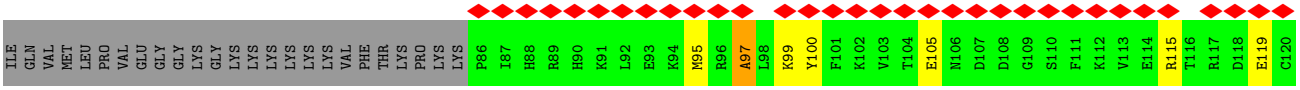


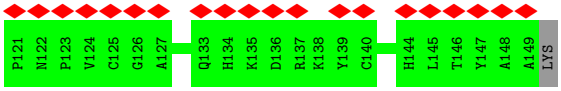


- Molecule 26: Ubiquitin/ribosomal protein S27a, putative

Chain j:

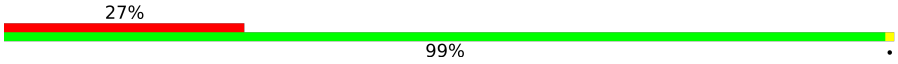


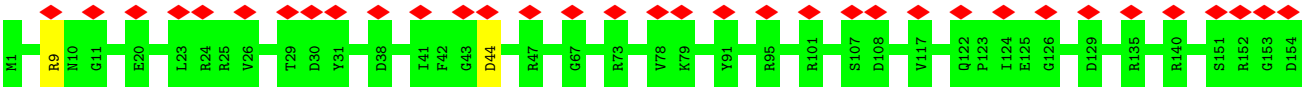


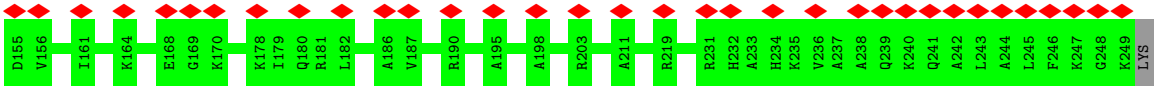


- Molecule 27: 40S ribosomal protein S6

Chain P:

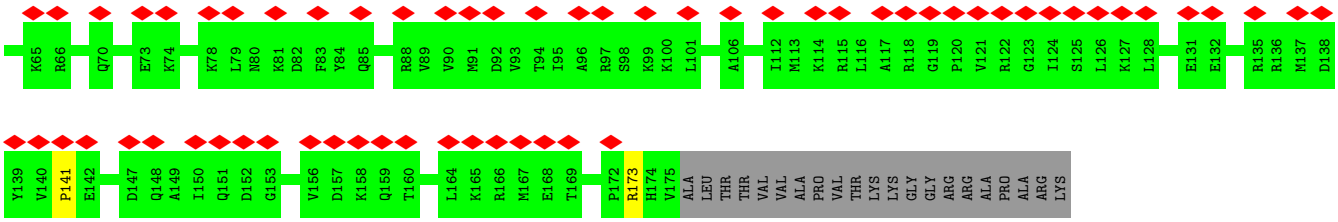






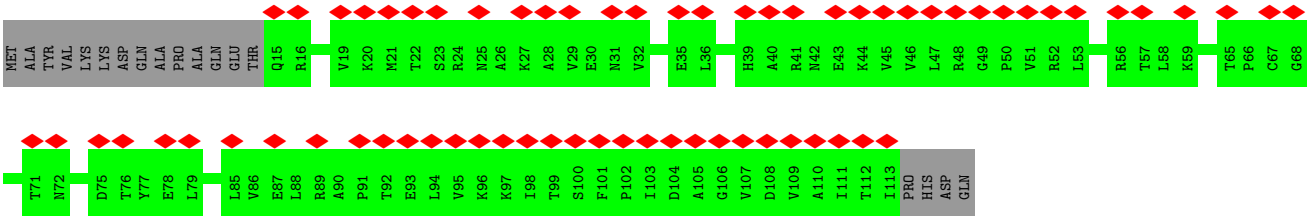
- Molecule 28: 40S ribosomal protein S17, putative

Chain k:



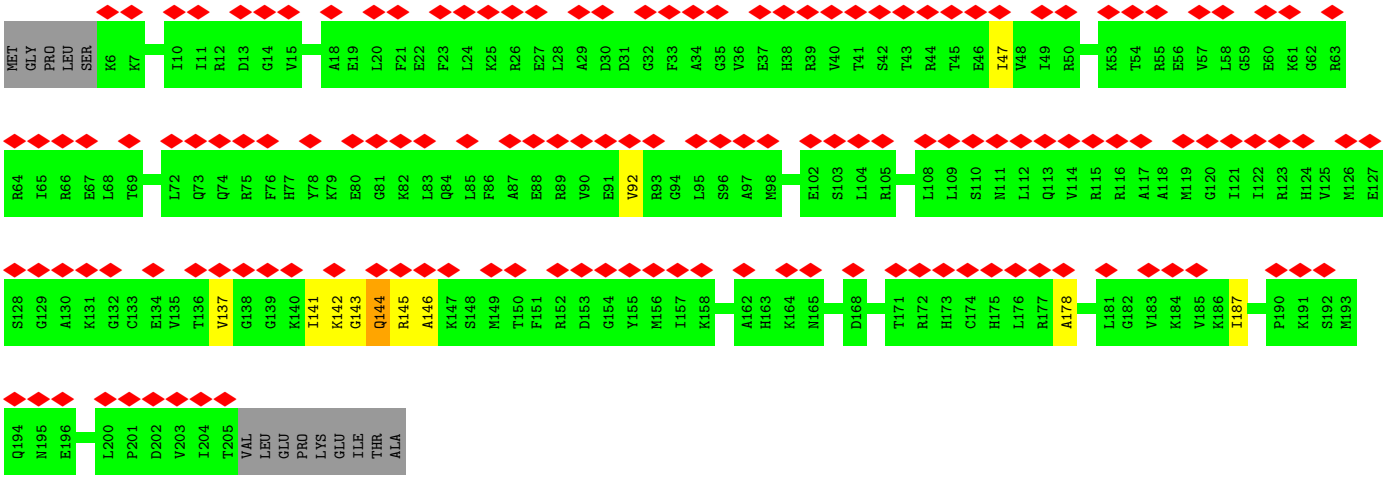
• Molecule 29: Ribosomal protein S20, putative

Chain l:



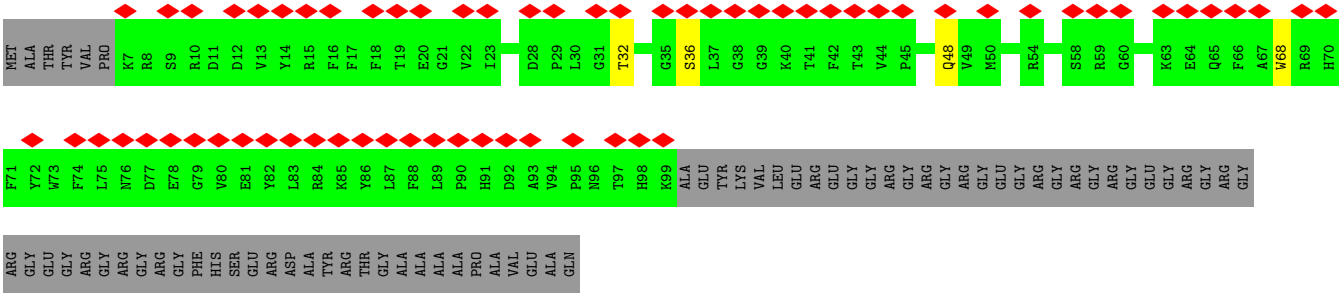
• Molecule 30: 40S ribosomal protein S3, putative

Chain m:



