wwPDB EM Validation Summary Report (i)

Jan 24, 2023 – 11:05 AM EST

PDB ID	:	7SYV
EMDB ID	:	EMD-25542
Title	:	Structure of the wt IRES eIF5B-containing pre-48S initiation complex, open conformation. Structure 14(wt)
Authors	:	Brown, Z.P.; Abaeva, I.S.; De, S.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.
Deposited on	:	2021-11-25
Resolution	:	3.90 Å(reported)
Based on initial models	:	6D9J, 5K0Y, 5FLX, 4UJD

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 (1)) were used in the production of this report:

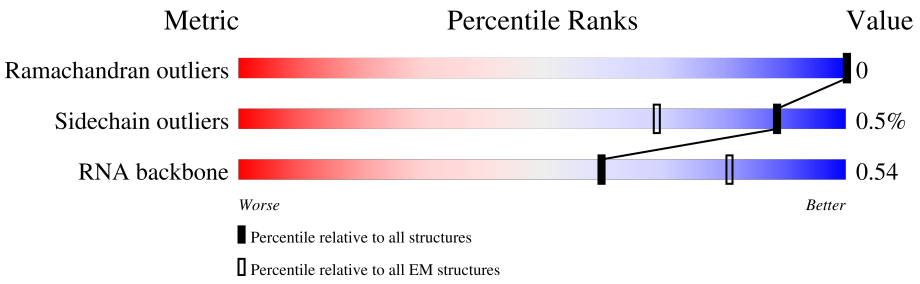
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	2	1870	5% 69% 20% • 10%
2	Z	131	• 94% • 5%
3	A	144	26% 70% • 29%
4	a	124	10% 61% • 38%
5	B	295	7% 73% 26%
6	b	101	9% 100%
7	C	264	• 81% 19%
8	c	84	11% 99% •

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Mol	Chain	Length	Quality of chain
9	D	221	8% 100%
10	d	69	10% 94%
11	E	281	21% 81% 19%
12	e	56	20% 98%
13	F	263	99%
14	f	133	17% 43% 57%
15	G	204	5% 93% 6%
16	g	188	35% 36% 64%
17	H	249	13% 94% 5%
18	h	317	36% 99%
19	I	432	12% 42% 57%
20	i	75	16% 80% 20%
21	J	208	11% 98%
22	n	25	16% 100%
23	K	194	95% 5%
24	x	627	32% 99%
25	L	149	32% 64% 36%
26	z	400	47% 16% 36%
27	M	158	14% 95%
28	N	132	87% 88% 11%
29	O	151	5% 99%
30	P	168	7% 79% 19%
31	Q	145	31% 82% 17%
32	R	172	6% 82% 17%
33	S	135	33% 97%

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Mol	Chain	Length	Quality of chain
34	T	152	25% 95% 5%
35	U	145	6% 97%
36	V	119	36% 82% 16%
37	W	83	99%
38	X	130	99%
39	Y	143	98%

2 Entry composition (i)

There are 43 unique types of molecules in this entry. The entry contains 87912 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 RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1680	35864	16009	6439	11737	1679	0	0

- Molecule 2 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Z	124	1011	640	198	168	5	0	0

- Molecule 3 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	102	822	517	147	154	4	0	0

- Molecule 4 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	a	77	614	393	114	106	1	0	0

- Molecule 5 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	217	1710	1086	300	316	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 6 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	b	101	814	507	170	132	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	28	ARG	CYS	conflict	UNP G1TFE8
b	56	ALA	VAL	conflict	UNP G1TFE8

- Molecule 7 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	213	1729	1098	309	308	14	0	0

- Molecule 8 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	c	83	651	408	121	115	7	0	0

- Molecule 9 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	D	221	1716	1111	295	301	9	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	73	MET	VAL	conflict	UNP G1TUT9
D	101	SER	ALA	conflict	UNP G1TUT9
D	119	GLY	ALA	conflict	UNP G1TUT9
D	194	ARG	HIS	conflict	UNP G1TUT9
D	215	MET	LEU	conflict	UNP G1TUT9
D	227	ARG	TRP	conflict	UNP G1TUT9
D	228	GLY	SER	conflict	UNP G1TUT9

- Molecule 10 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	d	67	530	321	108	99	2	0	0

- Molecule 11 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	E	228	1768	1126	318	316	8	0	0

- Molecule 12 is a protein called eS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	e	55	459	286	94	74	5	0	0

- Molecule 13 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	F	262	2076	1324	386	358	8	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	25	GLY	SER	conflict	UNP G1TK17
F	51	ARG	LYS	conflict	UNP G1TK17
F	78	THR	ALA	conflict	UNP G1TK17
F	156	VAL	MET	conflict	UNP G1TK17

- Molecule 14 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	f	57	457	282	101	73	1	0	0

- Molecule 15 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	191	1509	943	286	273	7	0	0

- Molecule 16 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	g	68	555	351	103	94	7	0	0

- Molecule 17 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	H	237	1923	1200	387	329	7	0	0

- Molecule 18 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	h	313	2436	1535	424	465	12	0	0

- Molecule 19 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	I	185	1488	952	271	264	1	0	0

- Molecule 20 is a RNA chain called Met-tRNA-i-Met.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	i	75	1604	717	298	515	74	0	0

- Molecule 21 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	J	206	1686	1058	332	291	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 22 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	n	25	239	145	64	27	3	0	0

- Molecule 23 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	K	185	1525	969	306	248	2	0	0

- Molecule 24 is a protein called Eukaryotic translation initiation factor 5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	x	627	4965	3157	856	929	23	0	0

- Molecule 25 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	L	96	810	530	143	131	6	0	0

- Molecule 26 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	z	258	5513	2456	989	1810	258	0	0

- Molecule 27 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	M	151	1233	785	231	211	6	0	0

- Molecule 28 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	N	117	908	570	161	169	8	0	0

- Molecule 29 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	O	149	1202	770	228	203	1	0	0

- Molecule 30 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	P	136	1016	621	199	190	6	0	0

- Molecule 31 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Q	120	997	635	187	168	7	0	0

- Molecule 32 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	R	142	1128	717	213	195	3	0	0

- Molecule 33 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	S	132	1068	670	199	195	4	0	0

- Molecule 34 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	T	144	1190	746	241	202	1	0	0

- Molecule 35 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	U	141	1097	688	211	195	3	0	0

- Molecule 36 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	V	100	795	498	152	141	4	0	0

- Molecule 37 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	W	83	636	393	117	121	5	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	3	ASN	SER	conflict	UNP G1TM82
W	4	ASP	ASN	conflict	UNP G1TM82
W	33	GLN	PRO	conflict	UNP G1TM82
W	50	PHE	SER	conflict	UNP G1TM82
W	75	ALA	SER	conflict	UNP G1TM82
W	76	ASP	HIS	conflict	UNP G1TM82
W	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 38 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	X	129	1034	659	193	176	6	0	0

- Molecule 39 is a protein called uS12.

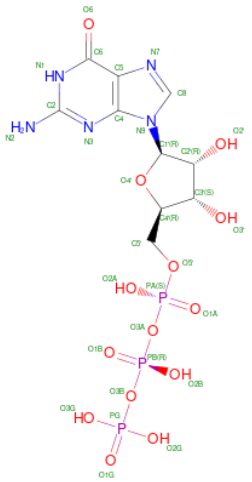
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Y	141	1098	693	219	183	3	0	0

- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
40	b	1	1	1	0
40	g	1	1	1	0

- Molecule 41 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

GTP



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
41	x	1	32	10	5	14	3	0

- Molecule 42 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
42	x	1	1	1	0

- Molecule 43 is SODIUM ION (three-letter code: NA) (formula: Na).

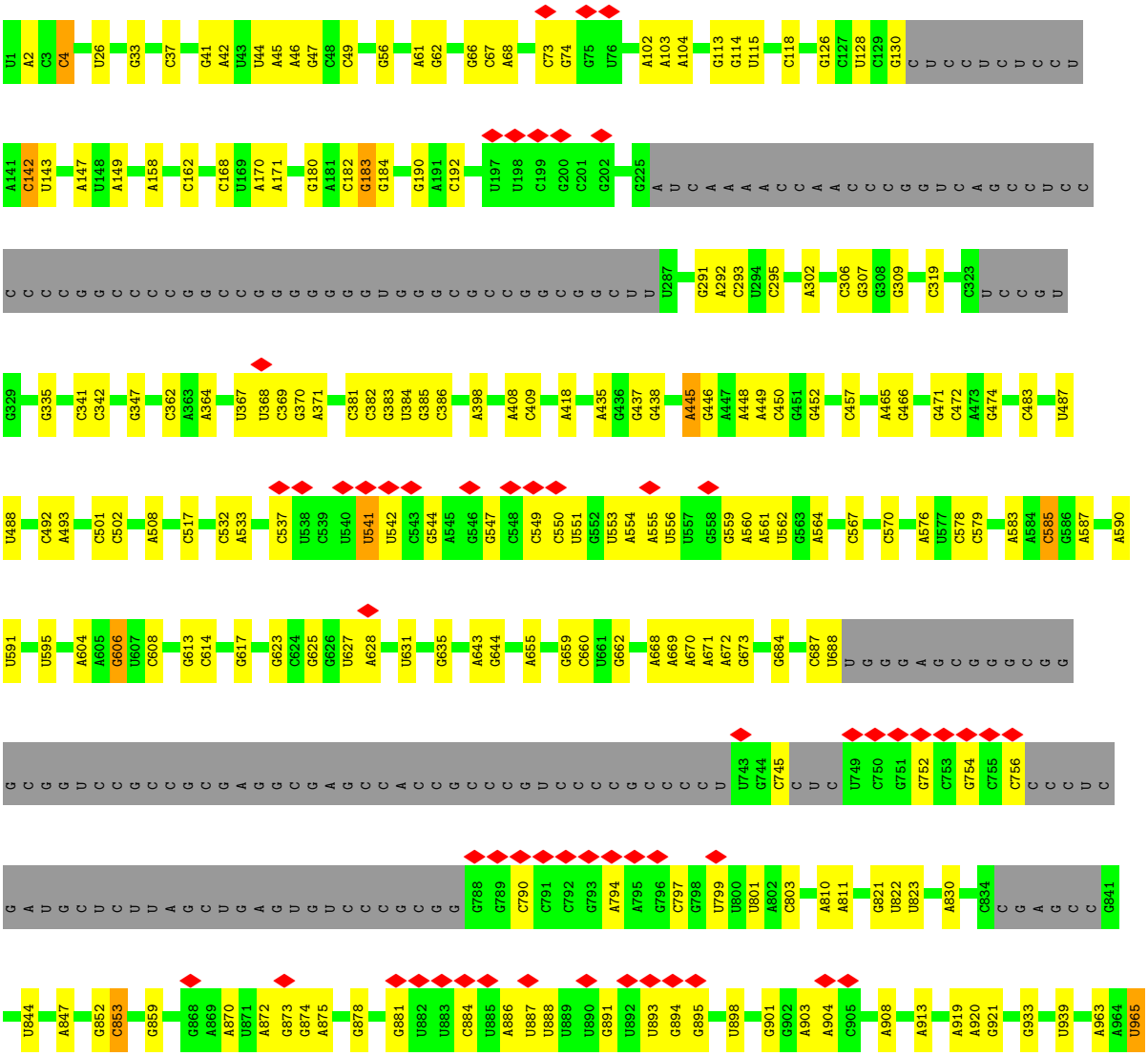
Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
43	x	1	1	1	0

