wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 10:05 pm GMT

PDB ID	:	6FEC
EMDB ID	:	EMD-4242
Title	:	Human cap-dependent 48S pre-initiation complex
Authors	:	Schaffitzel, C.; Schaffitzel, C.
Deposited on	:	2017-12-31
Resolution	:	6.30 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:

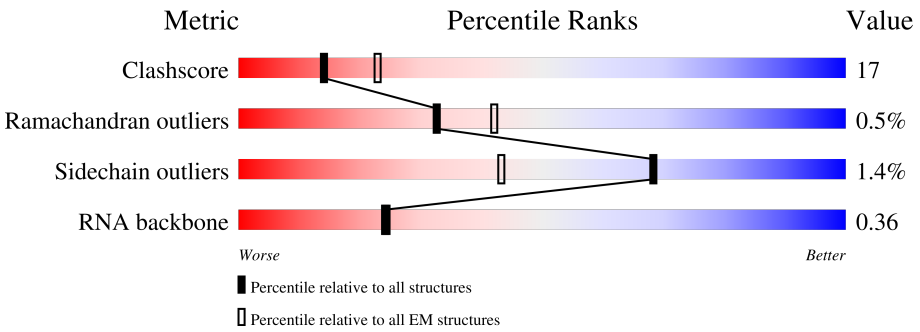
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 6.30 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	1	1362	23% 20% • 56%
2	2	843	40% 25% • 34%
3	3	445	54% 38% • 6%
4	4	364	39% 34% • 25%
5	5	352	7% 56% 34% • 8%
6	6	218	59% 40% •
7	7	564	44% 22% • 34%

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Mol	Chain	Length	Quality of chain
8	8	374	53% 43%
9	9	368	9% 60% 36%
10	A	1776	54% 39% 7%
11	F	26	12% 46% 54%
12	G	158	8% 96%
13	H	141	6% 96%
14	I	263	97%
15	J	53	13% 100%
16	K	182	98%
17	L	137	97%
18	N	75	67% 32%
19	P	266	27% 92% 8%
20	Q	142	6% 99%
21	R	141	99%
22	S	422	27% 98%
23	U	191	6% 96%
24	V	59	97%
25	W	75	97%
26	X	190	93% 6%
27	Y	84	5% 96%
28	Z	150	100%
29	a	129	99%
30	b	82	94% 5%
31	c	226	99%
32	d	17	35% 100%

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Mol	Chain	Length	Quality of chain
33	e	126	7% 97%
34	f	208	95%
35	g	227	97%
36	h	104	98%
37	i	215	97%
38	j	136	98%
39	k	99	97%
40	l	64	98%
41	m	313	98%
42	n	127	93% 6%
43	o	206	97%
44	p	71	7% 90% 10%
45	q	237	97%
46	r	124	96%
47	s	131	98%
48	t	98	95%
49	u	636	11% 88%
50	w	1121	25% 36% 64%

2 Entry composition (i)

There are 51 unique types of molecules in this entry. The entry contains 117189 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 Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	600	4935	3107	893	914	21	0	1

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	558	4529	2842	805	849	33	0	1

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	420	3466	2220	587	639	20	0	1

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	272	2111	1330	359	410	12	0	0

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	324	2624	1654	452	503	15	0	0

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	216	1738	1109	286	330	13	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	166	THR	SER	conflict	UNP Q9UBQ5
6	172	MET	VAL	conflict	UNP Q9UBQ5

- Molecule 7 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	7	373	3110	2010	520	563	17	0	1

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	13	VAL	ALA	conflict	UNP Q9Y262
7	53	ARG	LYS	conflict	UNP Q9Y262
7	117	THR	ALA	conflict	UNP Q9Y262
7	151	ALA	GLU	conflict	UNP Q9Y262
7	430	SER	ASN	conflict	UNP Q9Y262

- Molecule 8 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	8	366	2919	1850	494	558	17	0	1

- Molecule 9 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	9	356	2867	1804	500	548	15	0	0

- Molecule 10 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	A	1776	37881	16910	6782	12414	1775	0	0

- Molecule 11 is a RNA chain called Messenger RNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	F	26	544	245	95	179	25	0	0

- Molecule 12 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	G	158	1296	827	241	221	7	0	0

- Molecule 13 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	H	141	1124	715	212	194	3	0	0

- Molecule 14 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	I	263	2083	1329	385	359	10	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	25	SER	GLY	conflict	UNP P62701
I	51	LYS	ARG	conflict	UNP P62701
I	78	ALA	THR	conflict	UNP P62701
I	156	MET	VAL	conflict	UNP P62701

- Molecule 15 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	J	53	445	278	90	72	5	0	0

- Molecule 16 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	K	182	1499	952	300	245	2	0	0

- Molecule 17 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	L	137	1140	714	231	194	1	0	0

- Molecule 18 is a RNA chain called Transfer RNA (75-MER).

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

- Molecule 19 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	P	266	2147	1354	376	406	11	0	0

- Molecule 20 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Q	142	1107	698	220	185	4	0	0

- Molecule 21 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	R	141	1113	701	213	196	3	0	0

- Molecule 22 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	S	422	3214	2044	561	592	17	0	0

- Molecule 23 is a protein called 40S ribosomal protein S5.

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

- Molecule 24 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	V	59	473	293	104	75	1	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	83	VAL	ALA	conflict	UNP P62861
V	91	LEU	PRO	conflict	UNP P62861
V	102	ARG	LYS	conflict	UNP P62861

- Molecule 25 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	W	75	599	382	111	105	1	0	0

- Molecule 26 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	X	190	1530	975	281	273	1	0	0

- Molecule 27 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Y	84	659	413	122	116	8	0	0

- Molecule 28 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Z	150	1208	773	229	205	1	0	0

- Molecule 29 is a protein called 40S ribosomal protein S15a.

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

- Molecule 30 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	b	82	620	378	117	120	5	0	0

- Molecule 31 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	c	226	1743	1127	300	307	9	0	0

- Molecule 32 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT (eIF2-Beta).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	d	17	147	94	22	30	1	0	0

- Molecule 33 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	e	126	1020	639	188	188	5	0	0

- Molecule 34 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	f	208	1643	1045	289	301	8	0	0

- Molecule 35 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	g	227	1765	1124	317	316	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	195	SER	THR	conflict	UNP P23396

- Molecule 36 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	h	104	822	514	156	148	4	0	0

- Molecule 37 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	i	215	1742	1107	309	311	15	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	136	HIS	ARG	conflict	UNP P61247
i	146	CYS	ARG	conflict	UNP P61247

- Molecule 38 is a protein called 40S ribosomal protein S14.

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

- Molecule 39 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	k	99	790	491	162	131	6	0	0

- Molecule 40 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	l	64	507	308	102	95	2	0	0

- Molecule 41 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	m	313	2437	1535	424	466	12	0	0

- Molecule 42 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	n	127	1061	673	201	180	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	46	SER	ASN	conflict	UNP P62841

- Molecule 43 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	o	206	1680	1054	329	292	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
o	47	GLY	ARG	conflict	UNP P62241

- Molecule 44 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	p	71	582	367	109	99	7	0	0

- Molecule 45 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	q	237	1924	1200	387	330	7	0	0

- Molecule 46 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	r	124	958	600	170	179	9	0	0

- Molecule 47 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	s	131	1065	673	206	181	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
s	41	GLN	ARG	conflict	UNP P62847

- Molecule 48 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	t	98	828	539	148	135	6	0	0

- Molecule 49 is a protein called Eukaryotic translation initiation factor 4B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	u	76	608	385	104	119	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	-119	MET	-	initiating methionine	UNP P23588
u	-118	SER	-	expression tag	UNP P23588
u	-117	TYR	-	expression tag	UNP P23588
u	-116	TYR	-	expression tag	UNP P23588
u	-115	HIS	-	expression tag	UNP P23588
u	-114	HIS	-	expression tag	UNP P23588
u	-113	HIS	-	expression tag	UNP P23588
u	-112	HIS	-	expression tag	UNP P23588
u	-111	HIS	-	expression tag	UNP P23588
u	-110	HIS	-	expression tag	UNP P23588
u	-109	ASP	-	expression tag	UNP P23588
u	-108	TYR	-	expression tag	UNP P23588
u	-107	ASP	-	expression tag	UNP P23588
u	-106	ILE	-	expression tag	UNP P23588
u	-105	PRO	-	expression tag	UNP P23588
u	-104	THR	-	expression tag	UNP P23588
u	-103	THR	-	expression tag	UNP P23588
u	-102	GLU	-	expression tag	UNP P23588
u	-101	ASN	-	expression tag	UNP P23588
u	-100	LEU	-	expression tag	UNP P23588
u	-99	TYR	-	expression tag	UNP P23588
u	-98	PRO	-	expression tag	UNP P23588
u	-97	GLN	-	expression tag	UNP P23588
u	-96	GLY	-	expression tag	UNP P23588

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Chain	Residue	Modelled	Actual	Comment	Reference
u	-95	ALA	-	expression tag	UNP P23588

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	w	403	3308	2132	573	587	16	0	0

- Molecule 51 is water.