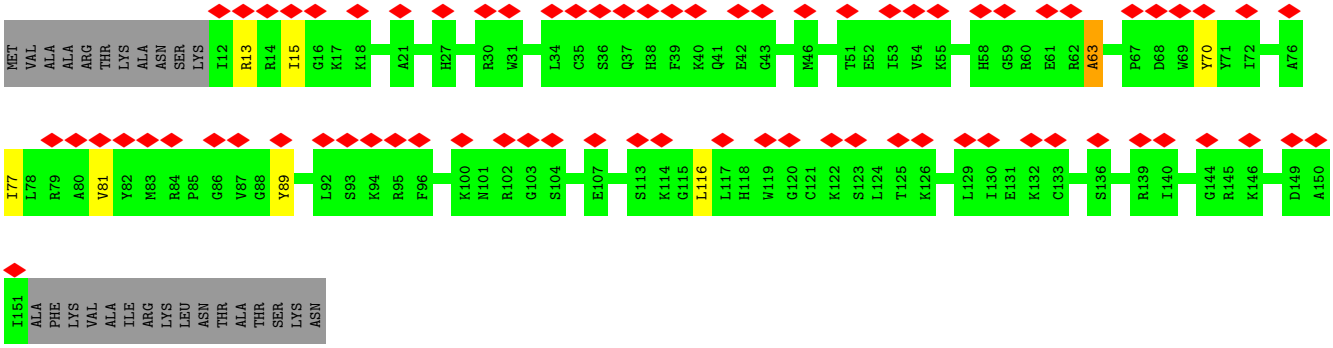
• Molecule 31: 40S ribosomal protein S10, putative

Chain n:



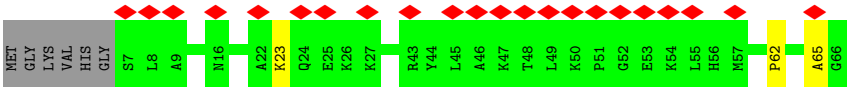
- Molecule 32: Ribosomal protein S19, putative

Chain o:



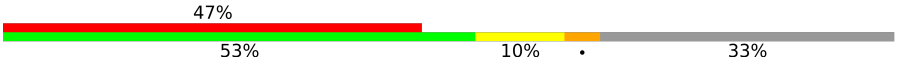
- Molecule 33: 40S ribosomal protein S30

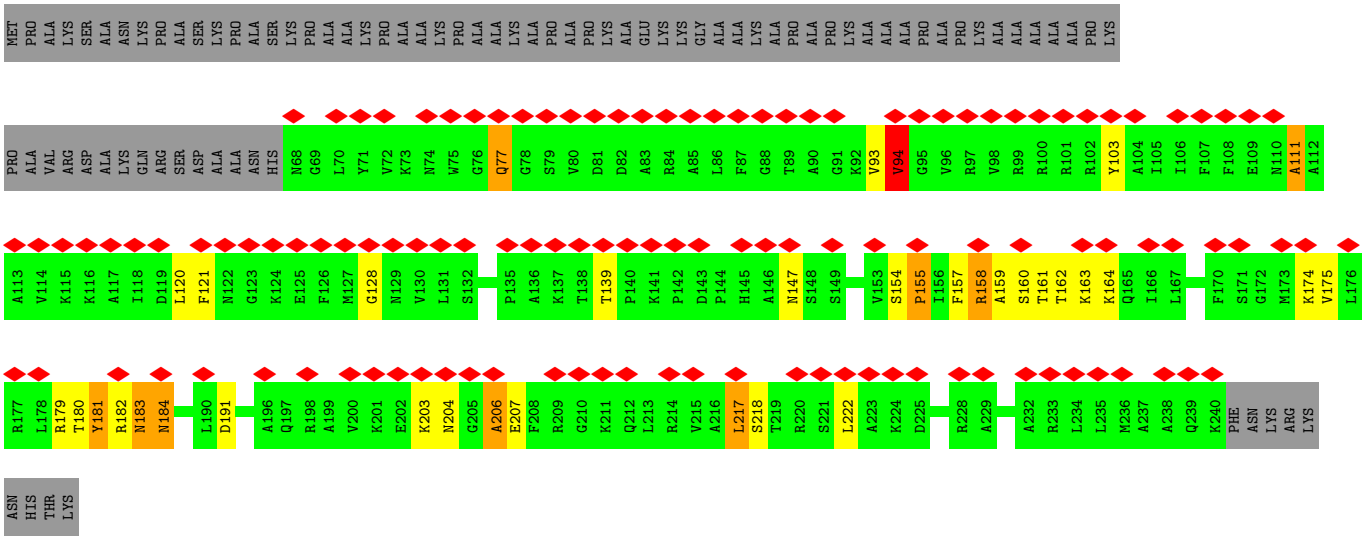
Chain c:



- Molecule 34: RNA-binding protein, putative

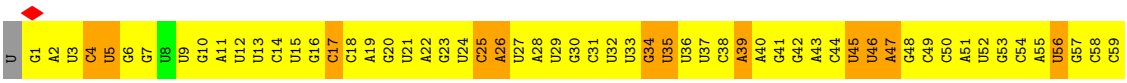
Chain h:

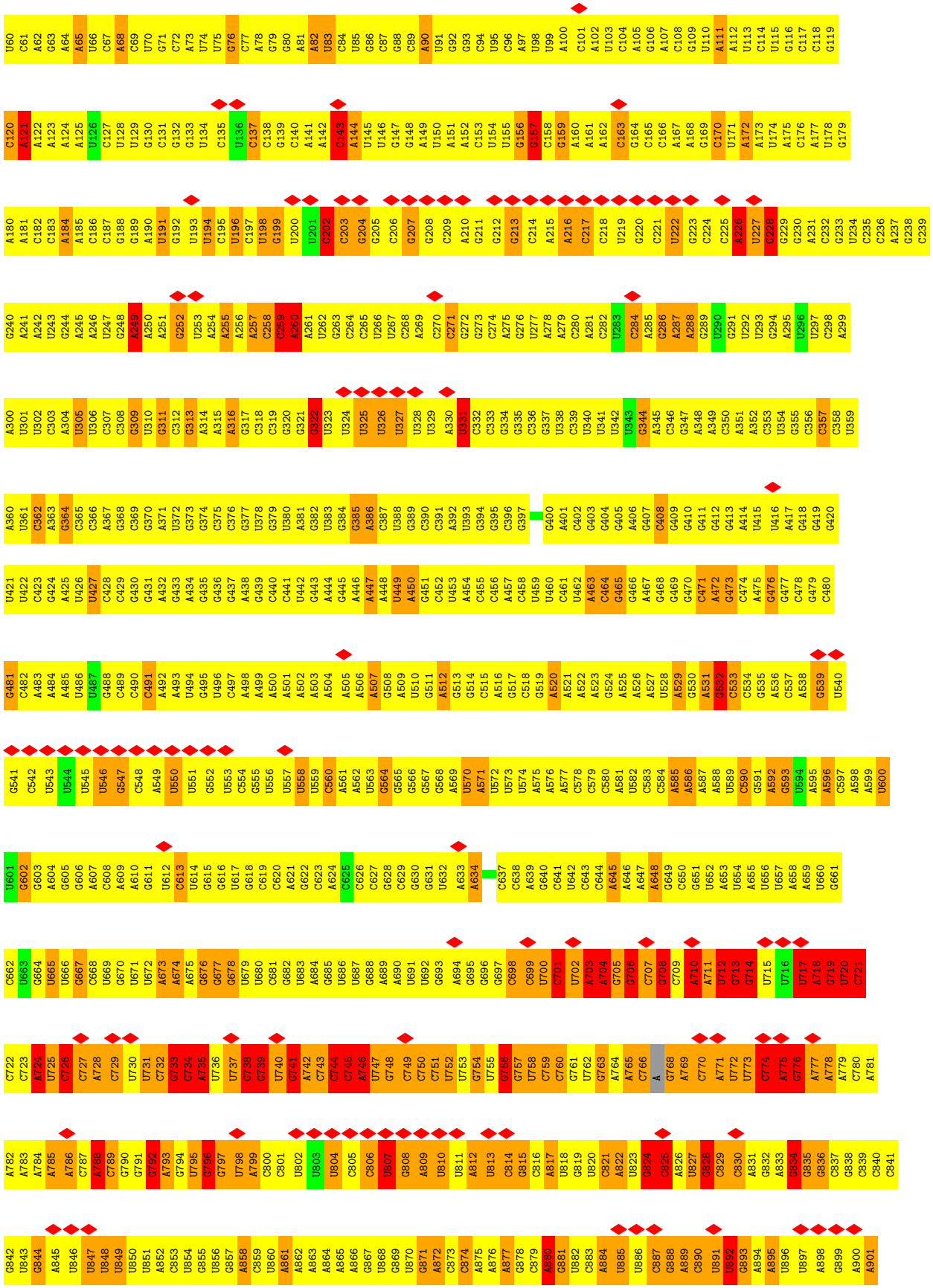




- Molecule 35: 18S rRNA

Chain E:

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A300 U301 U302 C303 A304 U305 U306 C307 C308 G309 U310 G311 C312 G313 A314 A315 A316 G317 C318 C319 G320 G321 G322 U323 U324 U325 U326 U327 U328 U329 A330 U331 C332 C333 G334 G335 C336 G337 U338 C339 U340 U341 U342 U343 G344 A345 C346 G347 A348 A349 C350 A351 A352 C353 U354 G355 C356 C357 C358 U359
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C662 U663 G664 U665 U666 G667 C668 U669 G670 U671 U672 A673 A674 A675 G676 G677 G678 U679 U680 C681 G682 U683 A684 G685 U686 U687 G688 A689 A690 U691 U692 G693 A694 G695 G696 G697 C698 C699 U700 C701 U702 A703 A704 G705 G706 C707 G708 C709 A710 A711 U712 G713 G714 U715 U716 U717 A718 G719 U720 C721
C722 C723 A724 U725 C726 C727 A728 C729 U730 U731 C732 G733 G734 A735 U736 U737 G738 G739 U740 G741 A742 C743 C744 C745 A746 U747 G748 C749 C750 C751 U752 U753 G754 U755 G756 G757 U758 C759 C760 G761 U762 G763 A764 A765 C766 A G768 A769 C770 A771 U772 U773 C774 A775 G776 A777 A778 A779 C780 A781
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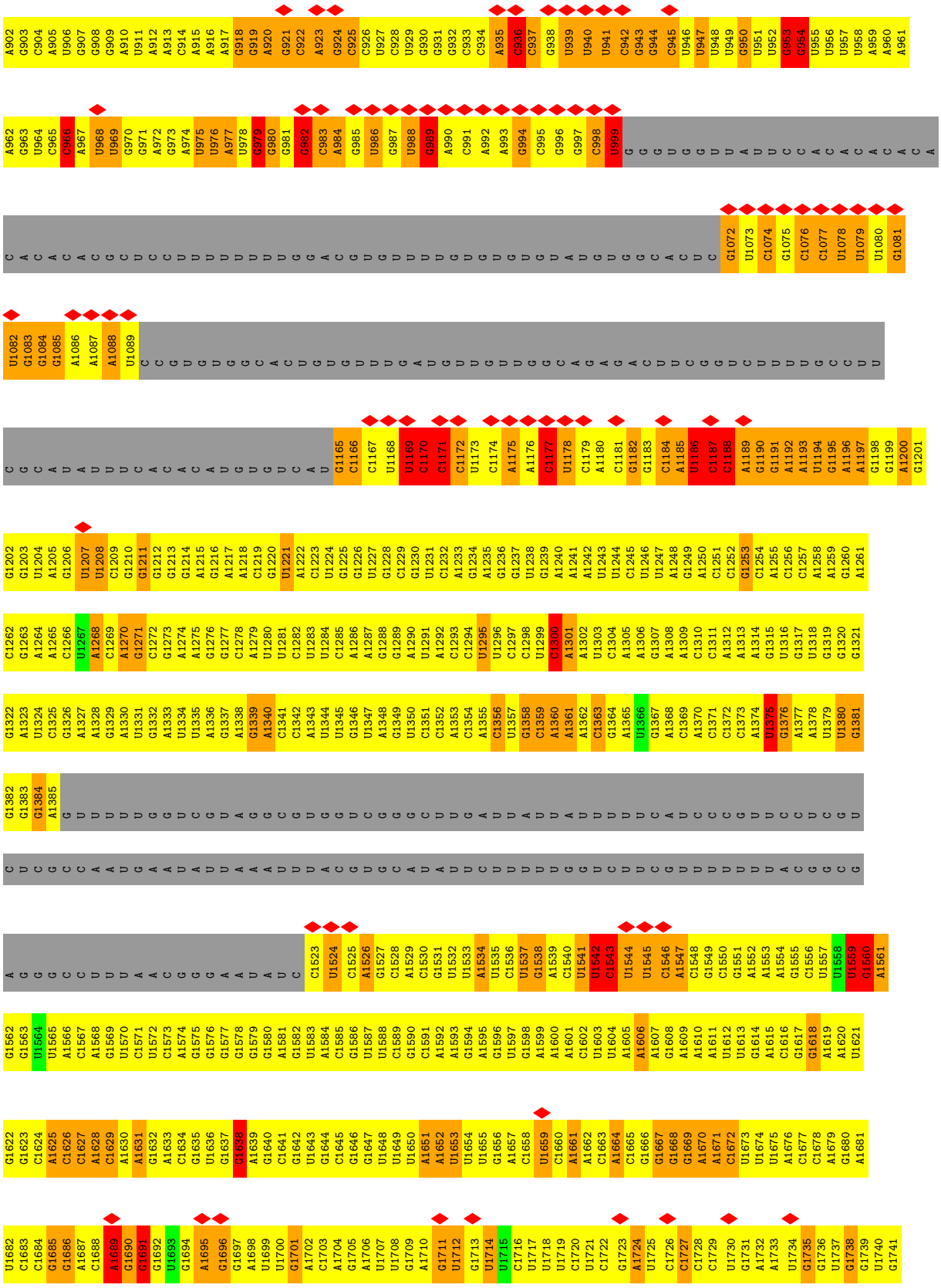
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A962 G963 U964 C965 C966 A967 U968 U969 G970 G971 A972 G973 A974 U975 U976 A977 U978 G979 G980 G981 G982 C983 A984 G985 U986 G987 U988 G989 A990 C991 A992 A993 G994 C995 G996 G997 C998 U999 G G G U C U A U U C C A C A C A C A
C A C A C A C G G C U C C U U U U U U U U U U U U G G A C G G U G U U U U G U U G U U U U G U G U G G U C A U G U G A G A C U U C G G U C U U U C
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C G C A U A U U U C A C A C A U G G U G U U U G A G A C U U C G G U C U U U U G C C U U
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G1382 G1383 G1384 A1385 G U U U U U G G U C G U A G G U C U U G U G G G G U A U U A U U U A U U U U A U U U U U C A U U C C C G G U
C U C G C C A U G A A U A A U U U G C A U A U U U U U U U U U U A A C G G C G
A G G G C C U U U A A C G G G A U A U U U U C C U U U C C C C U U U U U U U U U U C G G C G
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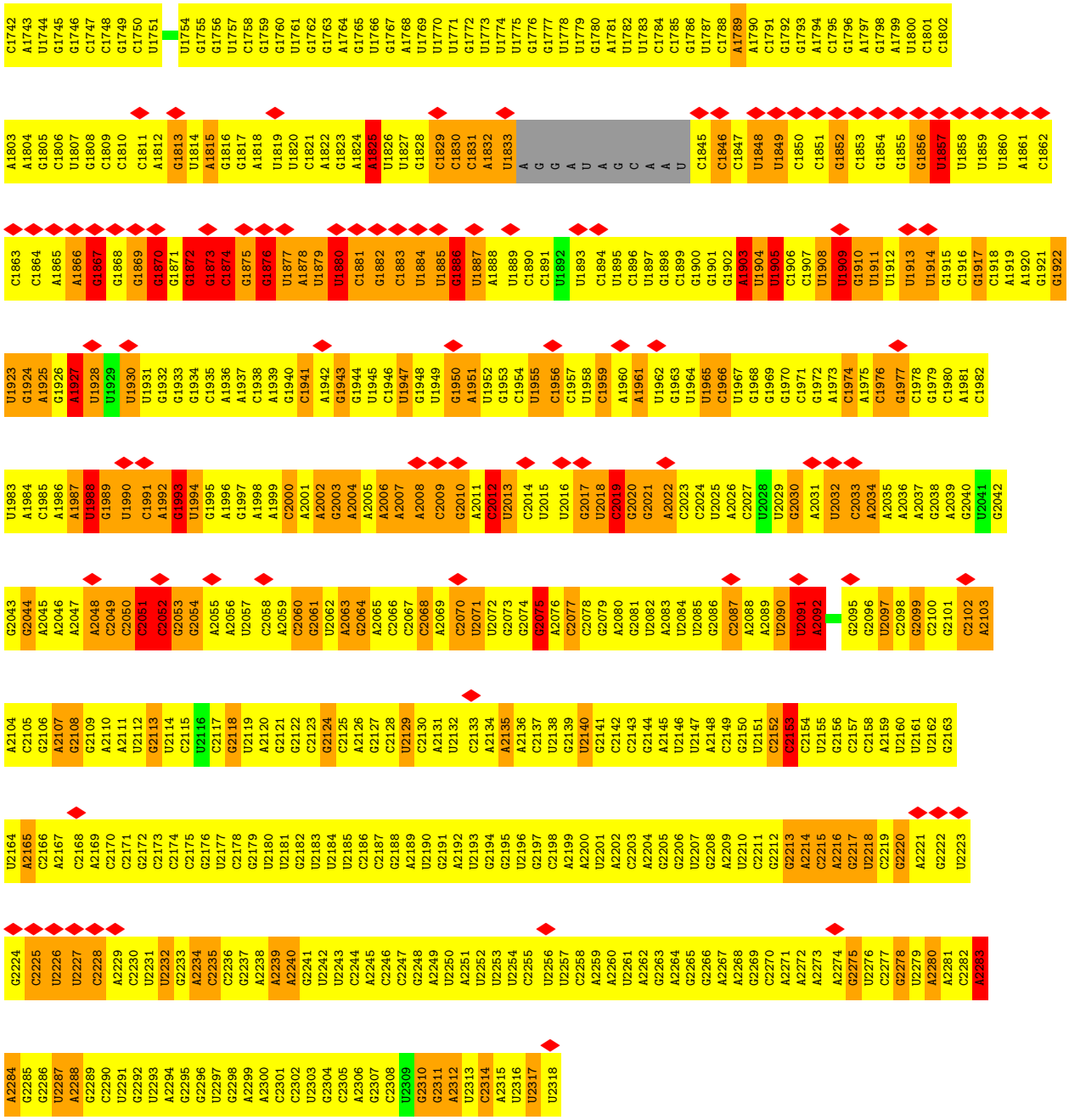
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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.132	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.0549	Depositor
Map size (Å)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.56, 1.56, 1.56	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	p	0.94	0/2461	1.01	3/3347 (0.1%)
2	q	1.09	0/314	1.04	1/416 (0.2%)
3	r	1.02	0/1131	1.11	5/1520 (0.3%)
4	t	1.02	0/988	1.05	3/1325 (0.2%)
5	u	1.05	0/996	1.10	5/1334 (0.4%)
6	L	0.99	0/2073	0.98	0/2787
7	M	0.97	0/1137	0.94	0/1520
8	O	0.99	0/1515	0.96	0/2034
9	Q	1.06	0/1703	1.01	0/2290
10	R	1.00	0/1164	0.96	0/1559
11	S	0.99	0/641	1.01	1/858 (0.1%)
12	T	1.13	0/845	1.00	0/1129
13	U	1.13	0/527	1.04	0/702
14	V	1.04	0/1026	1.02	1/1376 (0.1%)
15	W	1.03	0/1809	1.01	1/2437 (0.0%)
16	X	1.02	0/1238	0.96	0/1662
17	Y	1.01	0/1004	0.98	0/1335
18	Z	1.06	0/1424	1.01	0/1904
19	b	1.03	0/1394	0.95	0/1874
20	f	0.97	0/1693	1.01	5/2290 (0.2%)
21	d	0.94	0/1760	1.03	2/2376 (0.1%)
22	e	1.00	0/1037	1.03	0/1391
23	g	0.92	0/644	0.89	0/875
24	a	0.92	0/559	1.03	1/748 (0.1%)
25	i	0.98	0/966	0.97	2/1295 (0.2%)
26	j	0.98	0/530	1.10	3/707 (0.4%)
27	P	1.09	0/2008	0.98	0/2678
28	k	1.00	0/985	0.98	0/1313
29	l	0.99	0/794	1.06	0/1076
30	m	1.03	0/1606	1.02	4/2141 (0.2%)
31	n	0.98	0/804	0.99	0/1082
32	o	1.00	0/1140	1.09	2/1524 (0.1%)
33	c	0.98	0/488	0.97	0/644
34	h	1.06	0/1381	1.22	4/1857 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	E	1.63	86/48215 (0.2%)	2.51	5573/75140 (7.4%)
All	All	1.38	86/88000 (0.1%)	2.03	5616/128546 (4.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	p	0	3
3	r	0	7
4	t	0	2
5	u	0	4
8	O	0	3
9	Q	0	3
15	W	0	1
18	Z	0	1
22	e	0	1
24	a	0	2
26	j	0	1
27	P	0	2
28	k	0	1
30	m	0	2
32	o	0	2
33	c	0	2
34	h	0	22
35	E	4	121
All	All	4	180