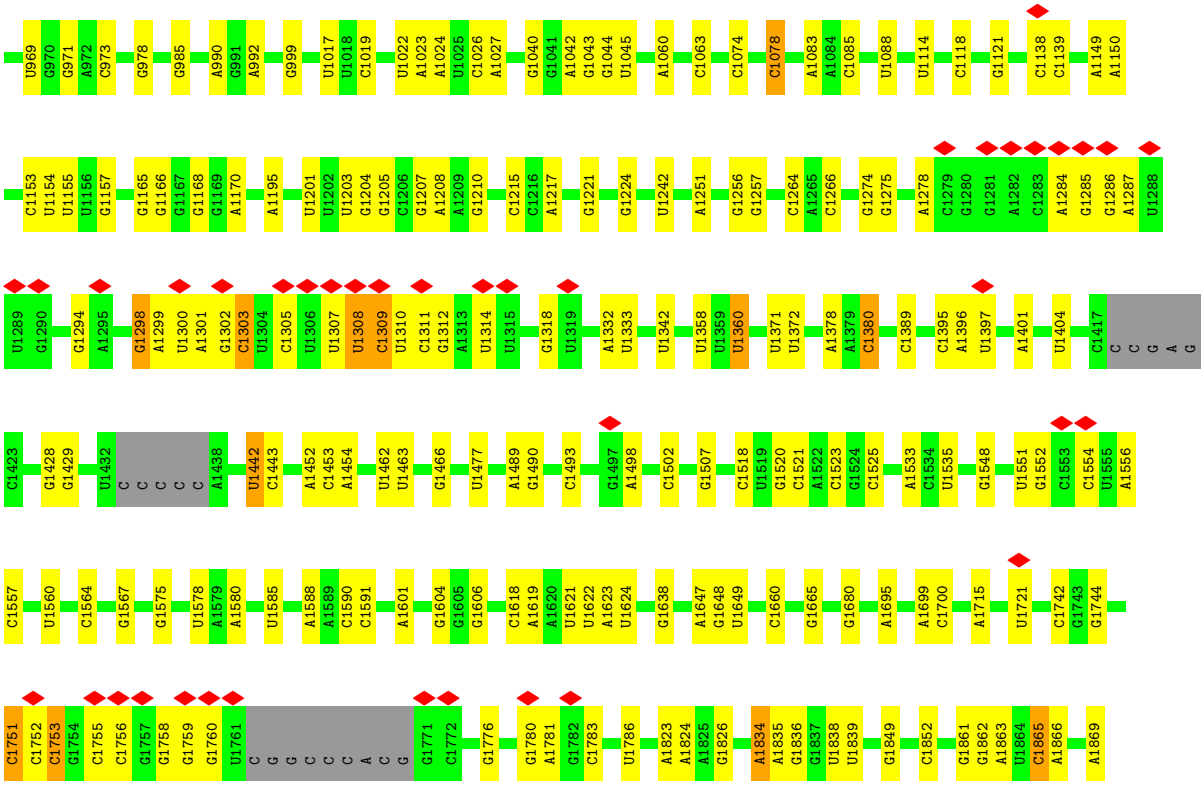
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 18S rRNA

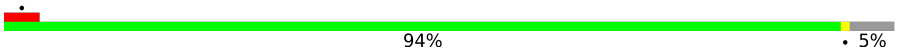
Chain 2:

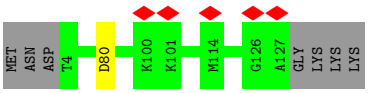




- Molecule 2: 40S ribosomal protein S24

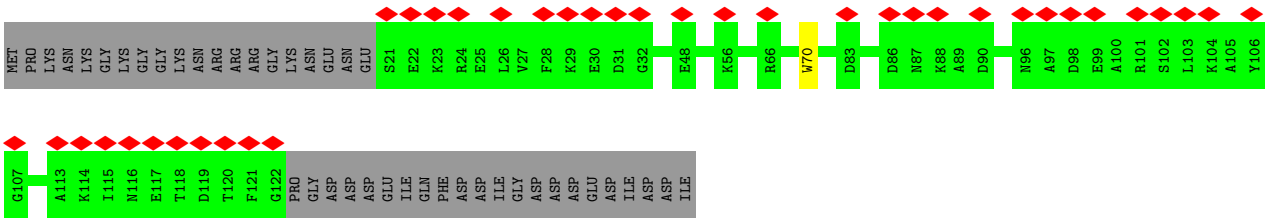
Chain Z:





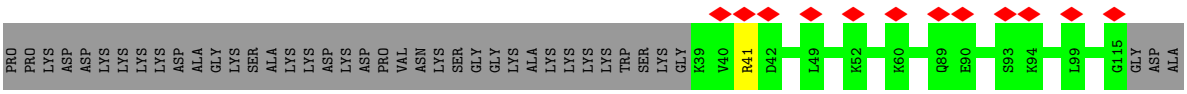
- Molecule 3: Eukaryotic translation initiation factor 1A, X-chromosomal

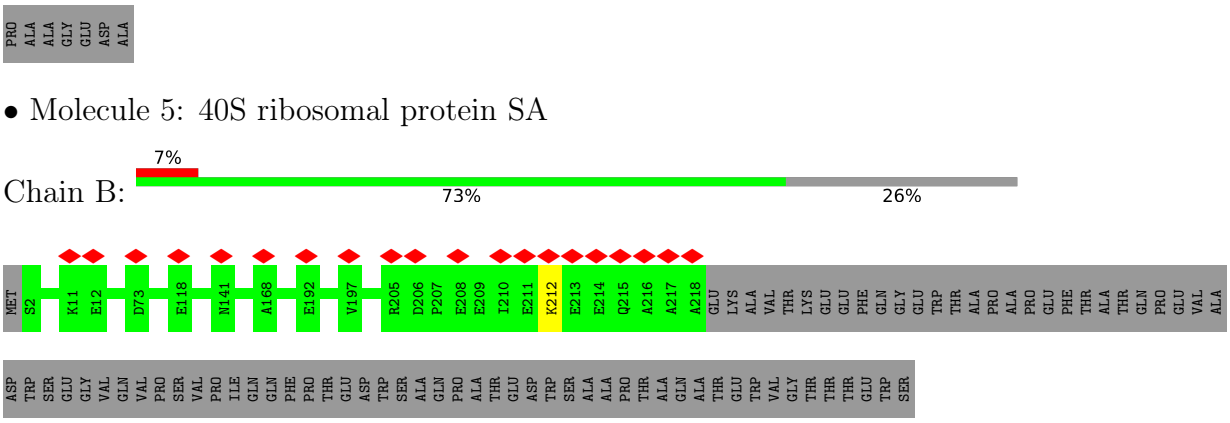
Chain A:

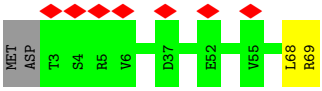


- Molecule 4: 40S ribosomal protein S25

Chain a:

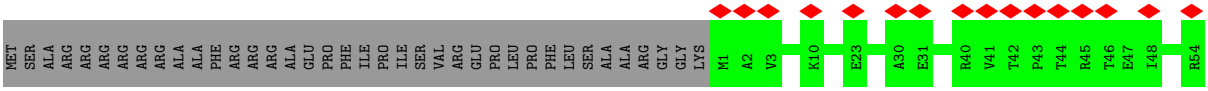


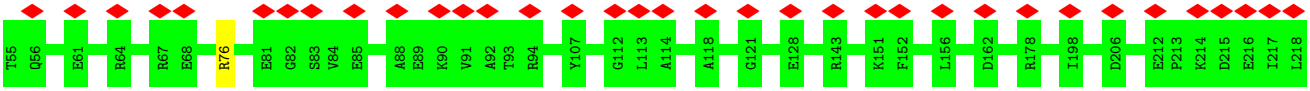

PRO ALA ALA GLY GLU ASP ALA
• Molecule 5: 40S ribosomal protein SA
Chain B:
7%
73%
26%
MET S2 K11 E12 D73 E118 N141 A168 E192 V197 R205 D206 P207 E208 E209 I210 E211 K212 E213 E214 Q215 A216 A217 A218 GLU LYS ALA VAL THR LYS GLU GLU PHE GLN GLY GLU TRP THR ALA PRO ALA PRO GLU PHE THR ALA THR GLN PRO GLU VAL ALA
ASP TRP SER GLU GLY VAL GLN VAL PRO SER VAL PRO ILE GLN GLN PHE PRO THR GLU ASP TRP SER ALA GLN PRO ALA THR GLU ASP TRP SER ALA ALA PRO THR ALA GLN ALA THR GLU TRP VAL GLY THR THR THR GLU TRP SER
• Molecule 6: eS26
Chain b:
9%
100%
T2 V45 E46 R51 E55 A61 R100 F101 R102
• Molecule 7: eS1
Chain C:
81%
19%
MET ALA VAL GLY LYS ASN LYS ARG LEU THR LYS GLY GLY LYS LYS GLY ALA LYS LYS LYS V21 Q53 N76 D77 E78 D108 D191 K222 P223 E224 G233 GLU GLY SER SER SER GLY LYS ALA THR GLY ASP GLU THR GLY ALA LYS VAL GLU ARG ALA ASP GLY TYR
GLU PRO PRO VAL GLN GLU SER VAL
• Molecule 8: eS27
Chain c:
11%
99%
MET P2 D6 L7 L8 G39 V57 G58 C59 S60 T61 E75 R81 H84
• Molecule 9: 40S ribosomal protein S2
Chain D:
8%
100%
K58 D72 D95 A100 K103 R117 A118 G119 D220 E258 E268 F269 T270 D271 K275 T276 H277 T278
• Molecule 10: eS28
Chain d:
10%
94%

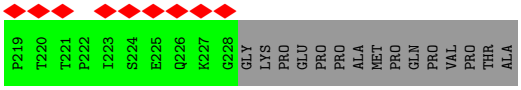


- Molecule 11: uS3

Chain E:

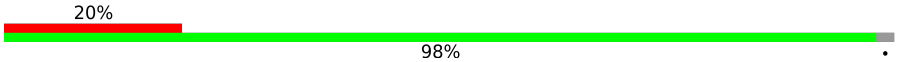


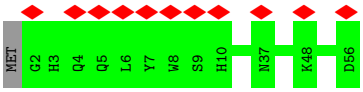




- Molecule 12: eS29

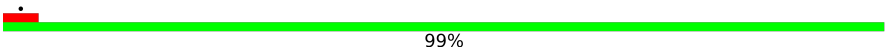
Chain e:

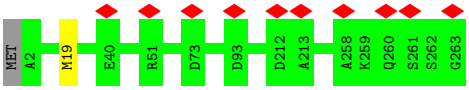




- Molecule 13: 40S ribosomal protein S4

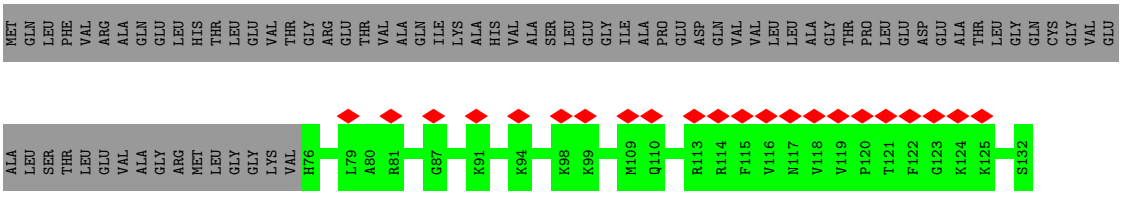
Chain F:





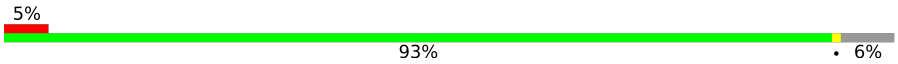
- Molecule 14: eS30

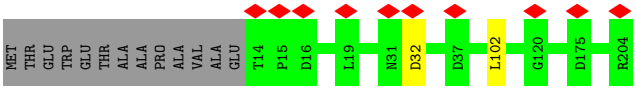
Chain f:



- Molecule 15: uS7

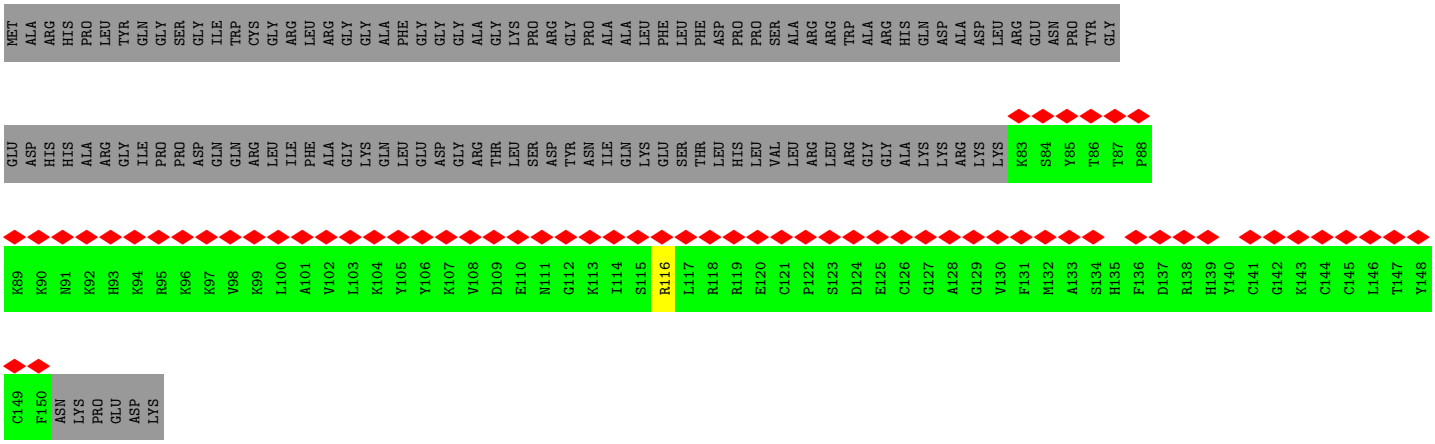
Chain G:





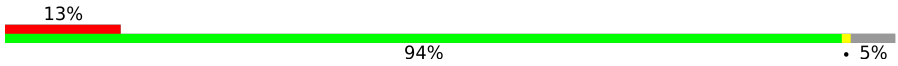
- Molecule 16: 40S ribosomal protein S27a

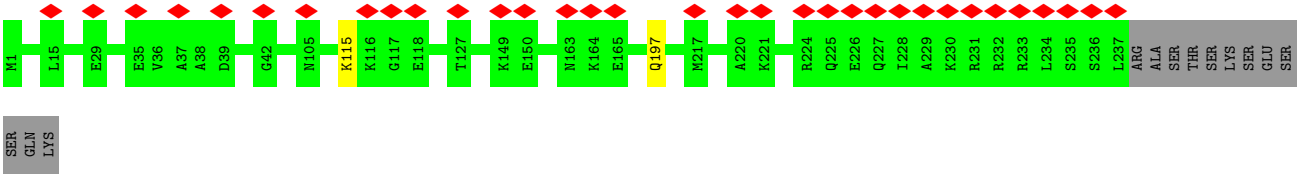
Chain g:



- Molecule 17: eS6

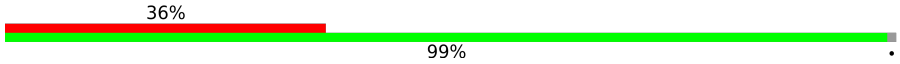
Chain H:

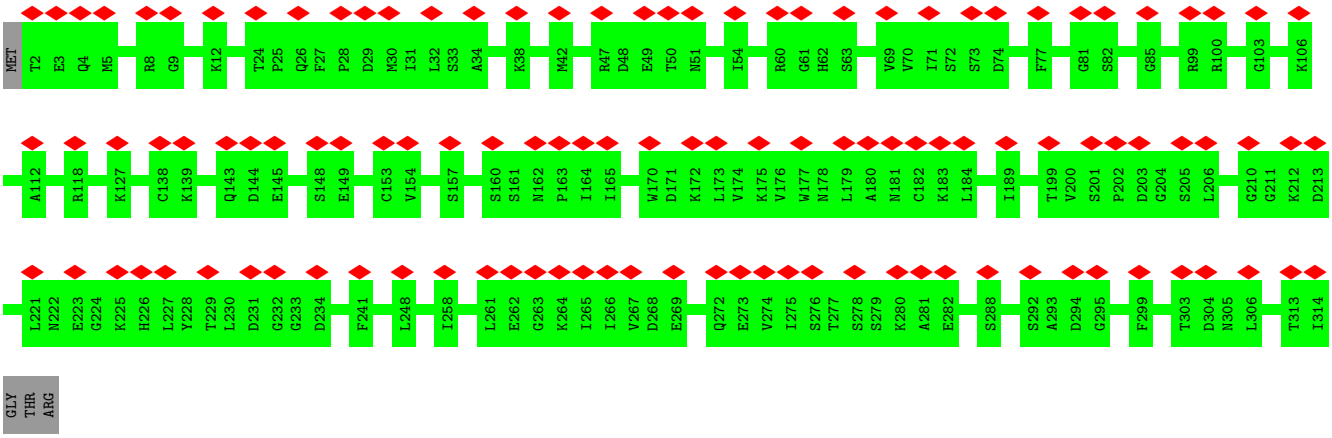




- Molecule 18: RACK1

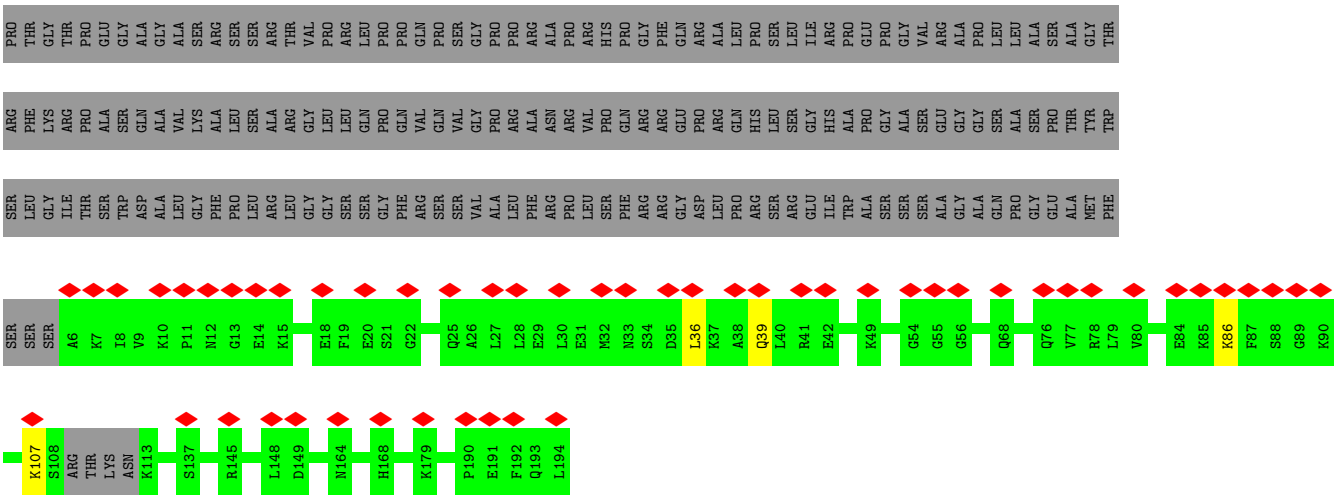
Chain h:





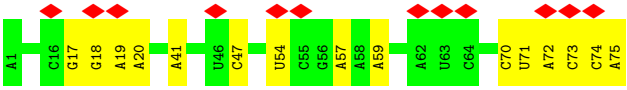
- Molecule 19: 40S ribosomal protein S7

Chain I:



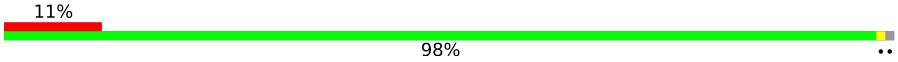
- Molecule 20: Met-tRNA-i-Met

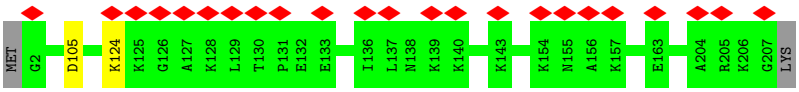
Chain i:



- Molecule 21: eS8

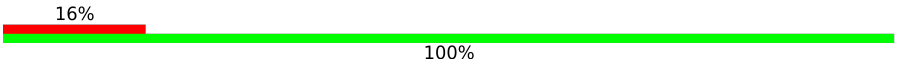
Chain J:

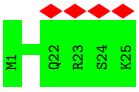




- Molecule 22: 60s ribosomal protein l41

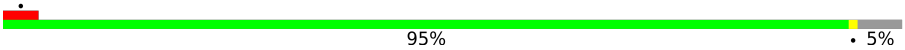
Chain n:

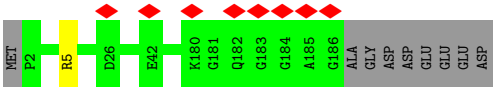




- Molecule 23: uS4

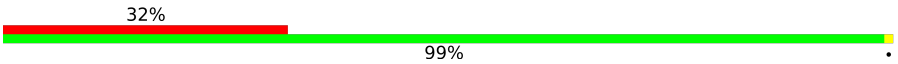
Chain K:

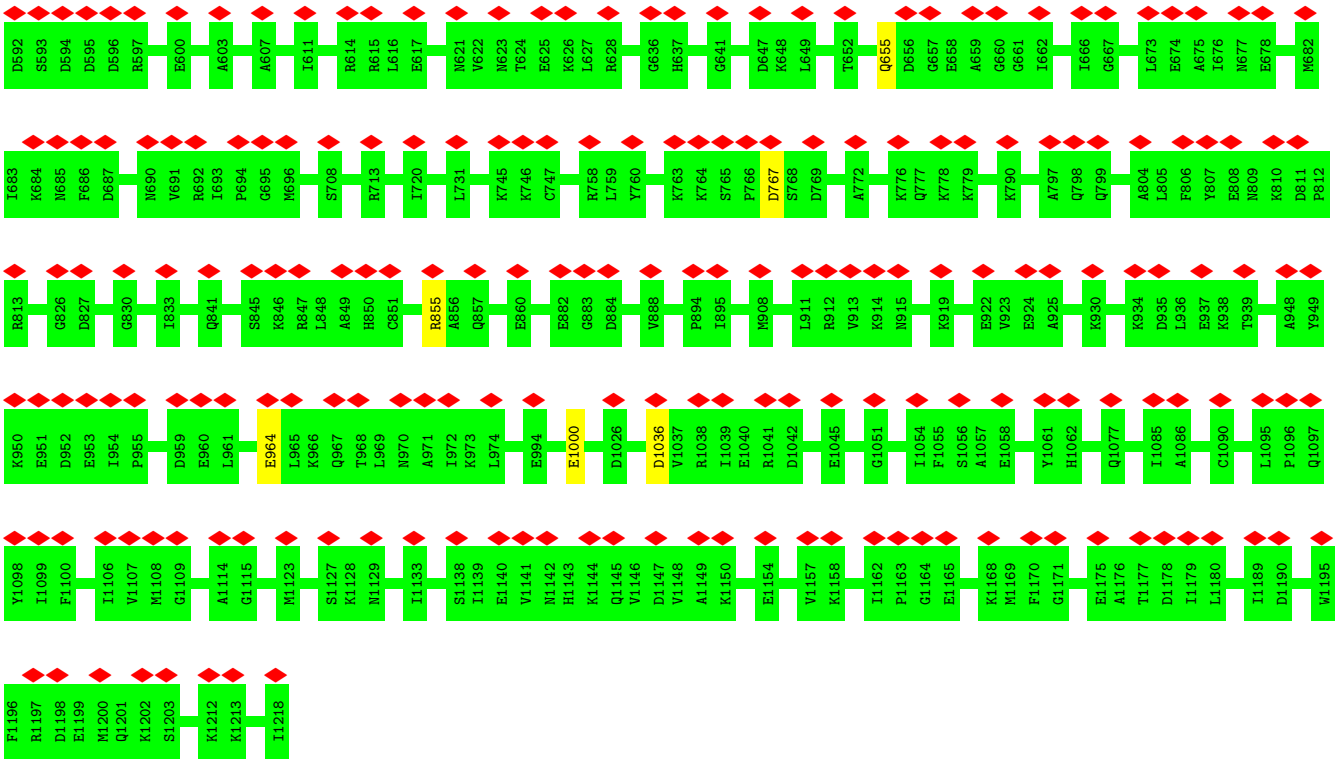




- Molecule 24: Eukaryotic translation initiation factor 5B

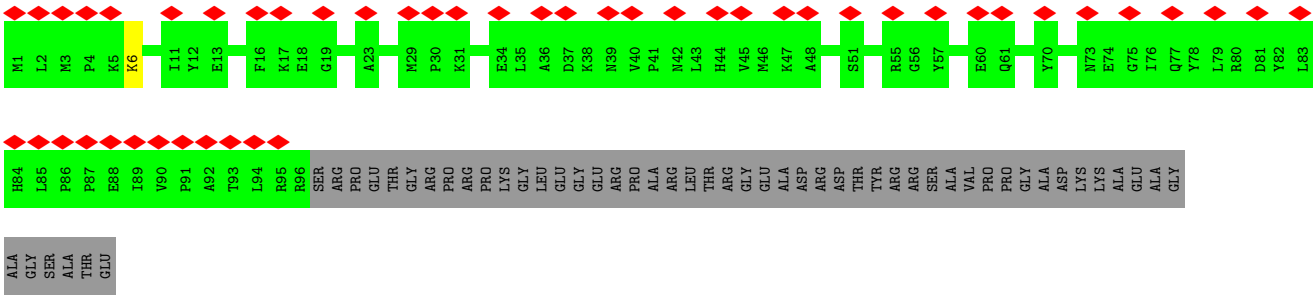
Chain x:





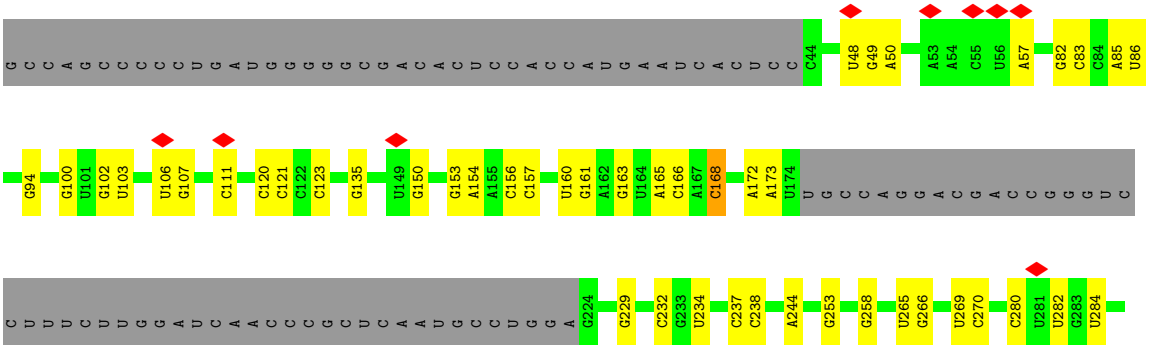
- Molecule 25: eS10

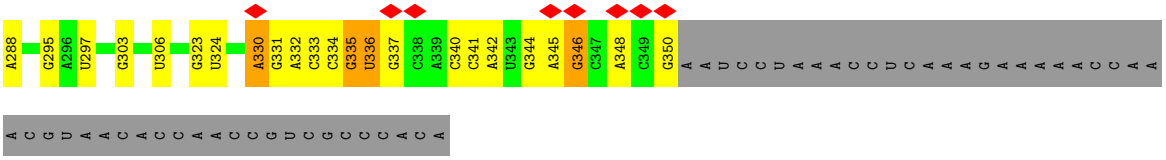
Chain L:



- Molecule 26: HCV IRES

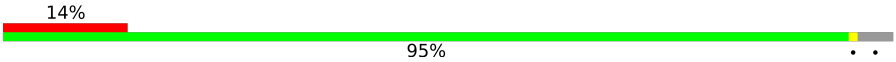
Chain z:

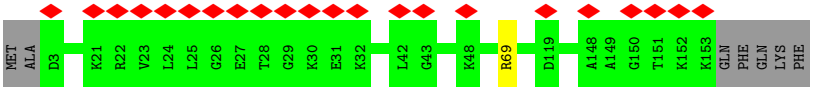




- Molecule 27: uS17

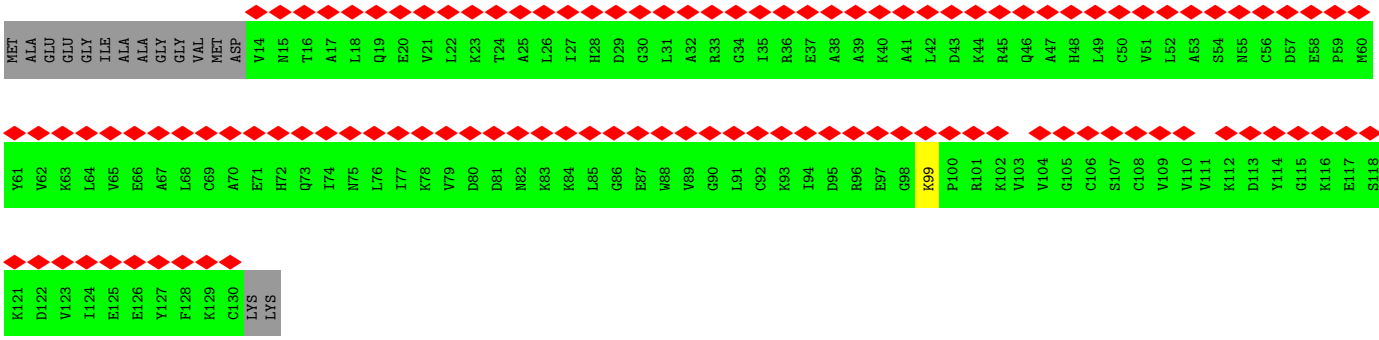
Chain M:





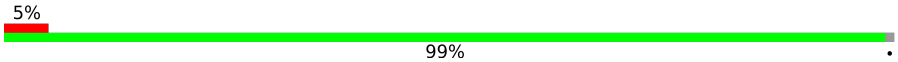
- Molecule 28: eS12

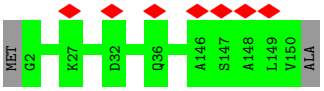
Chain N:



- Molecule 29: uS15

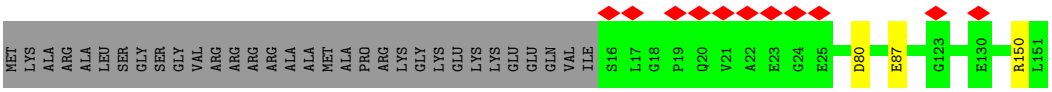
Chain O:





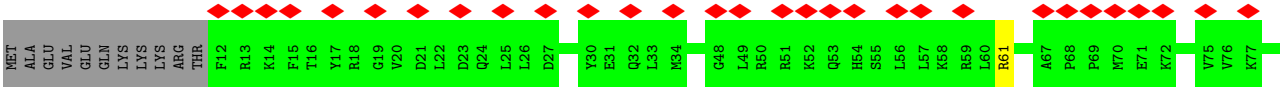
- Molecule 30: uS11

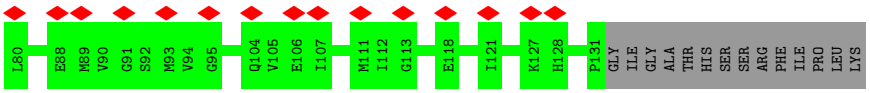
Chain P:



- Molecule 31: uS19

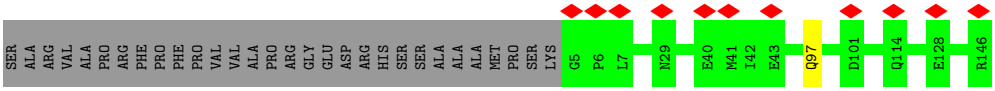
Chain Q:





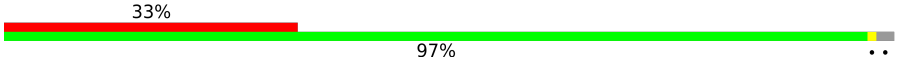
- Molecule 32: uS9

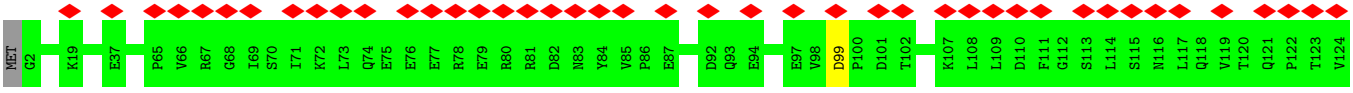
Chain R:

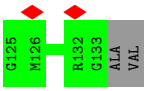


- Molecule 33: eS17

Chain S:

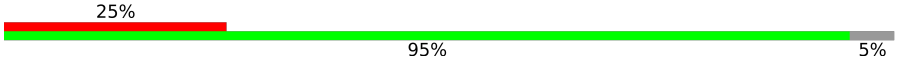


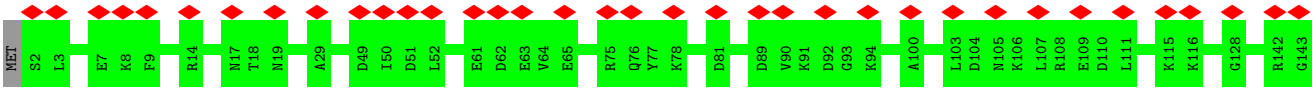


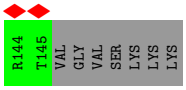


- Molecule 34: uS13

Chain T:

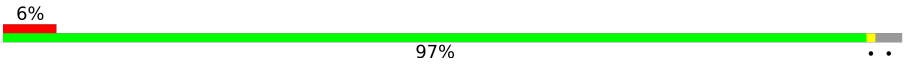


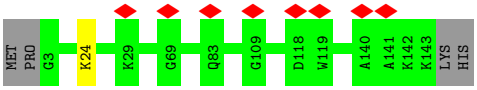




- Molecule 35: eS19

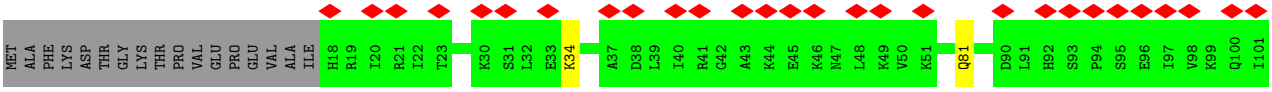
Chain U:

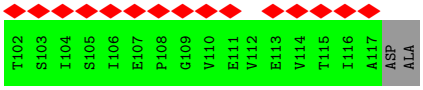




- Molecule 36: uS10

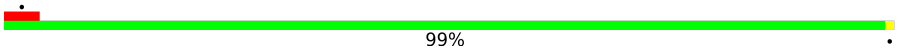
Chain V:

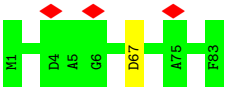




- Molecule 37: 40S ribosomal protein S21

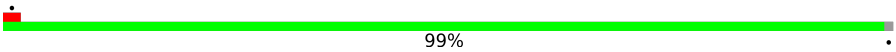
Chain W:

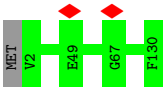




- Molecule 38: uS8

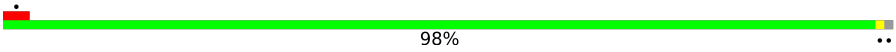
Chain X:

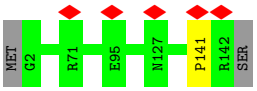




- Molecule 39: uS12

Chain Y:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60578	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	70.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	52000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.033	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	380.0, 380.0, 380.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GTP, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	2	0.28	0/40102	1.01	169/62495 (0.3%)
2	Z	0.32	0/1028	0.62	1/1366 (0.1%)
3	A	0.28	0/833	0.69	0/1114
4	a	0.30	0/620	0.66	0/831
5	B	0.27	0/1747	0.56	0/2374
6	b	0.28	0/828	0.65	0/1109
7	C	0.27	0/1756	0.56	0/2350
8	c	0.27	0/665	0.62	0/891
9	D	0.29	0/1753	0.66	1/2369 (0.0%)
10	d	0.29	0/532	0.73	0/712
11	E	0.26	0/1796	0.60	0/2417
12	e	0.27	0/470	0.58	0/623
13	F	0.29	0/2118	0.63	1/2849 (0.0%)
14	f	0.27	0/462	0.68	0/607
15	G	0.29	0/1531	0.67	2/2059 (0.1%)
16	g	0.25	0/567	0.54	0/753
17	H	0.27	0/1946	0.63	1/2590 (0.0%)
18	h	0.26	0/2493	0.56	0/3394
19	I	0.29	0/1510	0.65	1/2022 (0.0%)
20	i	0.16	0/1795	0.75	0/2798
21	J	0.26	0/1715	0.61	1/2287 (0.0%)
22	n	0.29	0/240	0.88	0/305
23	K	0.30	0/1550	0.68	0/2069
24	x	0.30	0/5047	0.66	4/6803 (0.1%)
25	L	0.27	0/834	0.59	0/1125
26	z	0.34	2/6161 (0.0%)	0.93	14/9604 (0.1%)
27	M	0.29	0/1254	0.61	0/1677
28	N	0.28	0/918	0.58	0/1233
29	O	0.29	0/1226	0.60	0/1649
30	P	0.30	0/1029	0.68	2/1380 (0.1%)
31	Q	0.27	0/1017	0.66	0/1358
32	R	0.29	0/1146	0.65	0/1534

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	S	0.30	0/1082	0.75	1/1452 (0.1%)
34	T	0.27	0/1208	0.63	0/1618
35	U	0.26	0/1115	0.56	0/1493
36	V	0.25	0/805	0.68	0/1081
37	W	0.32	0/643	0.77	1/860 (0.1%)
38	X	0.30	0/1051	0.66	0/1406
39	Y	0.27	0/1116	0.62	1/1490 (0.1%)
All	All	0.29	2/93709 (0.0%)	0.85	200/136147 (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
36	V	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	z	336	U	O3'-P	9.74	1.72	1.61
26	z	346	G	C1'-N9	-6.91	1.37	1.46