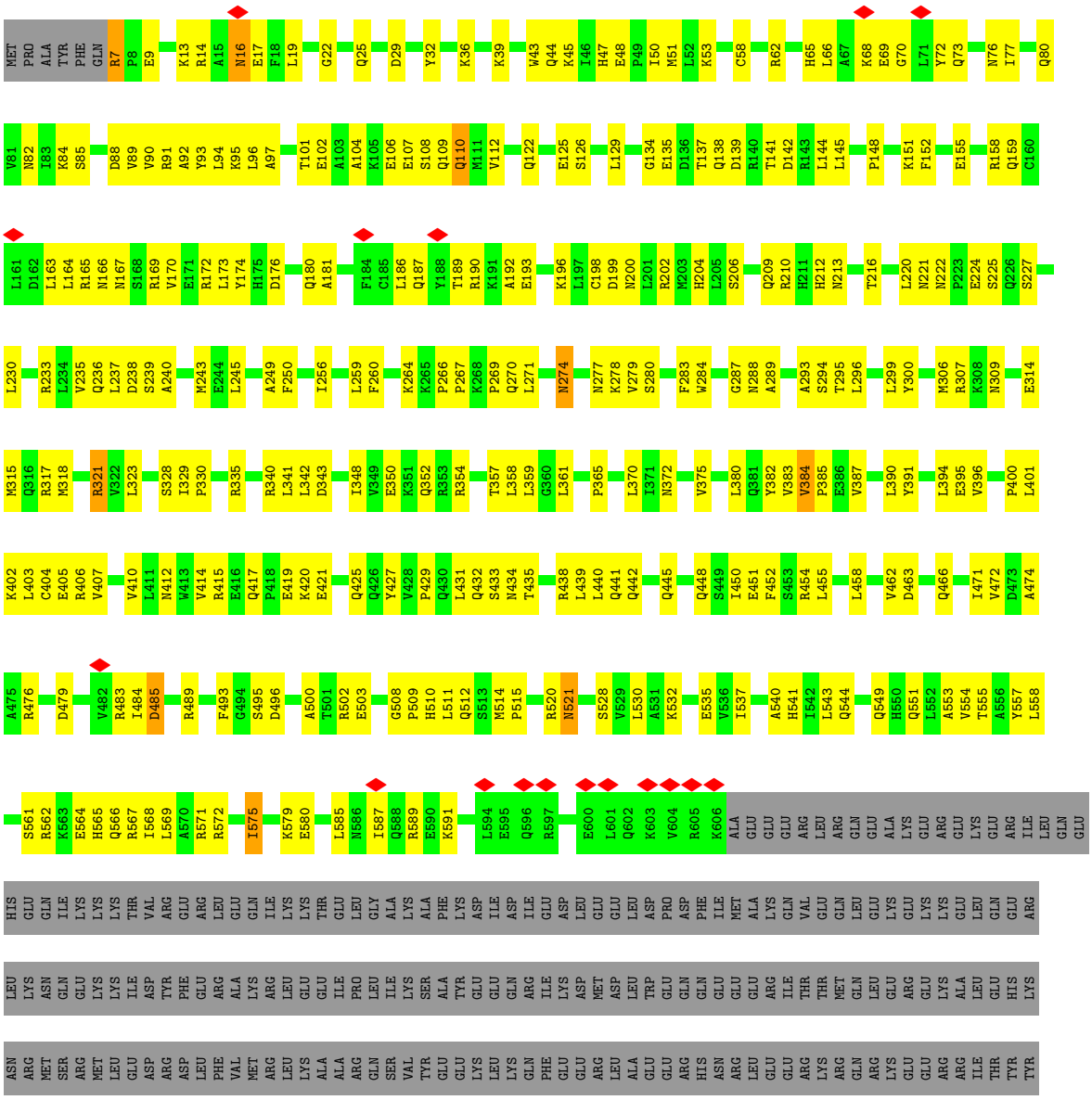
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
51	1	1	1	1	0
51	9	376	376	376	0
51	A	6	6	6	0
51	H	5	5	5	0
51	U	13	13	13	0
51	j	1	1	1	0
51	l	8	8	8	0
51	m	5	5	5	0

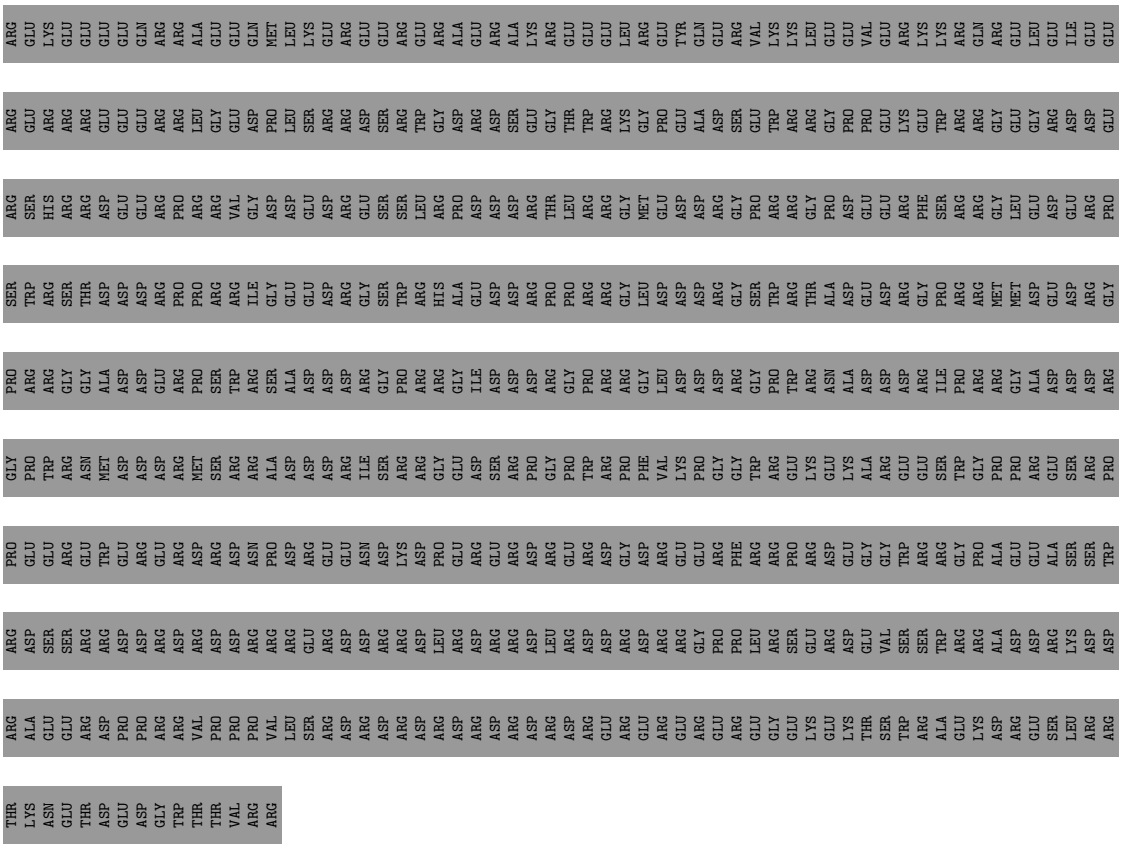
3 Residue-property plots (i)