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	E	724	A	N9-C4	-14.62	1.29	1.37
35	E	734	G	N9-C4	-13.56	1.27	1.38
35	E	711	A	N9-C4	-10.05	1.31	1.37
35	E	718	A	N9-C4	-9.61	1.32	1.37
35	E	738	G	N9-C4	-8.96	1.30	1.38

The worst 5 of 5616 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	774	C	P-O3'-C3'	37.91	165.19	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1187	C	P-O3'-C3'	33.90	160.37	119.70
35	E	976	U	O5'-P-OP2	-24.56	81.23	110.70
35	E	976	U	O5'-P-OP1	-24.39	81.44	110.70
35	E	703	A	P-O3'-C3'	23.77	148.22	119.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	E	325	U	C3'
35	E	702	U	C1'
35	E	810	U	C3'
35	E	1903	A	C3'

5 of 180 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	p	110	LYS	Peptide
1	p	261	ARG	Sidechain
1	p	43	TRP	Peptide
3	r	32	GLN	Peptide
3	r	42	VAL	Peptide

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	p	2405	0	2323	0	0
2	q	311	0	319	0	0
3	r	1113	0	1175	0	0
4	t	969	0	1003	0	0
5	u	981	0	1021	0	0
6	L	2038	0	2142	0	0
7	M	1116	0	1169	0	0
8	O	1493	0	1562	0	0
9	Q	1670	0	1778	1	0
10	R	1143	0	1226	1	0
11	S	630	0	630	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	T	829	0	866	0	0
13	U	526	0	550	0	0
14	V	1011	0	1019	0	0
15	W	1781	0	1853	0	0
16	X	1212	0	1250	0	0
17	Y	989	0	1065	0	0
18	Z	1404	0	1503	1	0
19	b	1365	0	1410	0	0
20	f	1658	0	1704	0	0
21	d	1726	0	1774	0	0
22	e	1019	0	1050	0	0
23	g	635	0	631	0	0
24	a	553	0	608	0	0
25	i	958	0	981	0	0
26	j	518	0	513	0	0
27	P	1983	0	2131	0	0
28	k	972	0	1031	0	0
29	l	784	0	848	0	0
30	m	1587	0	1662	0	0
31	n	780	0	771	0	0
32	o	1116	0	1166	0	0
33	c	480	0	532	0	0
34	h	1358	0	1419	0	0
35	E	43106	0	21756	87	0
All	All	82219	0	62441	87	0

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

The worst 5 of 87 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)
35:E:725:U:H3	35:E:733:G:H1	1.12	0.96
35:E:1849:U:H3	35:E:1869:G:H1	1.26	0.83
35:E:207:G:H1	35:E:222:U:H3	1.30	0.78
35:E:2220:G:H1	35:E:2232:U:H3	1.32	0.77
35:E:711:A:N1	35:E:746:A:N1	2.33	0.77