The worst 5 of 200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1752	C	C2-N1-C1'	13.46	133.61	118.80
1	2	1752	C	N1-C2-O2	13.27	126.86	118.90
1	2	1309	C	N1-C2-O2	11.06	125.54	118.90
1	2	1852	C	N3-C2-O2	-10.52	114.54	121.90
1	2	1752	C	N3-C2-O2	-10.10	114.83	121.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	V	81	GLN	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Z	122/131 (93%)	118 (97%)	4 (3%)	0	100	100
3	A	100/144 (69%)	89 (89%)	11 (11%)	0	100	100
4	a	75/124 (60%)	73 (97%)	2 (3%)	0	100	100
5	B	215/295 (73%)	202 (94%)	13 (6%)	0	100	100
6	b	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
7	C	211/264 (80%)	203 (96%)	8 (4%)	0	100	100
8	c	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
9	D	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
10	d	65/69 (94%)	57 (88%)	8 (12%)	0	100	100
11	E	226/281 (80%)	220 (97%)	6 (3%)	0	100	100
12	e	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
13	F	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
14	f	55/133 (41%)	45 (82%)	10 (18%)	0	100	100
15	G	189/204 (93%)	180 (95%)	9 (5%)	0	100	100
16	g	66/188 (35%)	64 (97%)	2 (3%)	0	100	100
17	H	235/249 (94%)	227 (97%)	8 (3%)	0	100	100
18	h	311/317 (98%)	289 (93%)	22 (7%)	0	100	100
19	I	181/432 (42%)	174 (96%)	7 (4%)	0	100	100
21	J	204/208 (98%)	191 (94%)	13 (6%)	0	100	100
22	n	23/25 (92%)	23 (100%)	0	0	100	100
23	K	183/194 (94%)	173 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	x	625/627 (100%)	577 (92%)	48 (8%)	0	100	100
25	L	94/149 (63%)	86 (92%)	8 (8%)	0	100	100
27	M	149/158 (94%)	144 (97%)	5 (3%)	0	100	100
28	N	115/132 (87%)	106 (92%)	9 (8%)	0	100	100
29	O	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
30	P	134/168 (80%)	126 (94%)	8 (6%)	0	100	100
31	Q	118/145 (81%)	111 (94%)	7 (6%)	0	100	100
32	R	140/172 (81%)	134 (96%)	6 (4%)	0	100	100
33	S	130/135 (96%)	115 (88%)	15 (12%)	0	100	100
34	T	142/152 (93%)	137 (96%)	5 (4%)	0	100	100
35	U	139/145 (96%)	133 (96%)	6 (4%)	0	100	100
36	V	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
37	W	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
38	X	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
39	Y	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
All	All	5551/6592 (84%)	5251 (95%)	300 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	107/113 (95%)	107 (100%)	0	100	100
3	A	87/123 (71%)	86 (99%)	1 (1%)	73	84
4	a	68/102 (67%)	67 (98%)	1 (2%)	65	80
5	B	180/245 (74%)	179 (99%)	1 (1%)	86	91
6	b	88/88 (100%)	88 (100%)	0	100	100
7	C	194/231 (84%)	194 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	c	75/76 (99%)	75 (100%)	0	100	100
9	D	187/187 (100%)	187 (100%)	0	100	100
10	d	60/62 (97%)	58 (97%)	2 (3%)	38	63
11	E	190/232 (82%)	189 (100%)	1 (0%)	88	93
12	e	48/49 (98%)	48 (100%)	0	100	100
13	F	224/225 (100%)	224 (100%)	0	100	100
14	f	47/106 (44%)	47 (100%)	0	100	100
15	G	161/170 (95%)	161 (100%)	0	100	100
16	g	61/154 (40%)	60 (98%)	1 (2%)	62	79
17	H	207/218 (95%)	206 (100%)	1 (0%)	88	93
18	h	272/275 (99%)	272 (100%)	0	100	100
19	I	165/360 (46%)	162 (98%)	3 (2%)	59	77
21	J	178/180 (99%)	177 (99%)	1 (1%)	86	91
22	n	24/24 (100%)	24 (100%)	0	100	100
23	K	161/168 (96%)	160 (99%)	1 (1%)	86	91
24	x	552/552 (100%)	550 (100%)	2 (0%)	91	94
25	L	87/125 (70%)	86 (99%)	1 (1%)	73	84
27	M	136/142 (96%)	135 (99%)	1 (1%)	84	90
28	N	99/108 (92%)	98 (99%)	1 (1%)	76	86
29	O	130/131 (99%)	130 (100%)	0	100	100
30	P	106/130 (82%)	105 (99%)	1 (1%)	78	87
31	Q	109/130 (84%)	108 (99%)	1 (1%)	78	87
32	R	117/140 (84%)	116 (99%)	1 (1%)	78	87
33	S	119/121 (98%)	119 (100%)	0	100	100
34	T	125/132 (95%)	125 (100%)	0	100	100
35	U	111/116 (96%)	110 (99%)	1 (1%)	78	87
36	V	92/107 (86%)	91 (99%)	1 (1%)	73	84
37	W	67/67 (100%)	67 (100%)	0	100	100
38	X	112/113 (99%)	112 (100%)	0	100	100
39	Y	113/115 (98%)	113 (100%)	0	100	100
All	All	4859/5617 (86%)	4836 (100%)	23 (0%)	89	93

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	x	855	ARG
28	N	99	LYS
27	M	69	ARG
30	P	150	ARG
16	g	116	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
12	e	5	GLN
24	x	655	GLN
30	P	94	HIS
33	S	31	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1669/1870 (89%)	342 (20%)	7 (0%)
20	i	74/75 (98%)	15 (20%)	0
26	z	256/400 (64%)	66 (25%)	0
All	All	1999/2345 (85%)	423 (21%)	7 (0%)

5 of 423 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	26	U
1	2	33	G
1	2	37	C

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1204	G
1	2	1308	U
1	2	1759	G
1	2	1395	C
1	2	561	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
41	GTP	x	1301	43,42	26,34,34	1.09	2 (7%)	32,54,54	1.69	10 (31%)

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
41	GTP	x	1301	43,42	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	x	1301	GTP	C5-C6	-3.87	1.39	1.47
41	x	1301	GTP	C8-N7	2.05	1.38	1.35

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	x	1301	GTP	C5-C6-N1	3.46	120.06	113.95
41	x	1301	GTP	N2-C2-N1	3.16	123.44	116.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	x	1301	GTP	O4'-C1'-C2'	-3.06	102.45	106.93
41	x	1301	GTP	C8-N7-C5	2.84	108.40	102.99
41	x	1301	GTP	N1-C2-N3	-2.62	118.42	123.32

There are no chirality outliers.

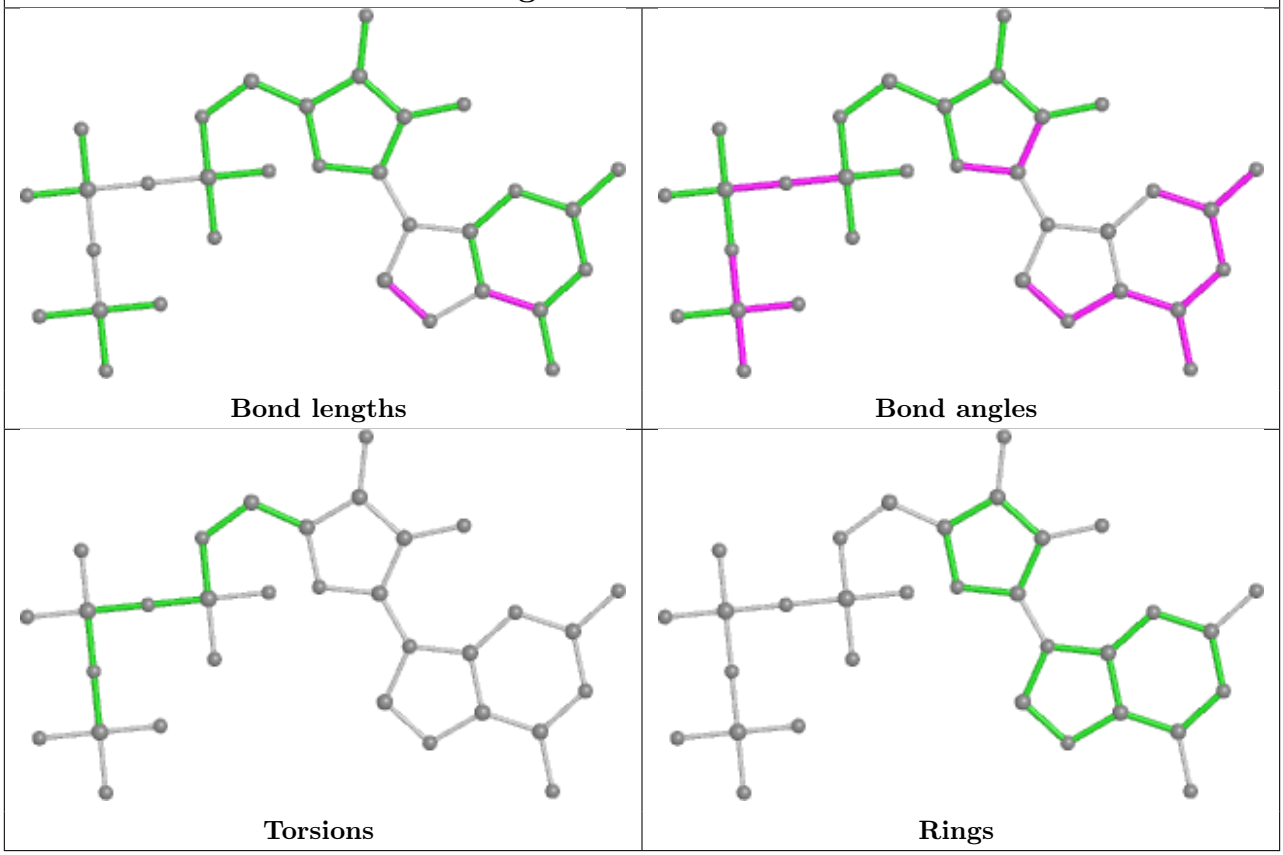
There are no torsion outliers.

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.

Ligand GTP x 1301



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.

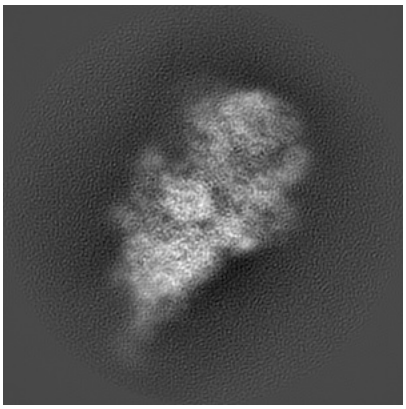
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-25542. These allow visual inspection of the internal detail of the map and identification of artifacts.

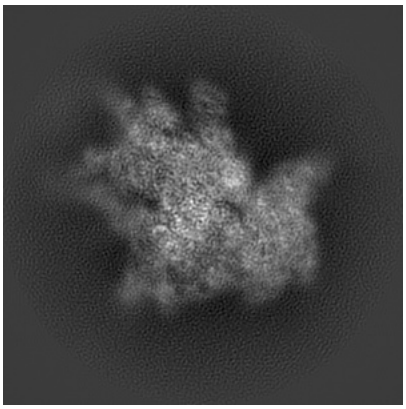
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