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: Eukaryotic translation initiation factor 3 subunit A

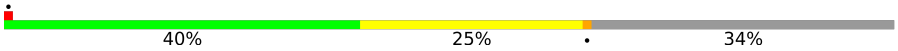
Chain 1: 23% 20% 56%

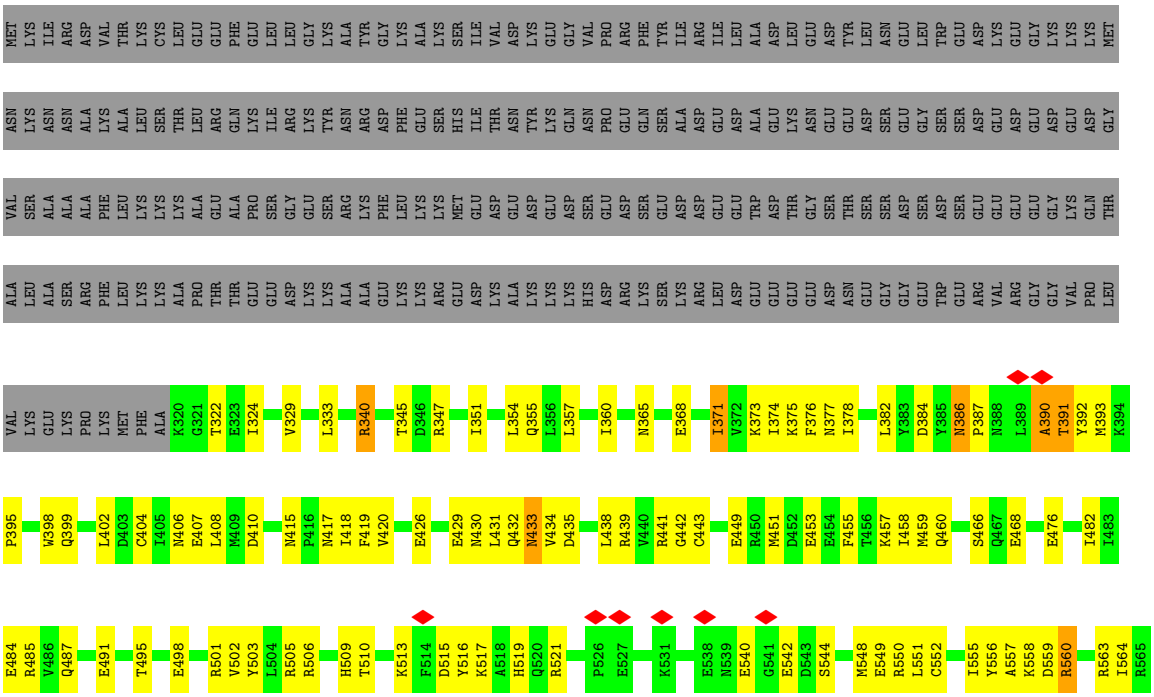


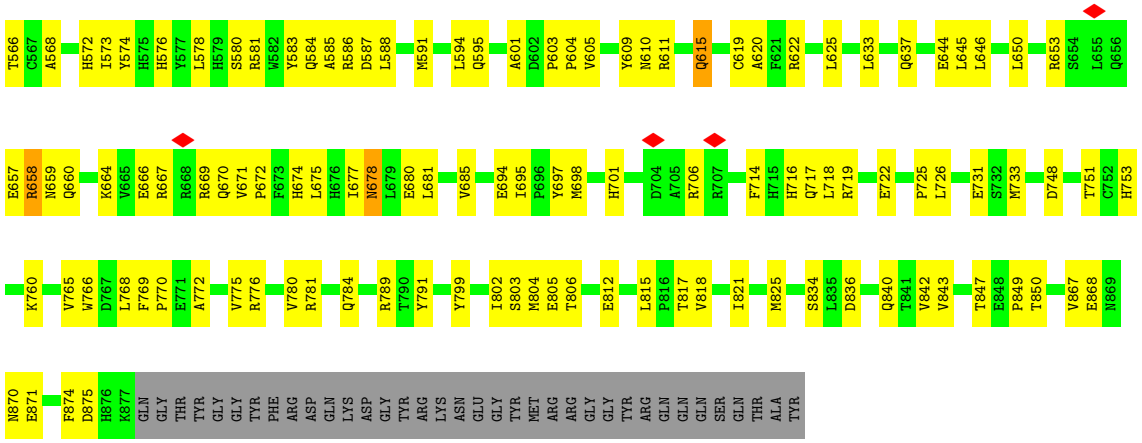


- Molecule 2: Eukaryotic translation initiation factor 3 subunit C

Chain 2:

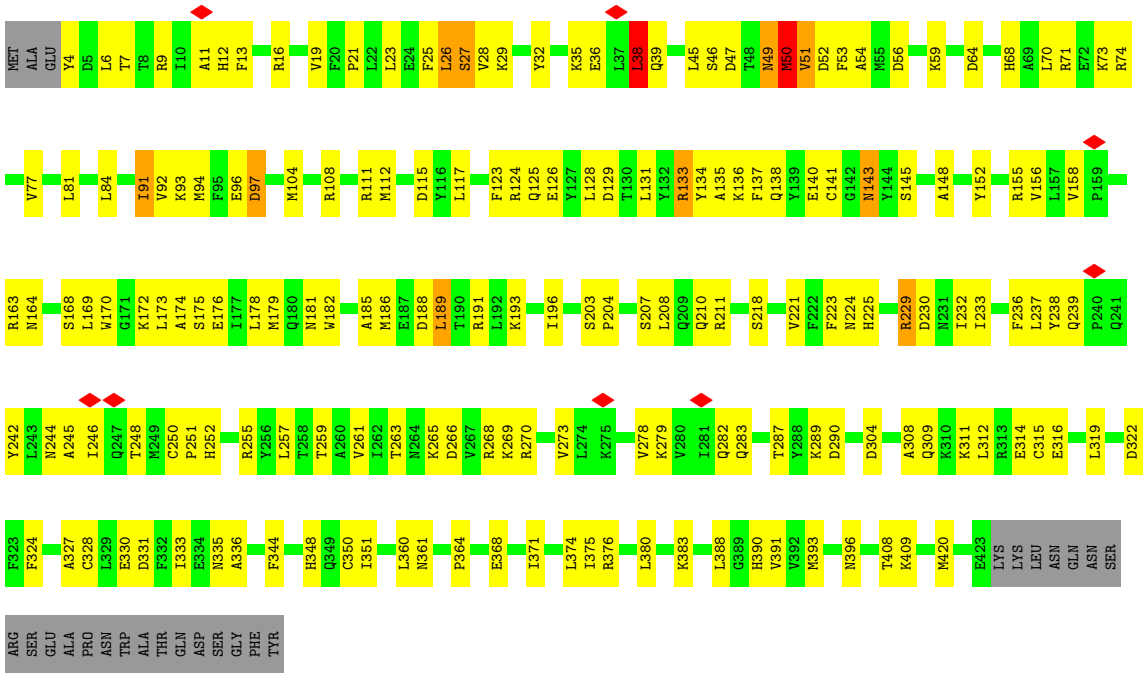






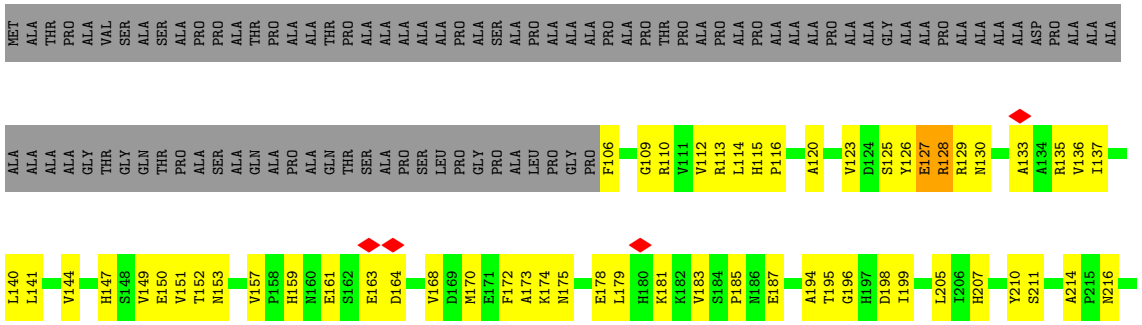
• Molecule 3: Eukaryotic translation initiation factor 3 subunit E