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	
1	p	308/318 (97%)	288 (94%)	18 (6%)	2 (1%)	25	63
2	q	36/57 (63%)	28 (78%)	6 (17%)	2 (6%)	2	20
3	r	138/149 (93%)	113 (82%)	18 (13%)	7 (5%)	2	22
4	t	117/152 (77%)	105 (90%)	8 (7%)	4 (3%)	3	30
5	u	118/153 (77%)	102 (86%)	13 (11%)	3 (2%)	5	35
6	L	256/273 (94%)	239 (93%)	16 (6%)	1 (0%)	34	71
7	M	140/143 (98%)	131 (94%)	8 (6%)	1 (1%)	22	61
8	O	188/190 (99%)	165 (88%)	16 (8%)	7 (4%)	3	28
9	Q	198/211 (94%)	178 (90%)	16 (8%)	4 (2%)	7	40
10	R	139/151 (92%)	127 (91%)	11 (8%)	1 (1%)	22	61
11	S	80/86 (93%)	73 (91%)	5 (6%)	2 (2%)	5	35
12	T	102/112 (91%)	90 (88%)	12 (12%)	0	100	100
13	U	66/112 (59%)	62 (94%)	3 (4%)	1 (2%)	10	45
14	V	133/144 (92%)	116 (87%)	16 (12%)	1 (1%)	19	58
15	W	215/261 (82%)	200 (93%)	13 (6%)	2 (1%)	17	55
16	X	146/173 (84%)	133 (91%)	11 (8%)	2 (1%)	11	46
17	Y	121/137 (88%)	113 (93%)	8 (7%)	0	100	100
18	Z	171/221 (77%)	157 (92%)	12 (7%)	2 (1%)	13	49
19	b	162/190 (85%)	143 (88%)	17 (10%)	2 (1%)	13	49
20	f	205/245 (84%)	190 (93%)	12 (6%)	3 (2%)	10	45
21	d	221/263 (84%)	205 (93%)	14 (6%)	2 (1%)	17	55
22	e	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	19	58
23	g	81/236 (34%)	78 (96%)	3 (4%)	0	100	100
24	a	68/110 (62%)	58 (85%)	6 (9%)	4 (6%)	1	19
25	i	119/141 (84%)	111 (93%)	7 (6%)	1 (1%)	19	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	j	62/150 (41%)	47 (76%)	11 (18%)	4 (6%)	1	18
27	P	247/250 (99%)	226 (92%)	21 (8%)	0	100	100
28	k	116/196 (59%)	102 (88%)	13 (11%)	1 (1%)	17	55
29	l	97/117 (83%)	82 (84%)	15 (16%)	0	100	100
30	m	198/214 (92%)	179 (90%)	14 (7%)	5 (2%)	5	35
31	n	91/161 (56%)	83 (91%)	5 (6%)	3 (3%)	4	30
32	o	138/167 (83%)	112 (81%)	21 (15%)	5 (4%)	3	28
33	c	58/66 (88%)	53 (91%)	4 (7%)	1 (2%)	9	43
34	h	171/257 (66%)	123 (72%)	31 (18%)	17 (10%)	0	9
All	All	4833/5936 (81%)	4330 (90%)	412 (8%)	91 (2%)	11	40

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	r	121	TYR
3	r	124	ILE
5	u	120	VAL
9	Q	138	CYS
21	d	81	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	p	262/268 (98%)	260 (99%)	2 (1%)	81	89
2	q	34/49 (69%)	34 (100%)	0	100	100
3	r	113/121 (93%)	113 (100%)	0	100	100
4	t	102/131 (78%)	102 (100%)	0	100	100
5	u	104/132 (79%)	104 (100%)	0	100	100
6	L	217/230 (94%)	217 (100%)	0	100	100
7	M	116/117 (99%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	O	160/160 (100%)	160 (100%)	0	100	100
9	Q	188/195 (96%)	188 (100%)	0	100	100
10	R	125/132 (95%)	124 (99%)	1 (1%)	81	89
11	S	70/73 (96%)	70 (100%)	0	100	100
12	T	87/93 (94%)	87 (100%)	0	100	100
13	U	57/97 (59%)	57 (100%)	0	100	100
14	V	103/112 (92%)	102 (99%)	1 (1%)	76	86
15	W	194/223 (87%)	192 (99%)	2 (1%)	76	86
16	X	137/157 (87%)	137 (100%)	0	100	100
17	Y	104/116 (90%)	104 (100%)	0	100	100
18	Z	143/184 (78%)	143 (100%)	0	100	100
19	b	148/165 (90%)	148 (100%)	0	100	100
20	f	182/211 (86%)	181 (100%)	1 (0%)	88	93
21	d	187/208 (90%)	187 (100%)	0	100	100
22	e	110/111 (99%)	109 (99%)	1 (1%)	78	88
23	g	68/186 (37%)	68 (100%)	0	100	100
24	a	64/96 (67%)	63 (98%)	1 (2%)	62	79
25	i	103/120 (86%)	99 (96%)	4 (4%)	32	58
26	j	55/123 (45%)	54 (98%)	1 (2%)	59	77
27	P	204/205 (100%)	204 (100%)	0	100	100
28	k	108/172 (63%)	108 (100%)	0	100	100
29	l	89/104 (86%)	89 (100%)	0	100	100
30	m	167/179 (93%)	166 (99%)	1 (1%)	86	92
31	n	84/125 (67%)	83 (99%)	1 (1%)	71	84
32	o	118/139 (85%)	117 (99%)	1 (1%)	81	89
33	c	49/53 (92%)	49 (100%)	0	100	100
34	h	138/191 (72%)	133 (96%)	5 (4%)	35	61
All	All	4190/4978 (84%)	4168 (100%)	22 (0%)	89	93

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	m	137	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	h	94	VAL
32	o	116	LEU
34	h	103	TYR
20	f	72	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
15	W	193	ASN
16	X	11	HIS
30	m	163	HIS
18	Z	64	ASN
20	f	121	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	E	2017/2319 (86%)	437 (21%)	86 (4%)

5 of 437 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	E	4	C
35	E	5	U
35	E	17	C
35	E	25	C
35	E	26	A

5 of 86 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	E	1187	C
35	E	1903	A
35	E	1191	G
35	E	1712	U
35	E	2017	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

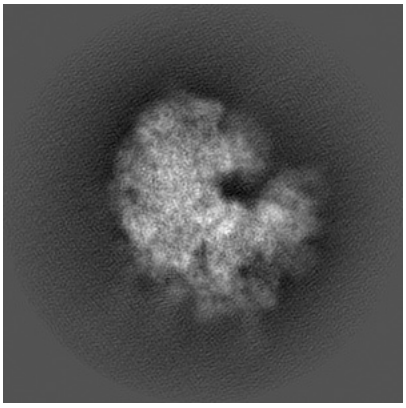
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3844. These allow visual inspection of the internal detail of the map and identification of artifacts.

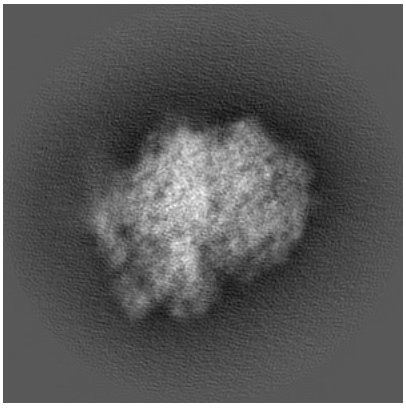
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

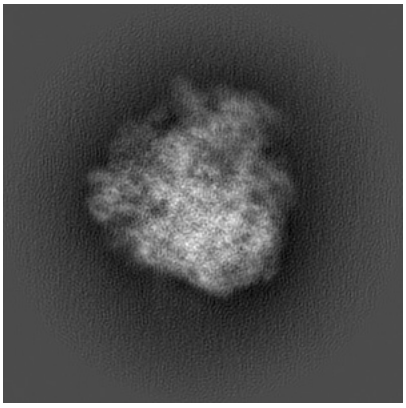
6.1.1 Primary map



X



Y

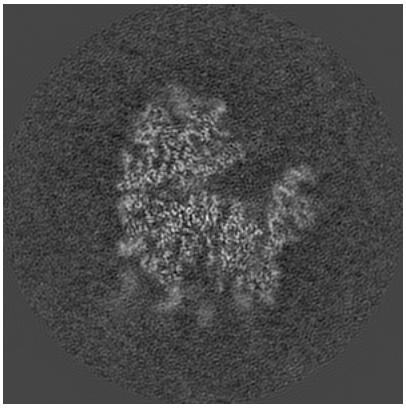


Z

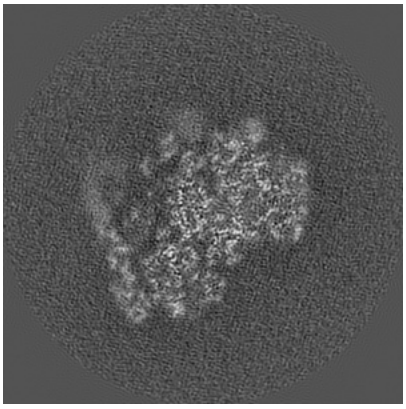
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