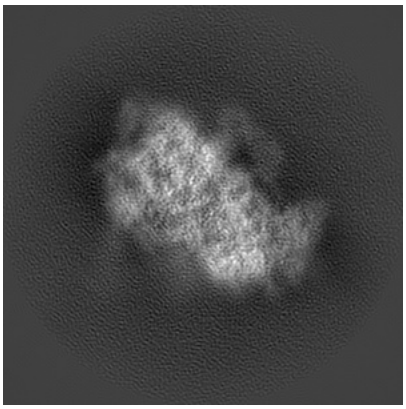
6.1.1 Primary map



X

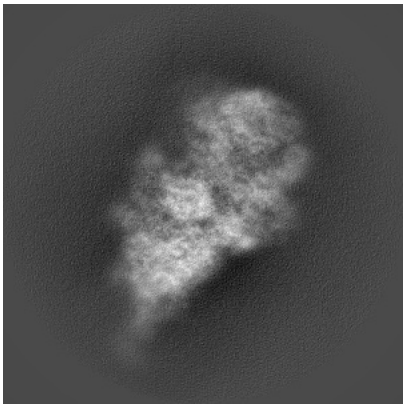


Y

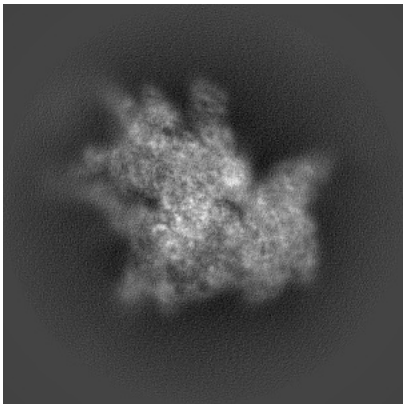


Z

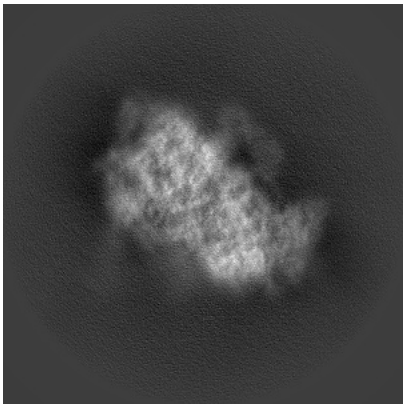
6.1.2 Raw map



X



Y

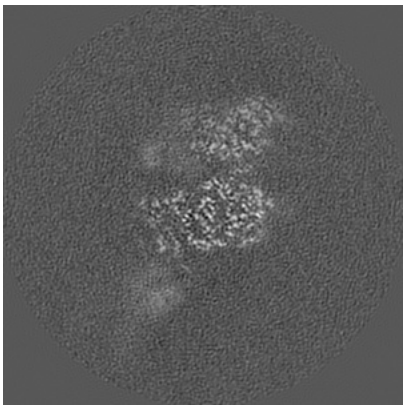


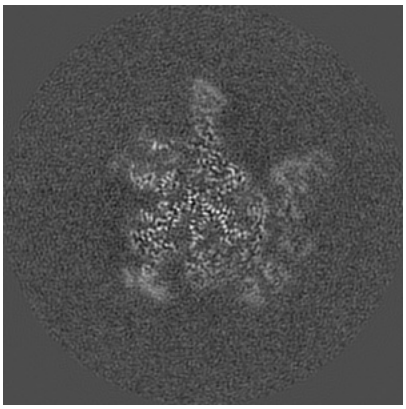
Z

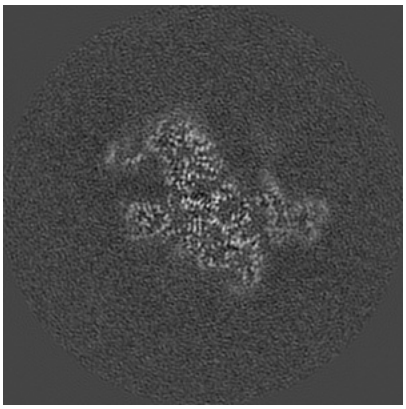
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

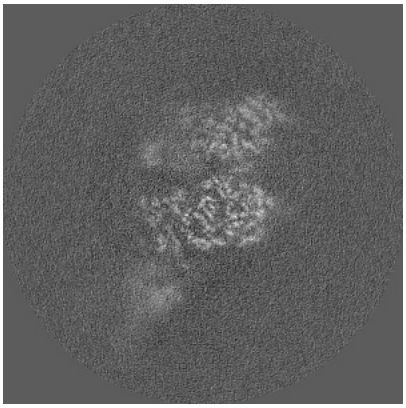
6.2.1 Primary map


X Index: 200


Y Index: 200


Z Index: 200

6.2.2 Raw map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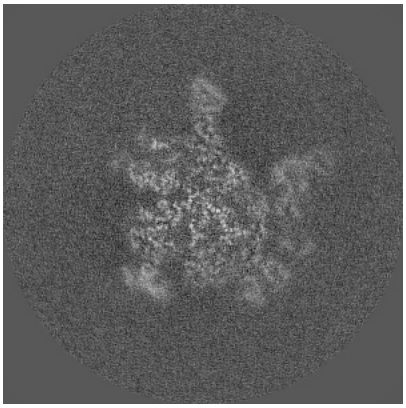
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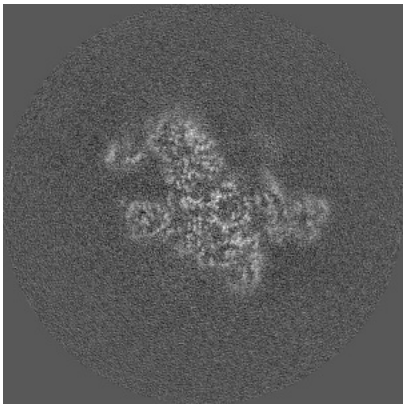
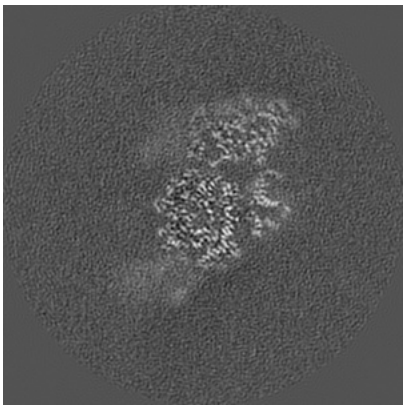
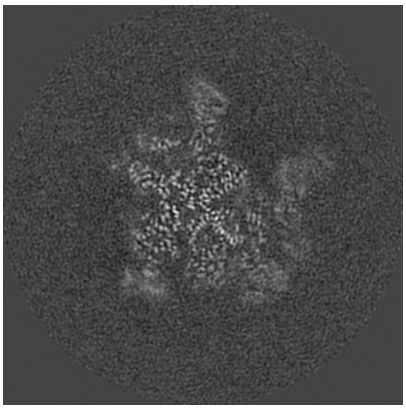

Z Index: 200

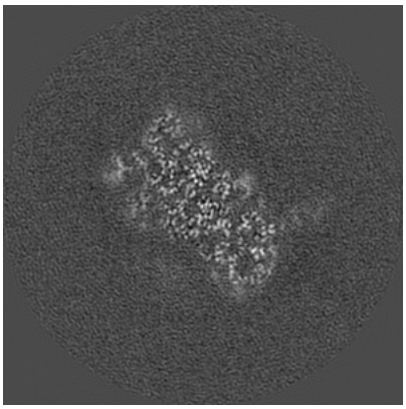
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

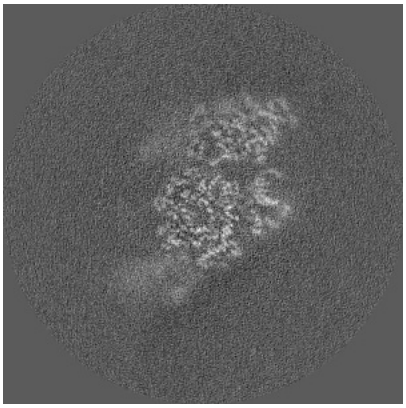
6.3.1 Primary map

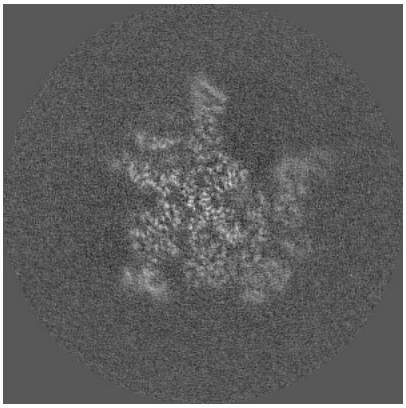

X Index: 188

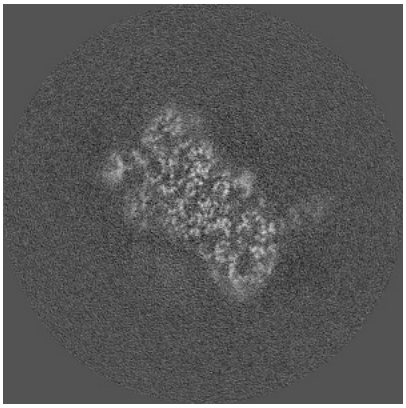

Y Index: 197


Z Index: 186

6.3.2 Raw map


X Index: 188

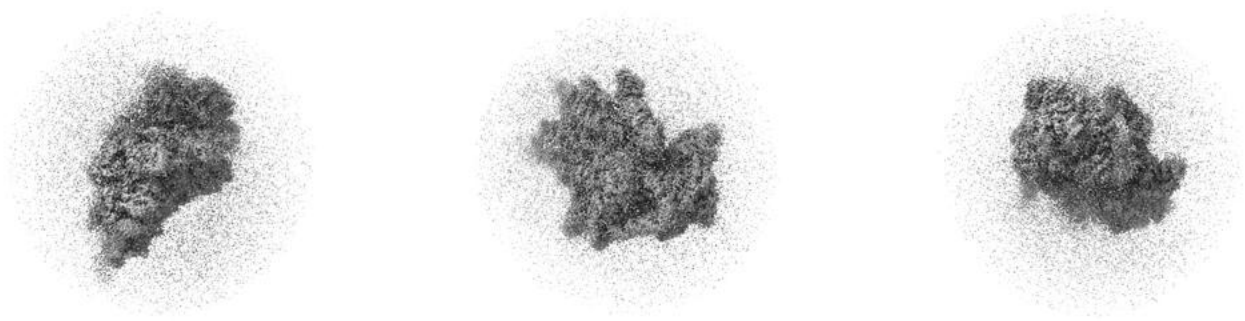

Y Index: 198


Z Index: 186

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

6.4 Orthogonal surface views (i)

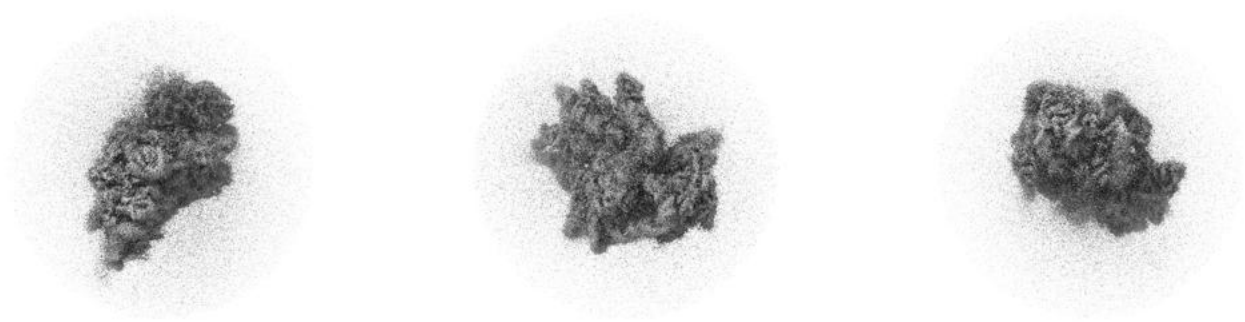
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

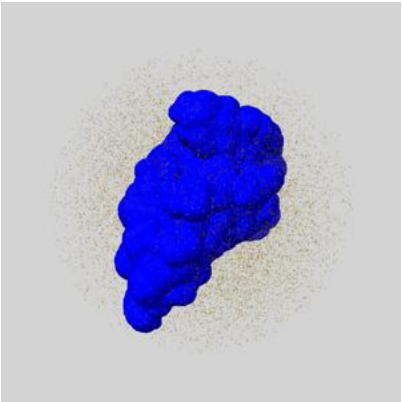
6.5 Mask visualisation (i)

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

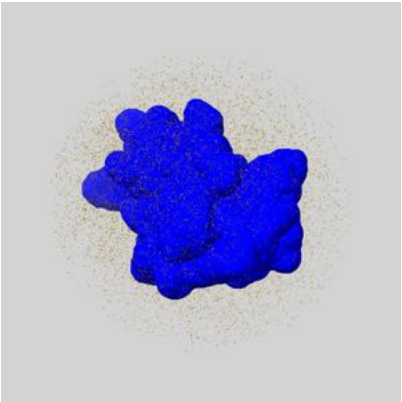
A mask typically either:

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

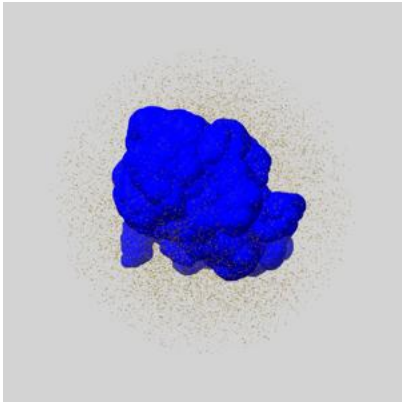
6.5.1 emd_25542_msk_1.map (i)