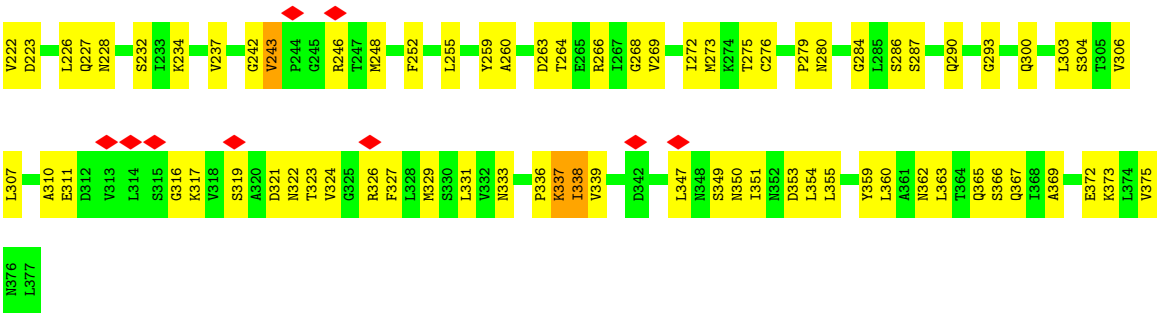
Chain 3:



• Molecule 4: Eukaryotic translation initiation factor 3 subunit F

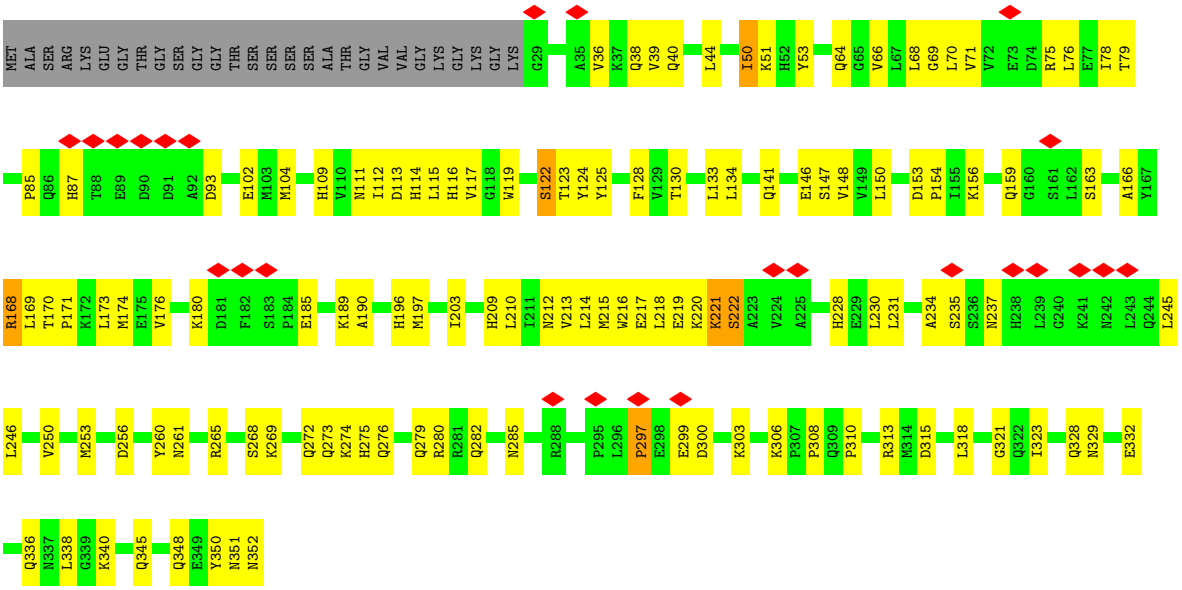
Chain 4:





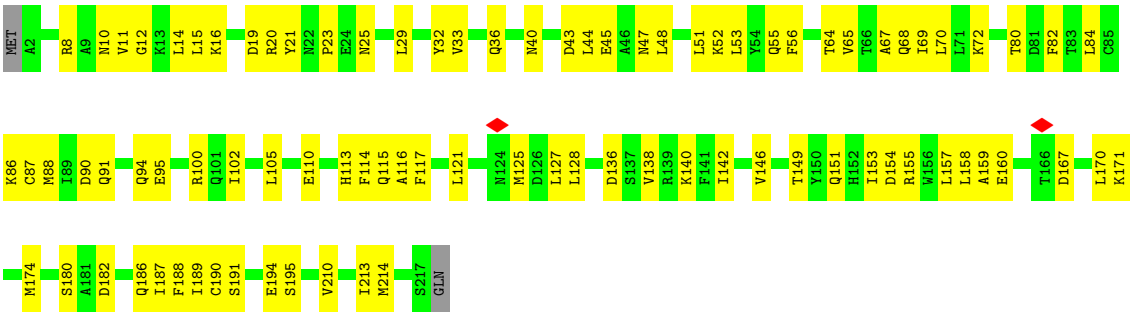
- Molecule 5: Eukaryotic translation initiation factor 3 subunit H

Chain 5:



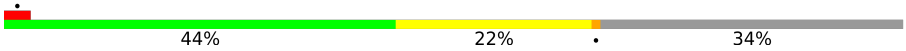
- Molecule 6: Eukaryotic translation initiation factor 3 subunit K

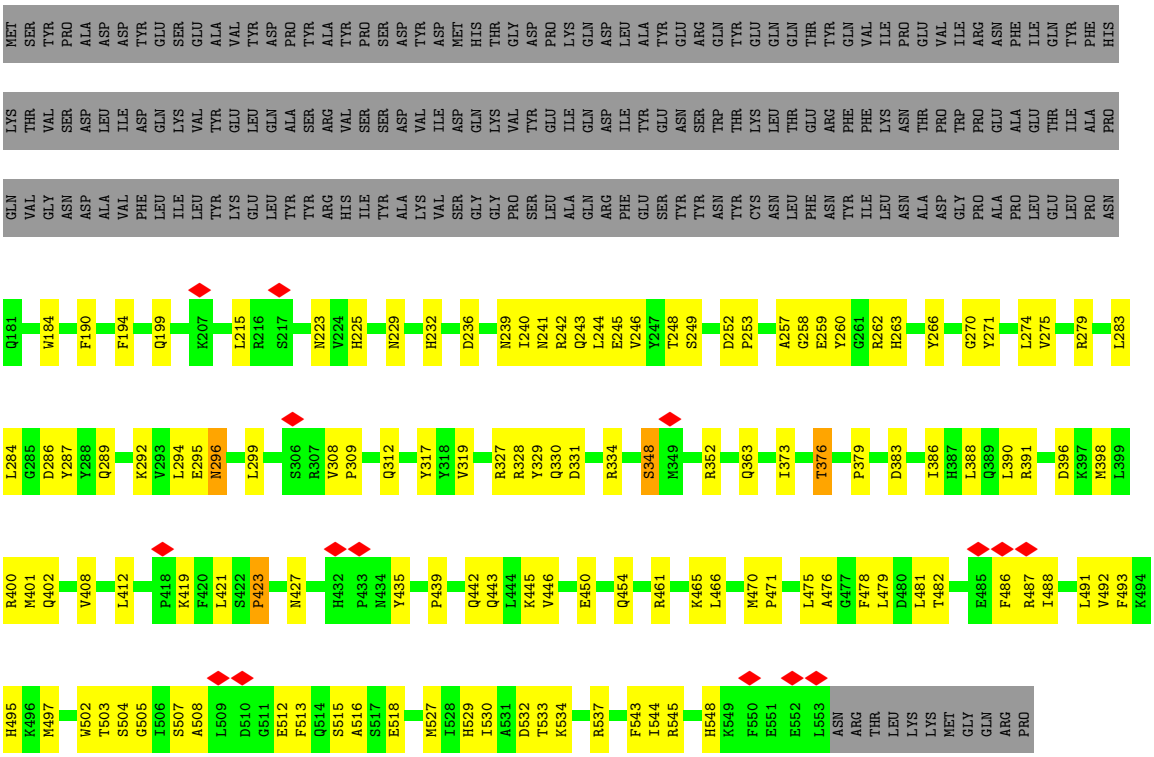
Chain 6:



- Molecule 7: Eukaryotic translation initiation factor 3 subunit L

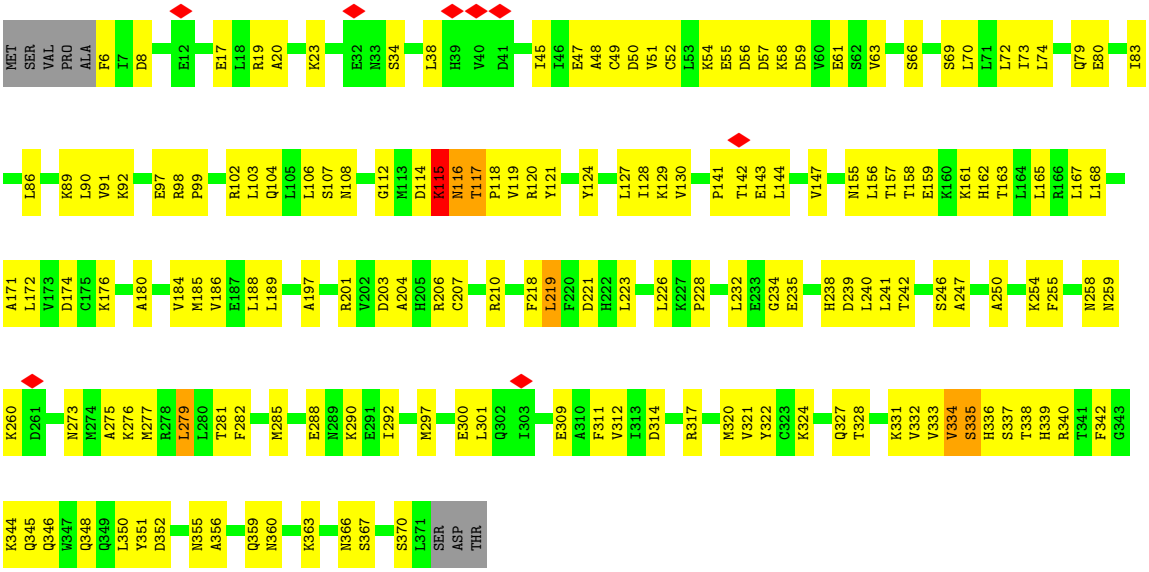
Chain 7:





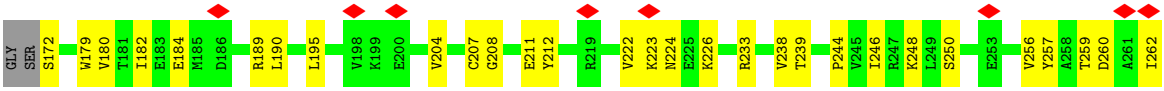
• Molecule 8: Eukaryotic translation initiation factor 3 subunit M

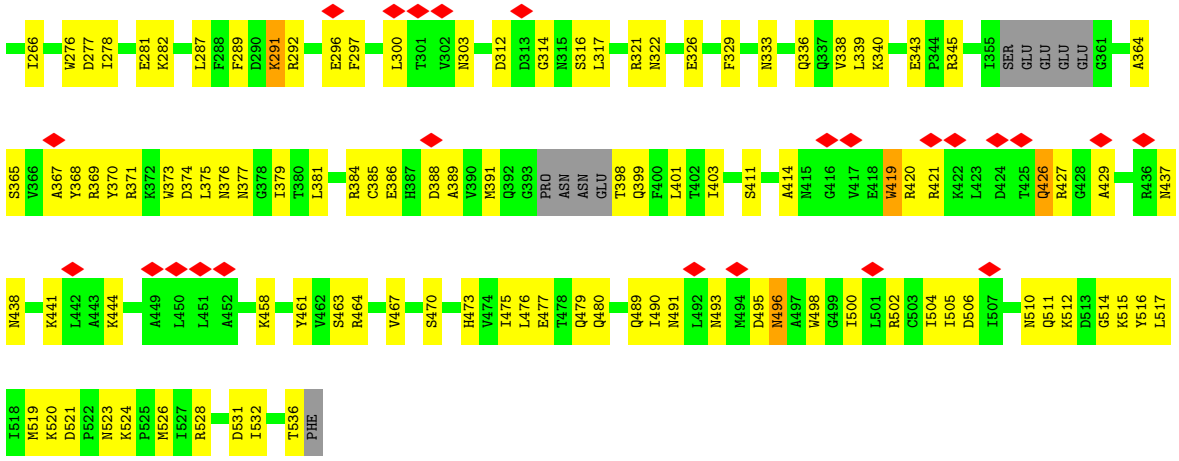
Chain 8:



• Molecule 9: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT D

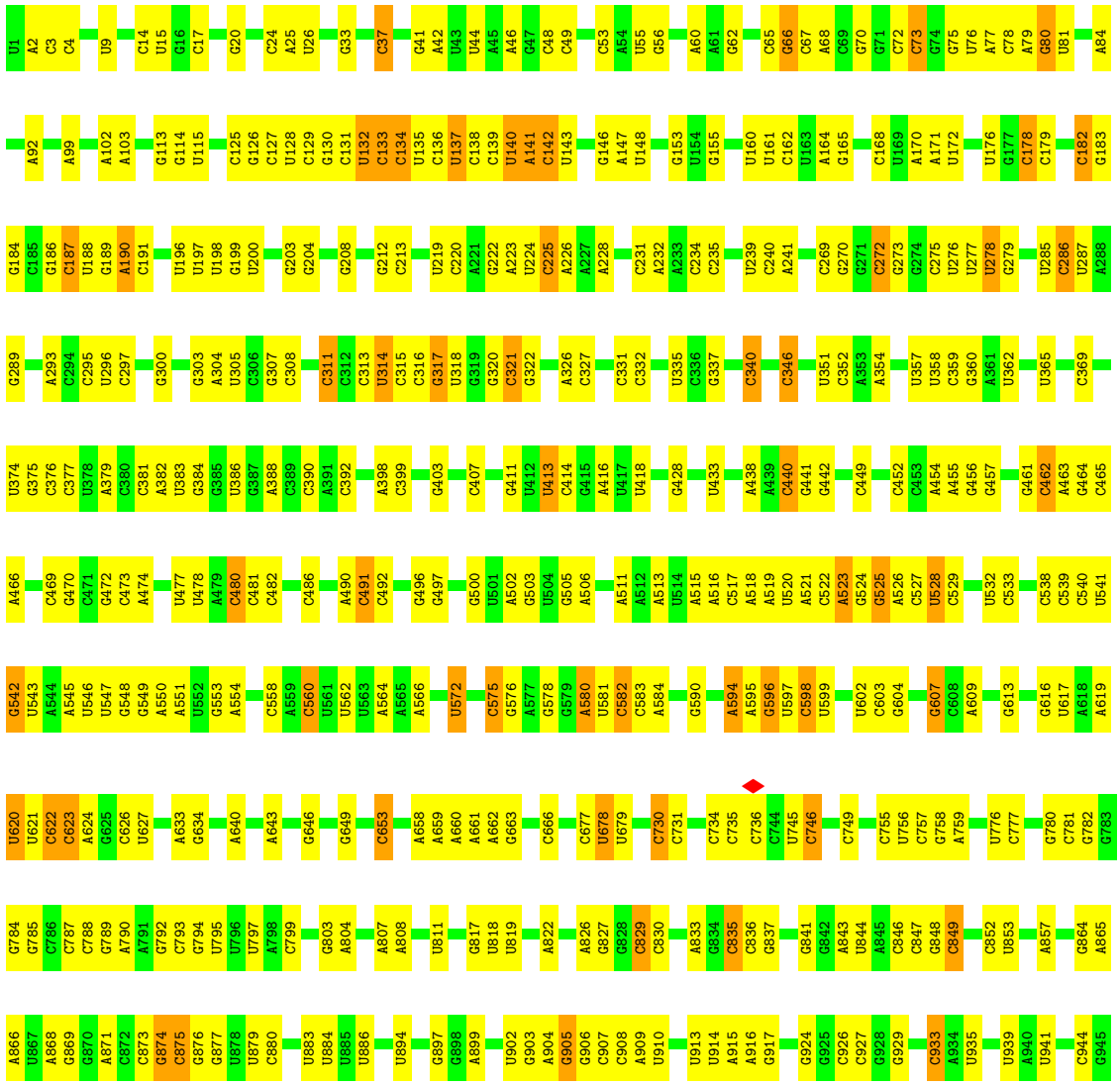
Chain 9:

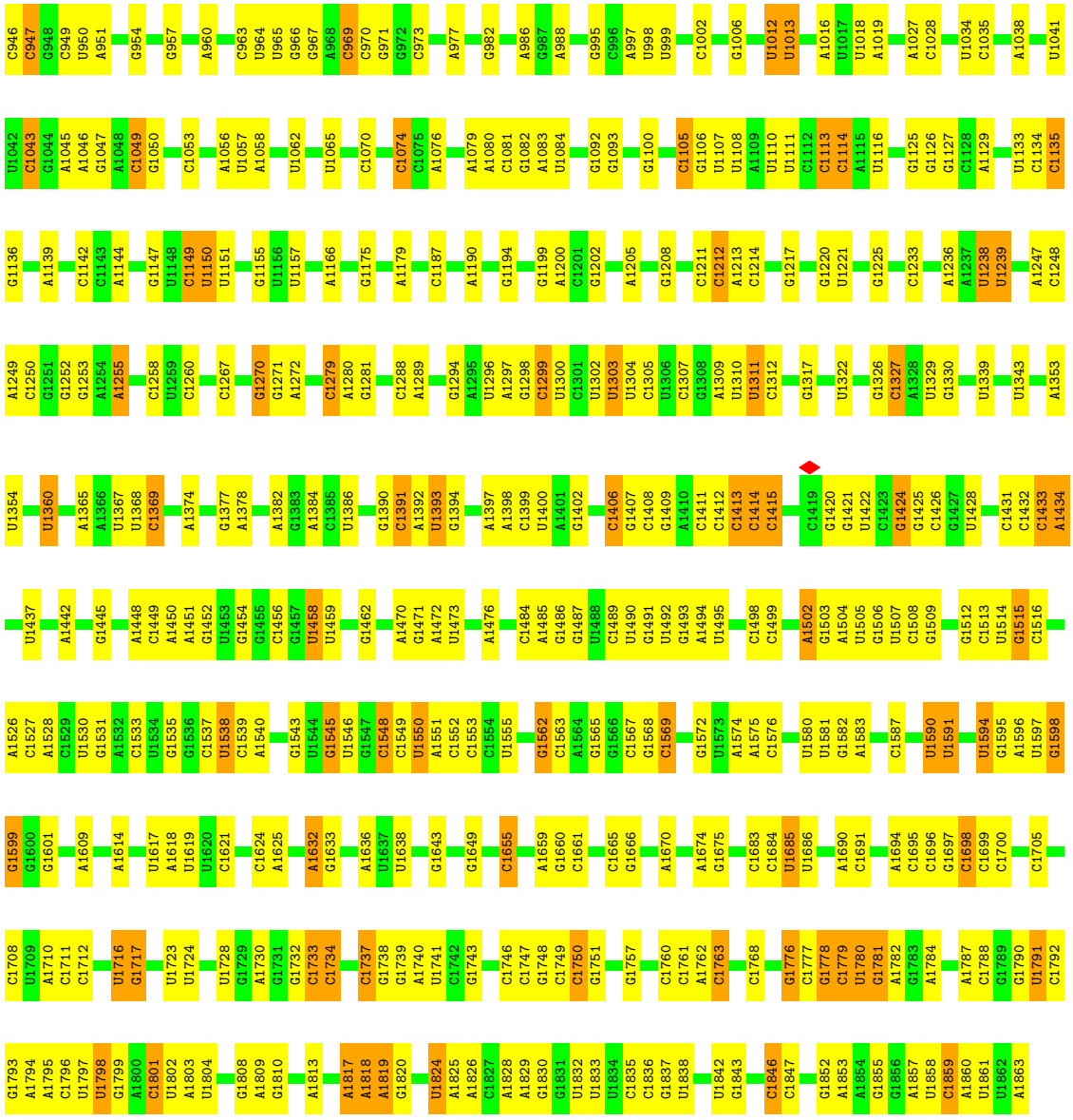




- Molecule 10: 18S ribosomal RNA

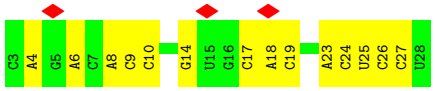
Chain A: 54% 39% 7%





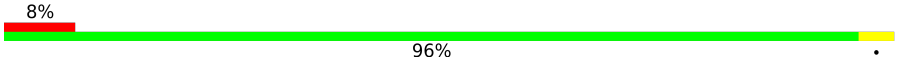
- Molecule 11: Messenger RNA (26-MER)

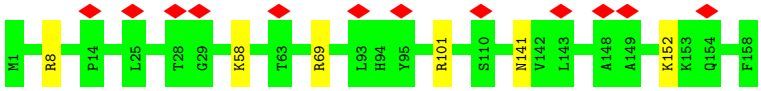
Chain F:



- Molecule 12: 40S ribosomal protein S11

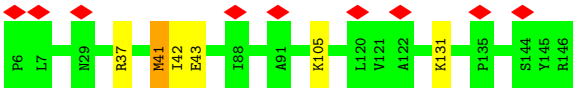
Chain G:





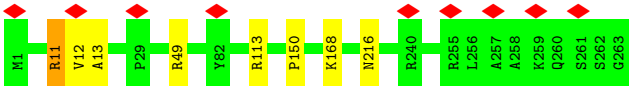
- Molecule 13: 40S ribosomal protein S16

Chain H: 6% 96%



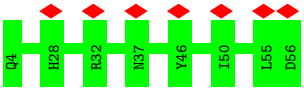
• Molecule 14: 40S ribosomal protein S4, X isoform

Chain I: 97%



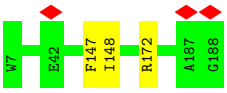
• Molecule 15: 40S ribosomal protein S29

Chain J: 13% 100%



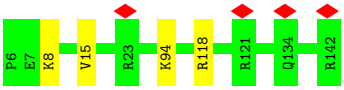
• Molecule 16: 40S ribosomal protein S9

Chain K: 98%



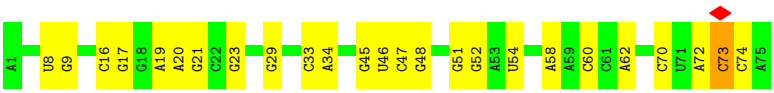
• Molecule 17: 40S ribosomal protein S18