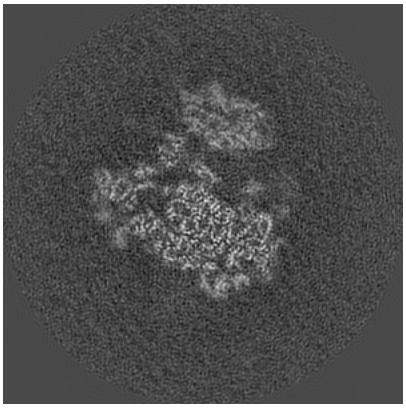
6.2.1 Primary map



X Index: 160



Y Index: 160

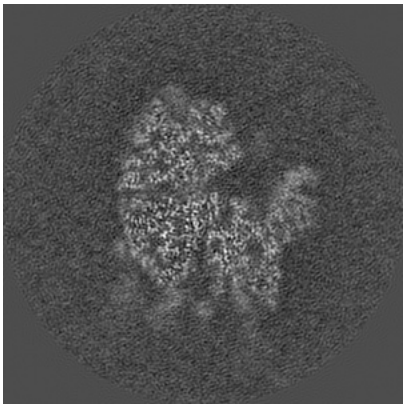


Z Index: 160

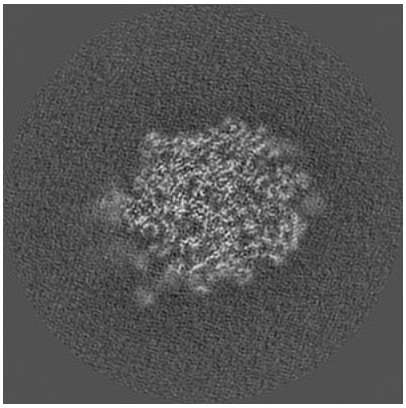
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

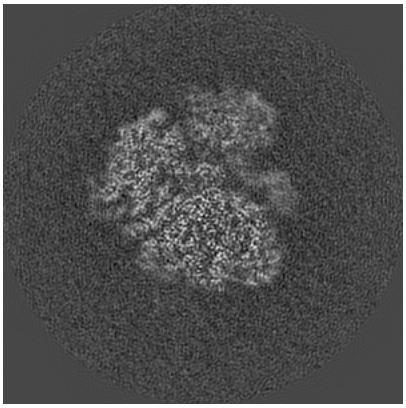
6.3.1 Primary map



X Index: 157



Y Index: 134

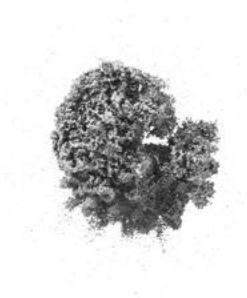


Z Index: 147

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

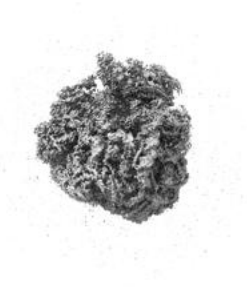
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0549. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

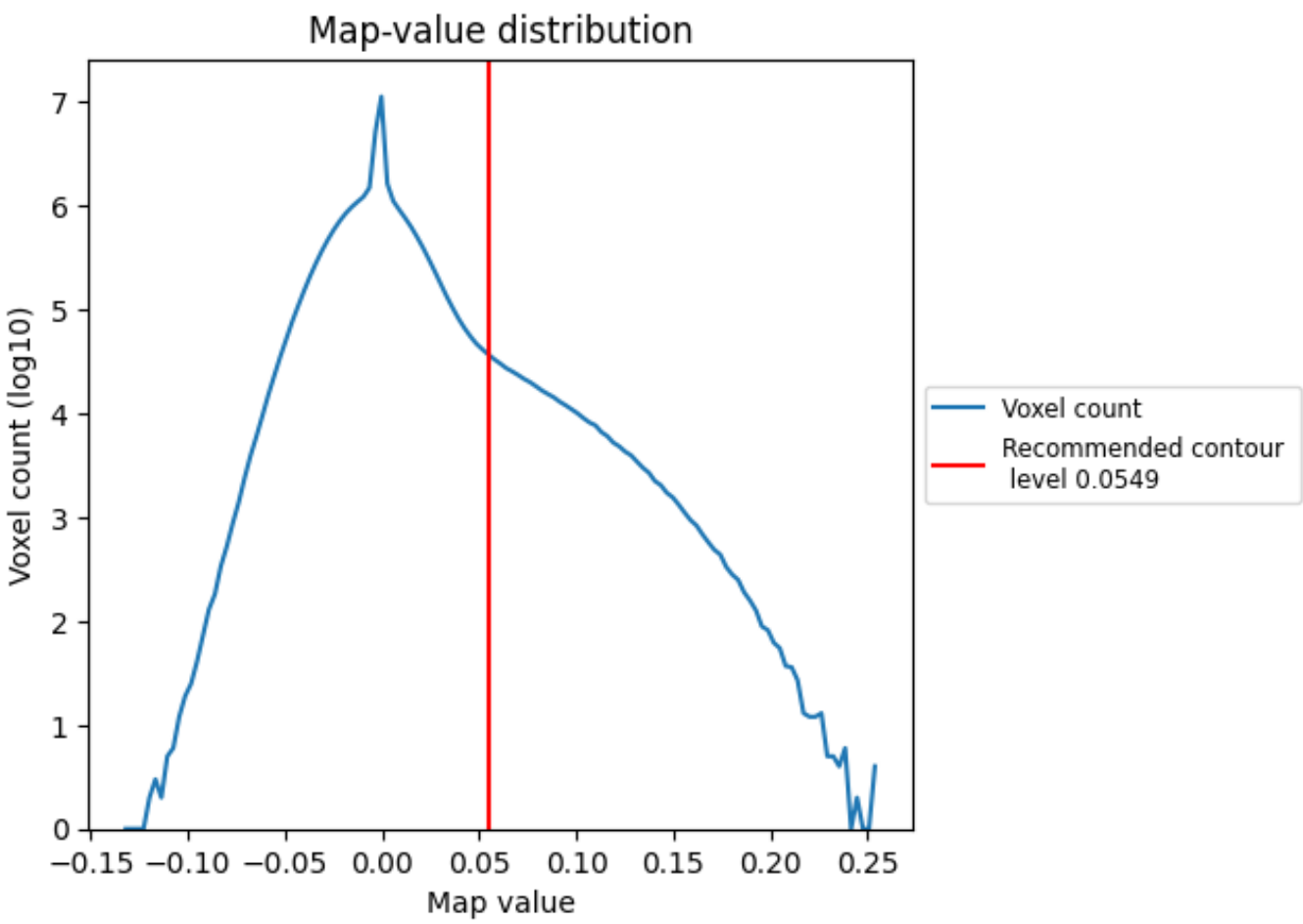
6.5 Mask visualisation (i)