X



Y

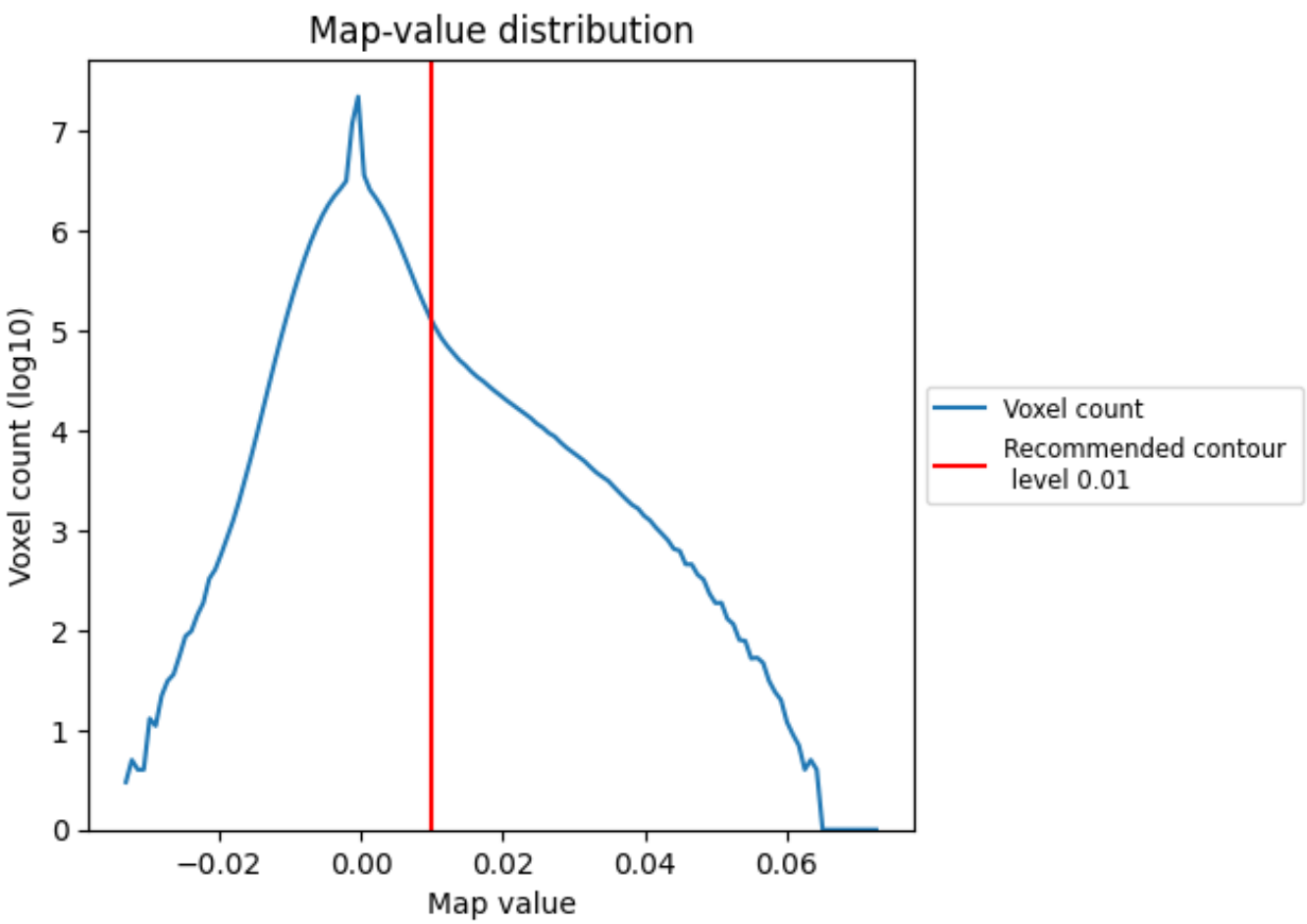


Z

7 Map analysis (i)

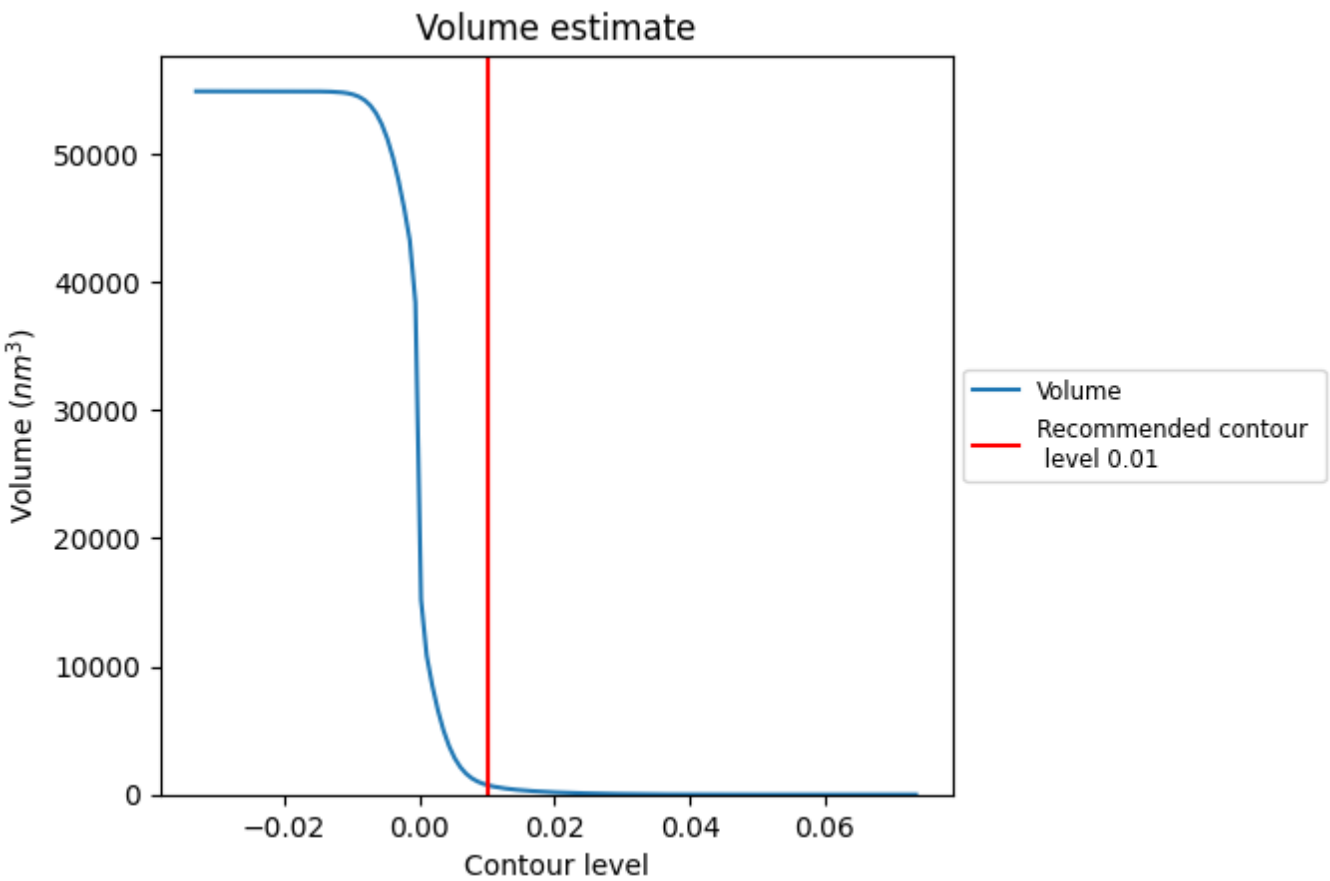
This section contains the results of statistical analysis of the map.

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.

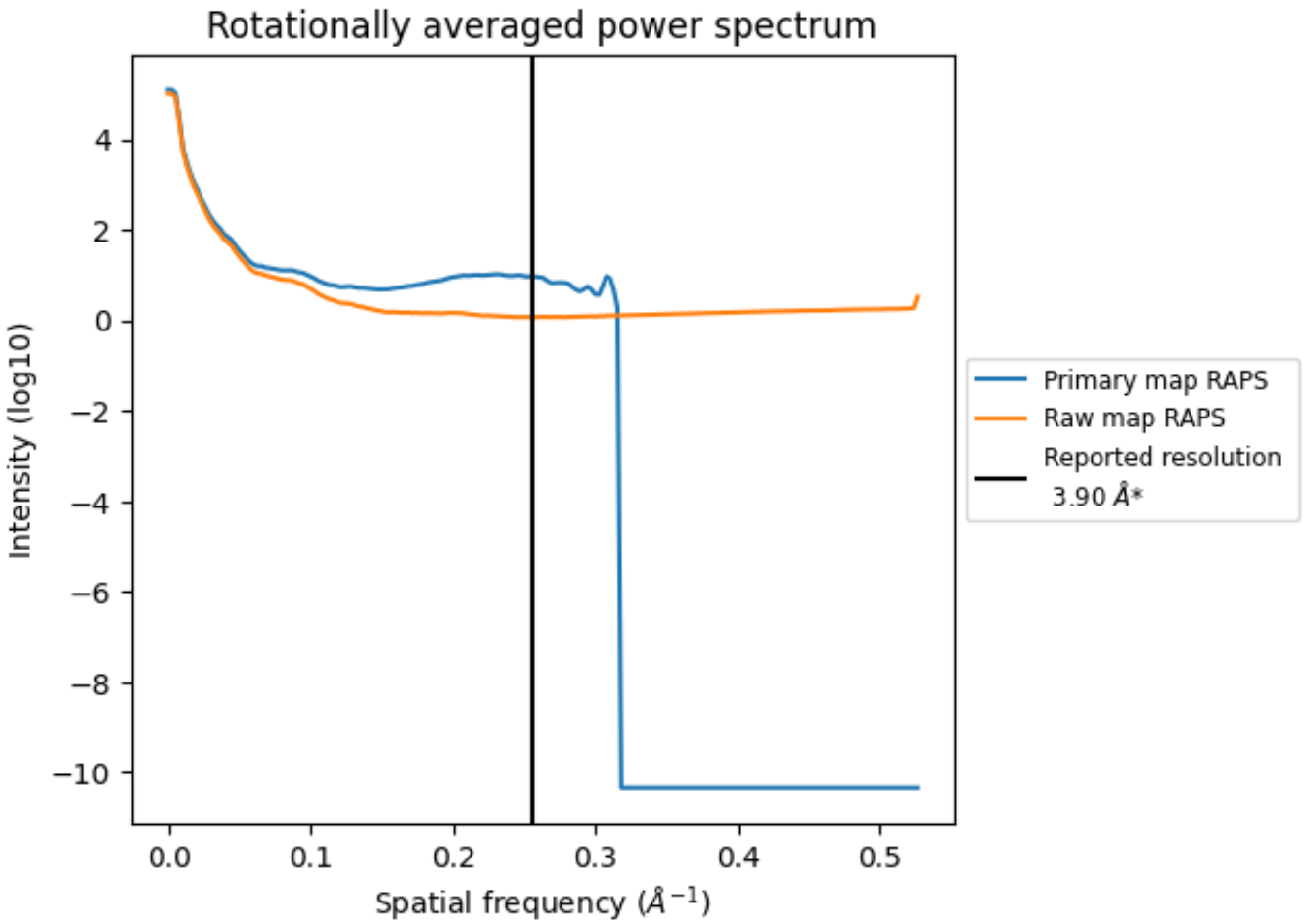
7.2 Volume estimate (i)



The volume at the recommended contour level is 753 nm^3; this corresponds to an approximate mass of 680 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)