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

7 Map analysis (i)

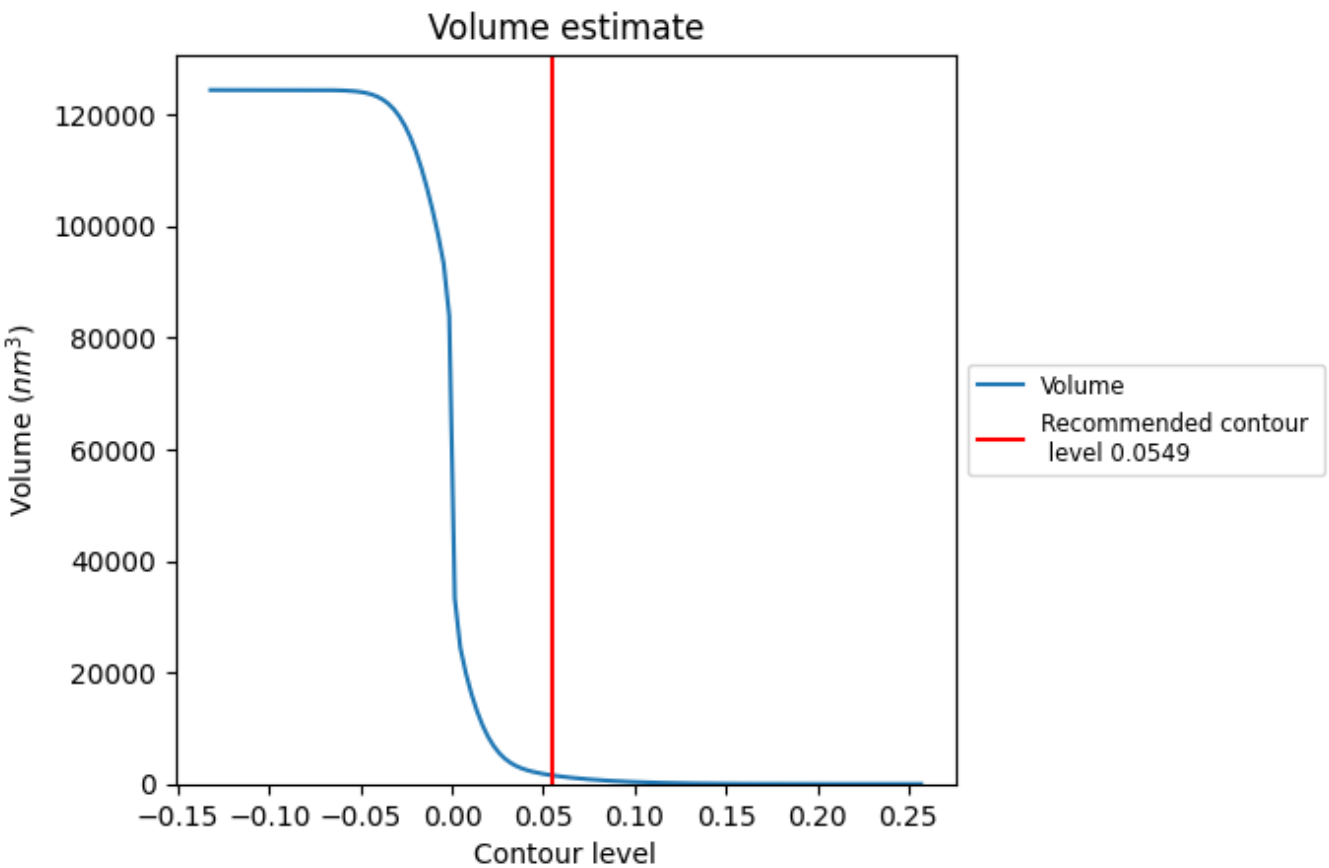
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

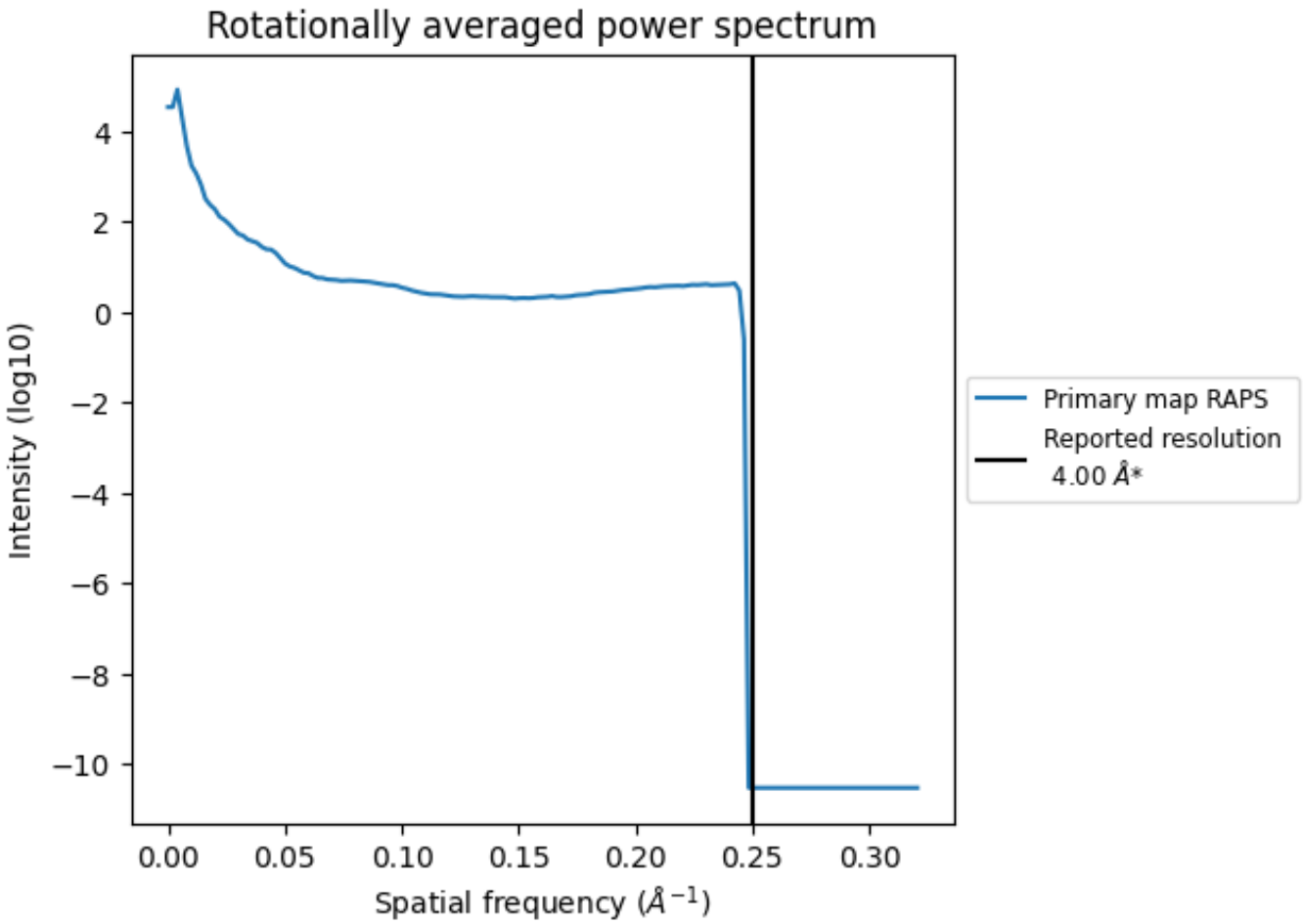
7.2 Volume estimate (i)



The volume at the recommended contour level is 1549 nm^3; this corresponds to an approximate mass of 1400 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 0.250 Å^{-1}

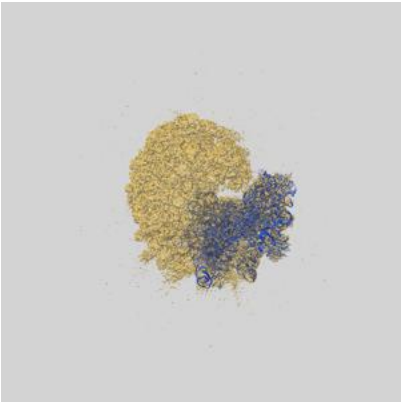
8 Fourier-Shell correlation (i)

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

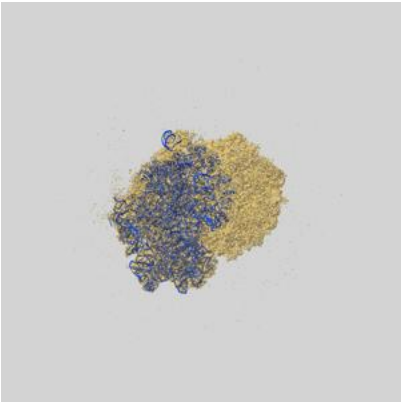
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3844 and PDB model 5OPT. Per-residue inclusion information can be found in section 3 on page 11.

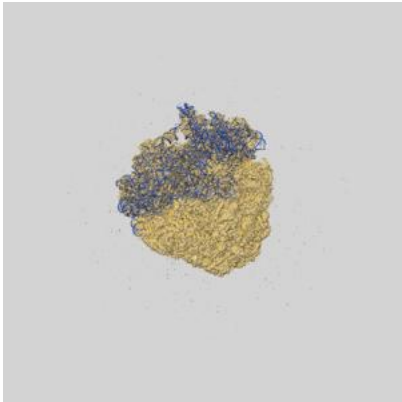
9.1 Map-model overlay (i)



X



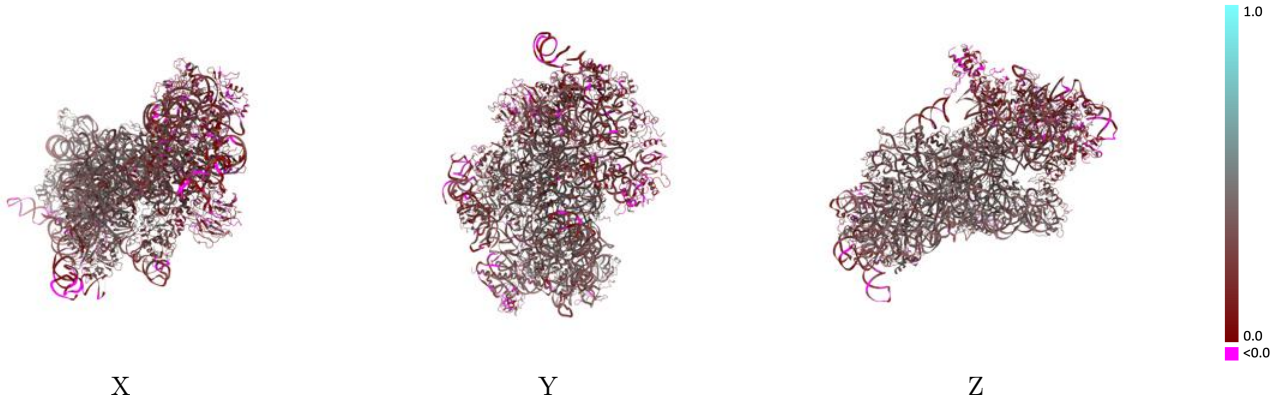
Y



Z

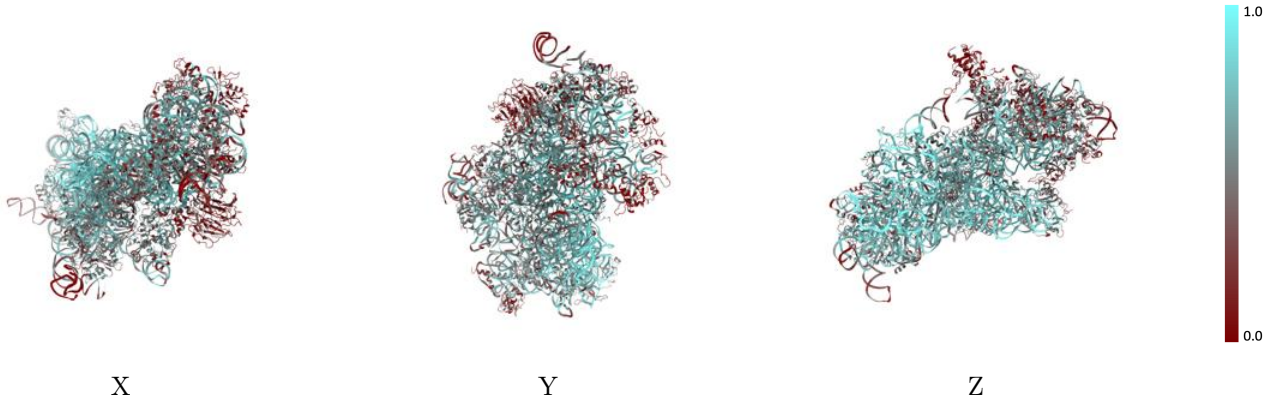
The images above show the 3D surface view of the map at the recommended contour level 0.0549 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



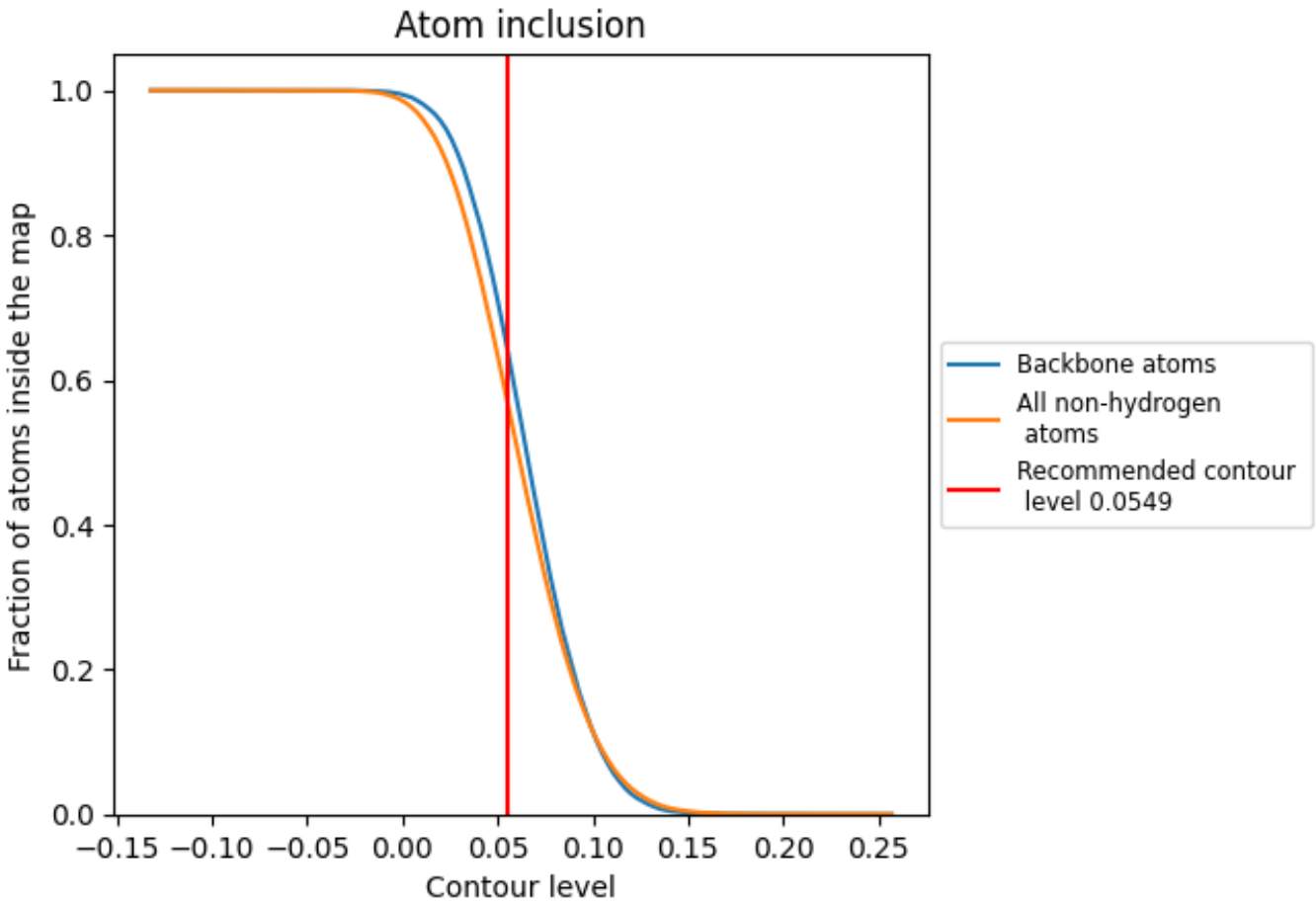
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.0549).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0549) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5724	0.2840
E	0.6987	0.2970
L	0.5232	0.3590
M	0.5606	0.3500
O	0.3579	0.2240
P	0.5280	0.2910
Q	0.5311	0.3060
R	0.5204	0.3280
S	0.4421	0.3200
T	0.5044	0.3360
U	0.2609	0.2090
V	0.4923	0.3140
W	0.5513	0.3340
X	0.5149	0.3370
Y	0.5848	0.3250
Z	0.5968	0.3600
a	0.2983	0.1260
b	0.5505	0.3240
c	0.4765	0.2910
d	0.5234	0.3260
e	0.5473	0.3480
f	0.5207	0.3120
g	0.5169	0.3330
h	0.2966	0.1270
i	0.1113	0.0940
j	0.1861	0.1000
k	0.3771	0.2550
l	0.2936	0.2240
m	0.2931	0.2600
n	0.2964	0.2120
o	0.3843	0.1690
p	0.1712	0.1680
q	0.3767	0.2290
r	0.3924	0.2380
t	0.2790	0.1820
u	0.3231	0.1910