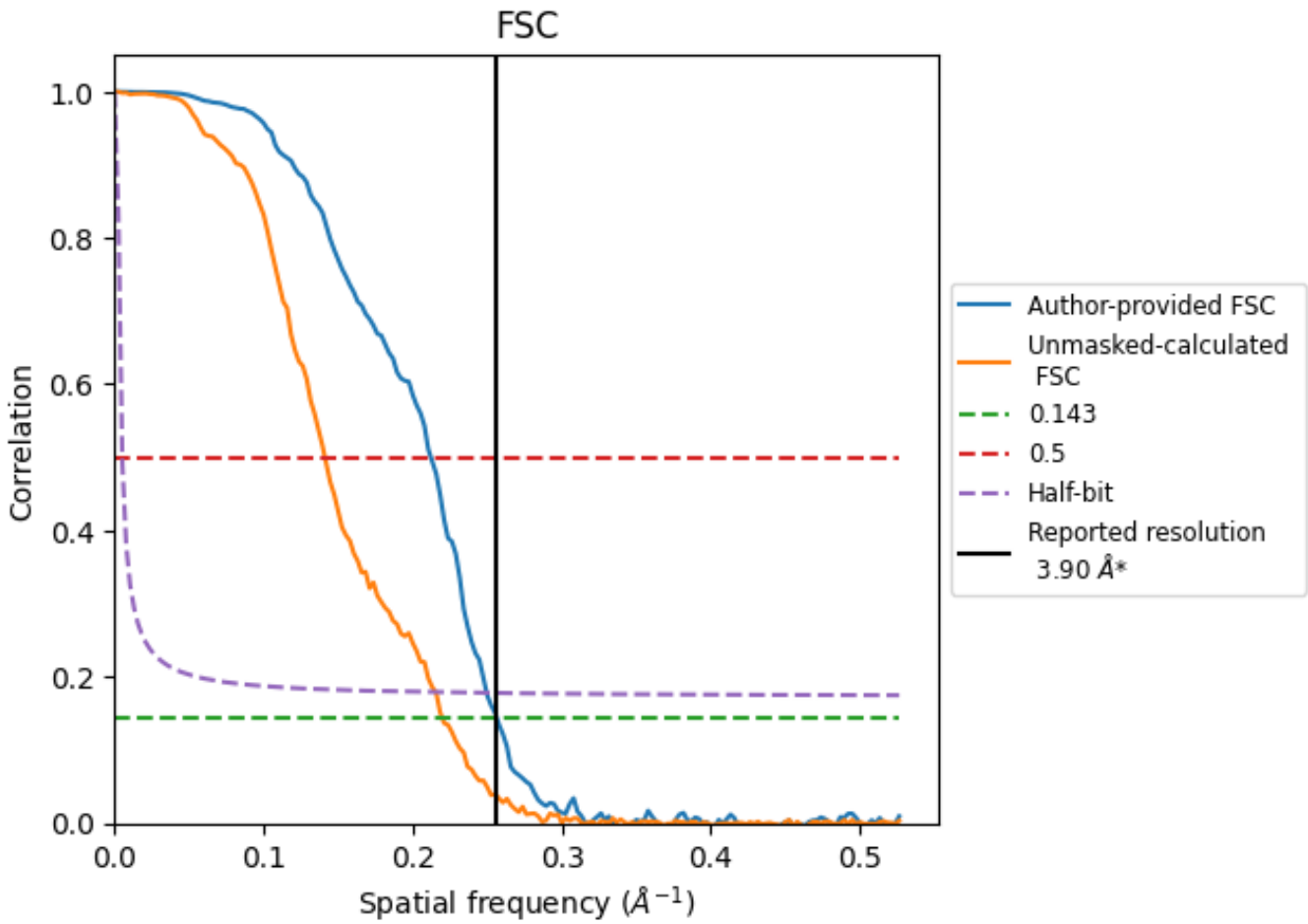


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

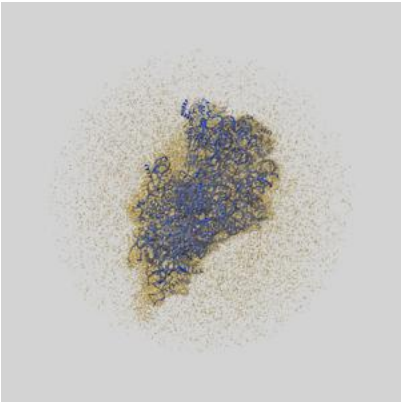
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.90	4.71	4.01
Unmasked-calculated*	4.55	7.09	4.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.55 differs from the reported value 3.9 by more than 10 %

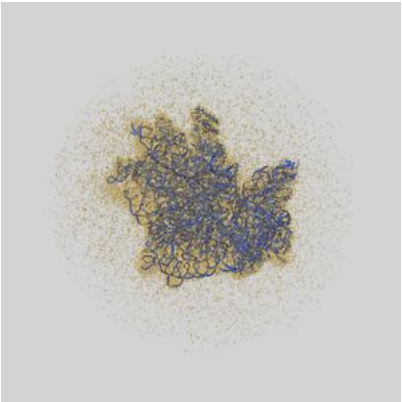
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-25542 and PDB model 7SYV. Per-residue inclusion information can be found in section 3 on page 13.

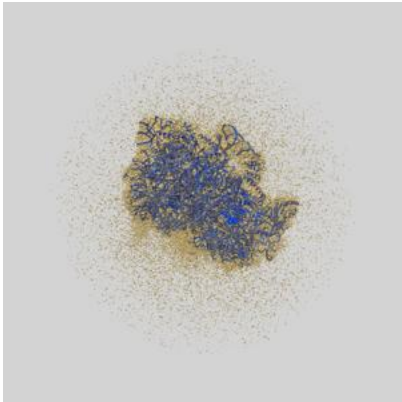
9.1 Map-model overlay (i)



X



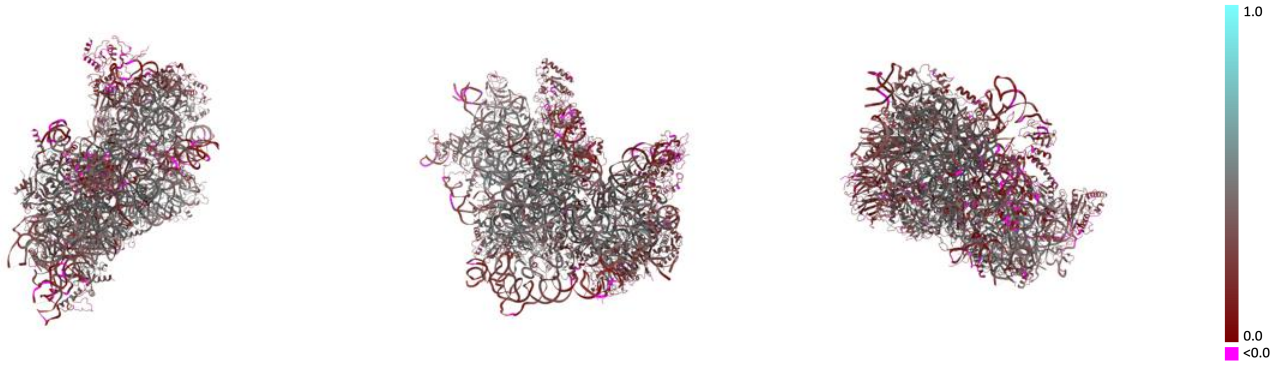
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

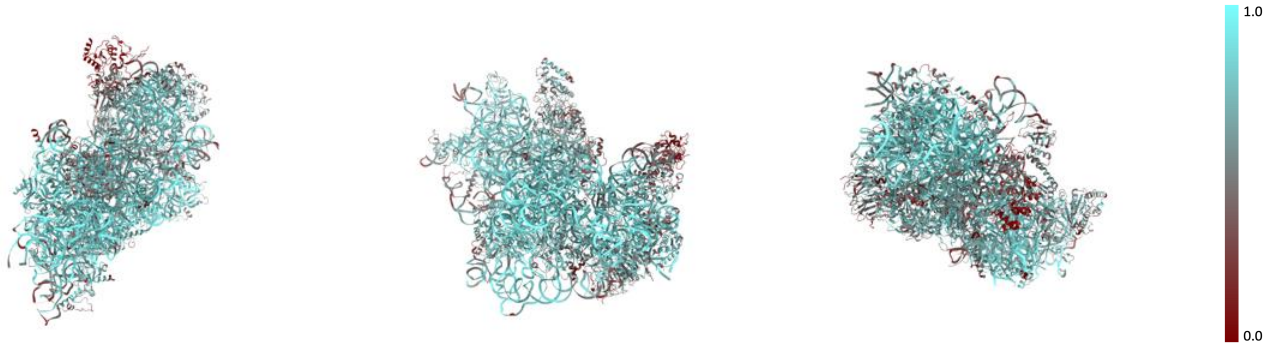
9.2 Q-score mapped to coordinate model (i)



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.

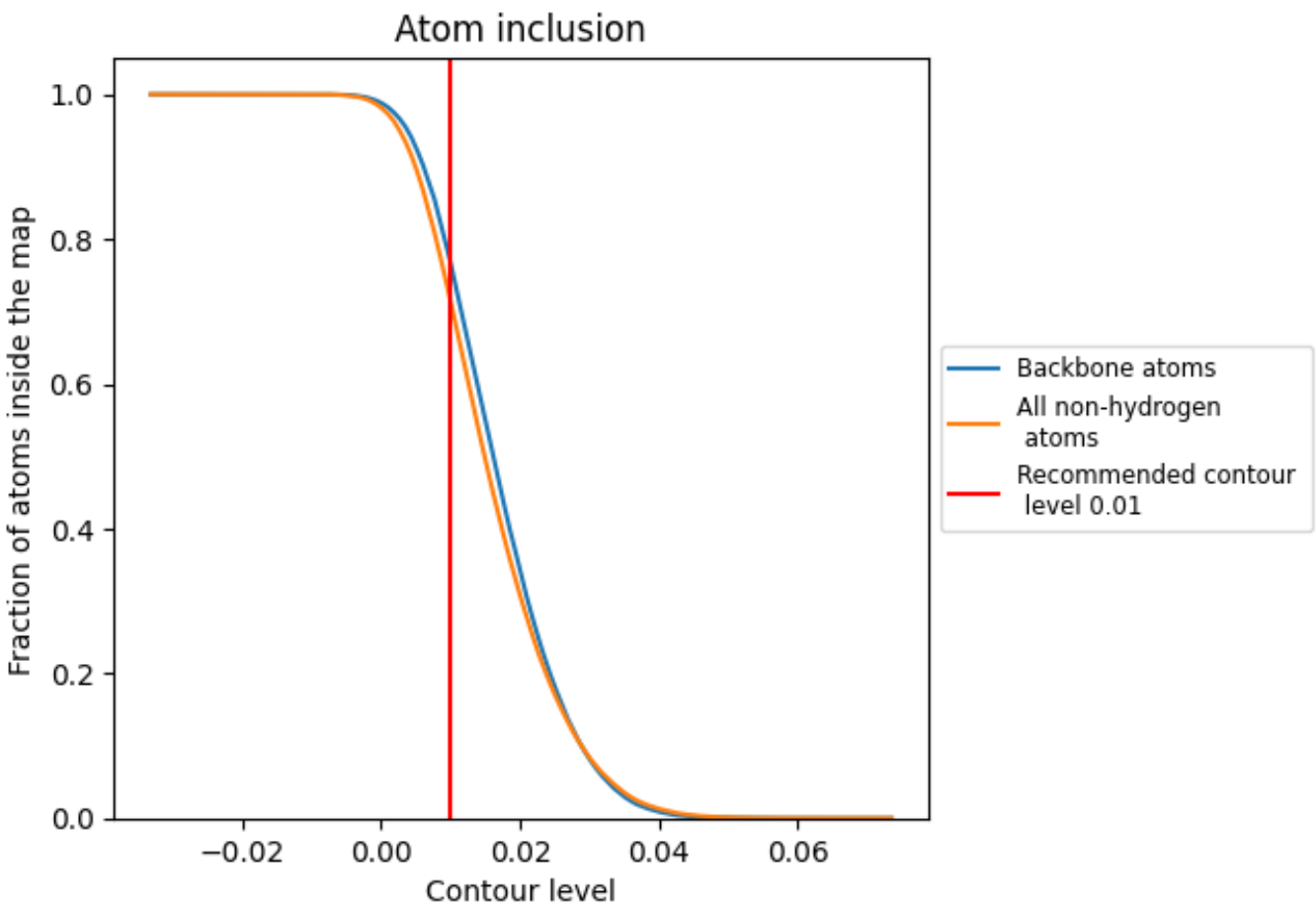
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 72% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7169	0.3470
2	0.8341	0.3850
A	0.4782	0.3010
B	0.7010	0.3830
C	0.7522	0.4010
D	0.7352	0.4140
E	0.5391	0.3070
F	0.7570	0.4050
G	0.7132	0.4020
H	0.6631	0.3060
I	0.5277	0.3110
J	0.7363	0.3800
K	0.7495	0.4070
L	0.4304	0.2220
M	0.7254	0.4160
N	0.0671	0.1230
O	0.7530	0.4120
P	0.7487	0.4060
Q	0.5119	0.2520
R	0.7179	0.3740
S	0.4855	0.2680
T	0.5729	0.3040
U	0.7432	0.3580
V	0.4703	0.2900
W	0.7170	0.3860
X	0.7703	0.4390
Y	0.7488	0.4370
Z	0.7482	0.3840
a	0.6077	0.3330
b	0.7609	0.4290
c	0.6901	0.3860
d	0.6398	0.3950
e	0.6349	0.3160
f	0.4614	0.2170
g	0.0869	0.1120

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Chain	Atom inclusion	Q-score
h	0.4898	0.2460
i	0.6596	0.2240
n	0.6927	0.3870
x	0.5100	0.2160
z	0.7272	0.2570