Chain L: 97%



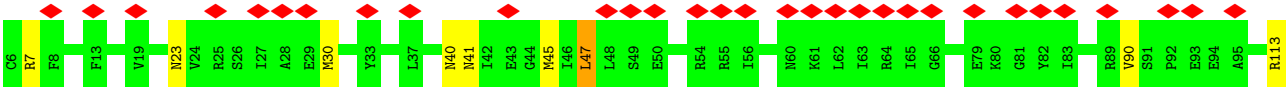
• Molecule 18: Transfer RNA (75-MER)

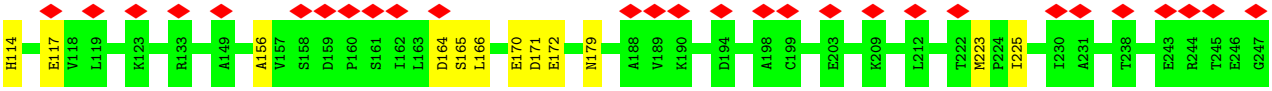
Chain N: 67% 32%

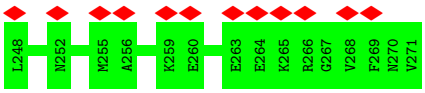


• Molecule 19: Eukaryotic translation initiation factor 2 subunit 1

Chain P: 27% 92% 8%

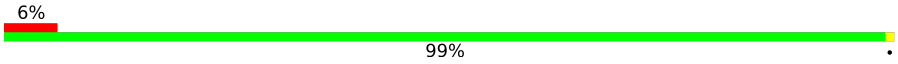


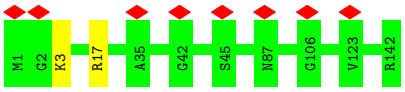




• Molecule 20: 40S ribosomal protein S23

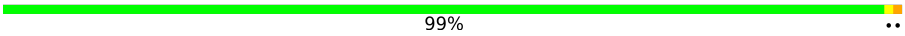
Chain Q:

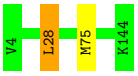




• Molecule 21: 40S ribosomal protein S19

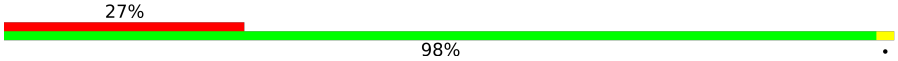
Chain R:

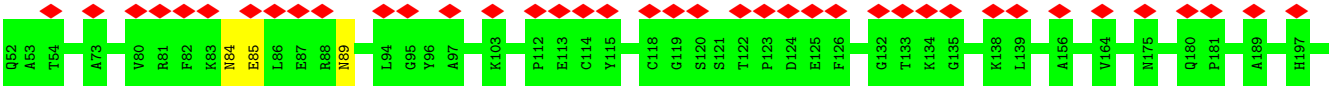


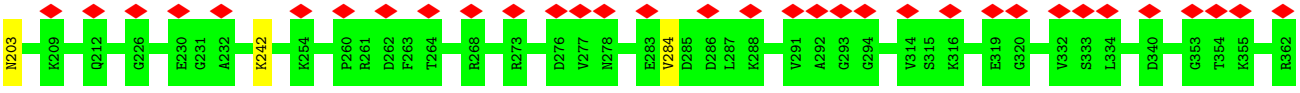


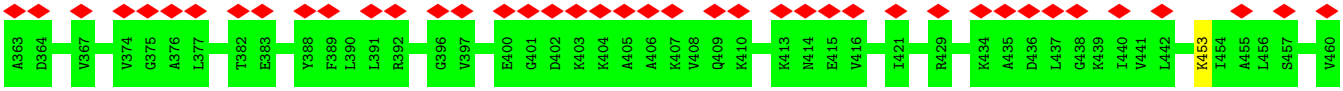
• Molecule 22: Eukaryotic translation initiation factor 2 subunit 3

Chain S:



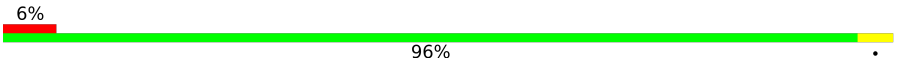


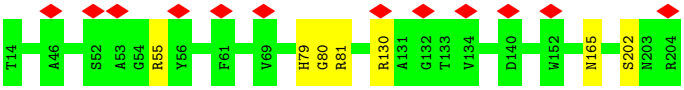




• Molecule 23: 40S ribosomal protein S5

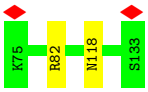
Chain U:





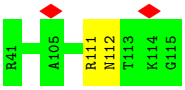
• Molecule 24: 40S ribosomal protein S30

Chain V: 97%



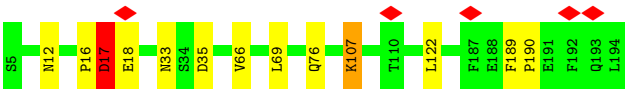
• Molecule 25: 40S ribosomal protein S25

Chain W: 97%



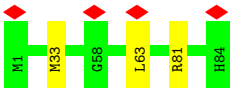
• Molecule 26: 40S ribosomal protein S7

Chain X: 93% 6%



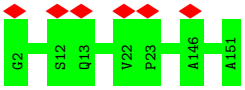
• Molecule 27: 40S ribosomal protein S27

Chain Y: 5% 96%



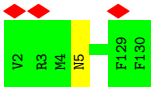
• Molecule 28: 40S ribosomal protein S13

Chain Z: 100%



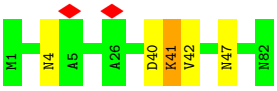
• Molecule 29: 40S ribosomal protein S15a

Chain a: 99%



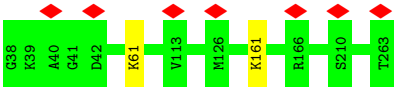
• Molecule 30: 40S ribosomal protein S21

Chain b: 94% 5%



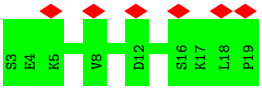
• Molecule 31: 40S ribosomal protein S2

Chain c: 99%



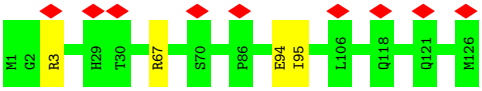
• Molecule 32: EUKARYOTIC TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT (eIF2-Beta)

Chain d: 35% 100%



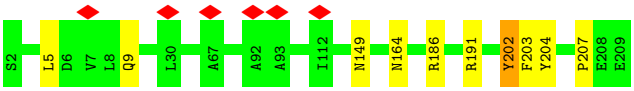
• Molecule 33: 40S ribosomal protein S17

Chain e: 7% 97%



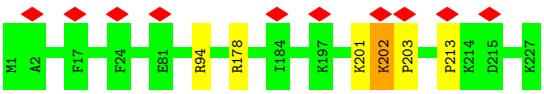
• Molecule 34: 40S ribosomal protein SA

Chain f: 95%



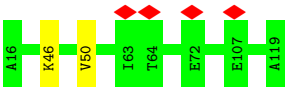
• Molecule 35: 40S ribosomal protein S3

Chain g: 97%



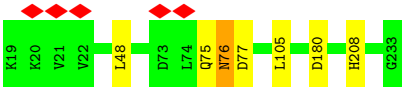
• Molecule 36: 40S ribosomal protein S20

Chain h: 98%



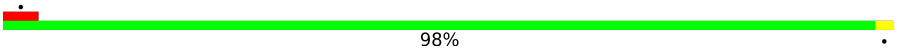
• Molecule 37: 40S ribosomal protein S3a

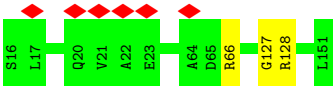
Chain i: 97%



• Molecule 38: 40S ribosomal protein S14

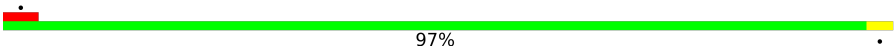
Chain j:

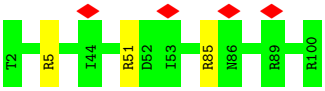




• Molecule 39: 40S ribosomal protein S26

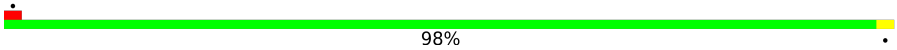
Chain k:

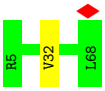




• Molecule 40: 40S ribosomal protein S28

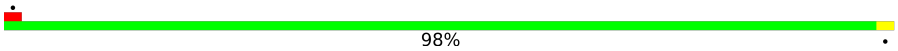
Chain l:

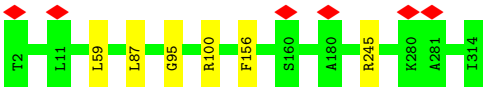




• Molecule 41: Receptor of activated protein C kinase 1

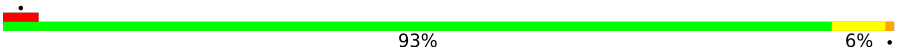
Chain m:

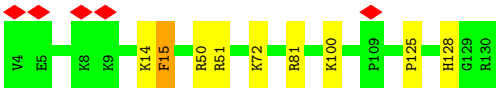




• Molecule 42: 40S ribosomal protein S15

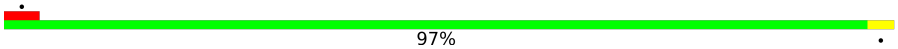
Chain n:

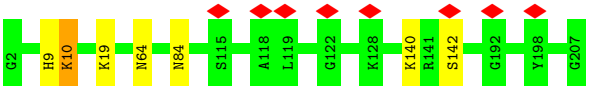




• Molecule 43: 40S ribosomal protein S8

Chain o:





• Molecule 44: Ubiquitin-40S ribosomal protein S27a

Chain p: 7% 90% 10%

K82 K83 T87 P88 K89 K90 K97 L100 K104 R118 H135 L146 K152

• Molecule 45: 40S ribosomal protein S6

Chain q: 97%

M1 F27 M32 V67 L68 T69 S82 E118 R131 N146 D151 D152 V153 R154 L234 S235 S236 L237

• Molecule 46: 40S ribosomal protein S12

Chain r: 96%

G9 D29 G30 D43 K44 R45 P59 K93 E97 S118 Q119 K132

• Molecule 47: 40S ribosomal protein S24

Chain s: 98%

D3 P30 R61 E86 R93 K100 K132 E133

• Molecule 48: 40S ribosomal protein S10

Chain t: 95%

M1 K24 M29 L43 H44 A48 R95 R98

• Molecule 49: Eukaryotic translation initiation factor 4B

Chain u: 11% 88%

MET SER TYR TYR HIS HIS HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PRO GLN GLY ALA MET ALA ALA SER ALA LYS LYS LYS ASN LYS LYS GLY LYS THR ILE SER LEU THR ASP PHE LEU ALA GLU ASP GLY GLY THR GLY GLY GLY SER THR TYR VAL SER

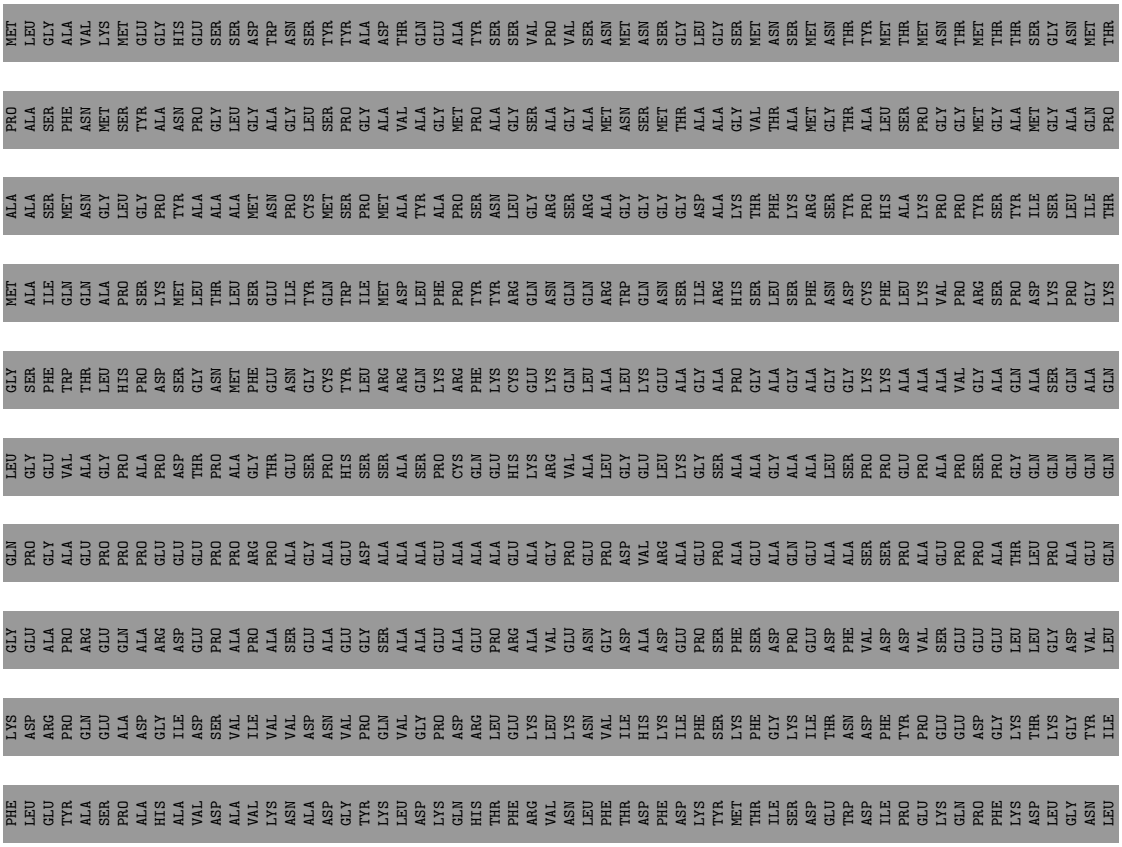
LYS PRO VAL SER TRP ALA ASP GLU THR ASP ASP LEU GLU GLY ASP VAL SER THR THR TRP HIS SER ASN ASP ASP ASP VAL TYR ARG ALA PRO PRO ILE ASP ARG SER ILE LEU PRO THR ALA PRO ARG ALA ALA ARG GLU PRO ASN ILE ASP ARG SER ARG LEU PRO LYS SER PRO PRO

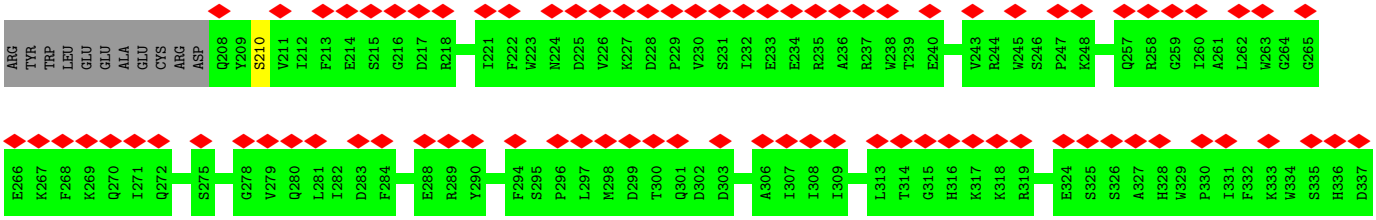
Y1 L8 P9 T13 E19 R22 S27 A28 L31 E34 N37 L41 F44 G45 F49 L59 A76 ASP GLN ALA GLN ASP LYS ASP ARG ASP ASP ARG SER PHE GLY ARG ASP ARG ASP MET ASP ARG ASN ARG ASP SER ASP LYS THR ASP THR ASP TRP ARG ALA

ARG PRO ALA THR ASP SER PHE ASP ASP TYR PRO PRO ARG ARG GLY ASP ASP SER PHE GLY ASP LYS TYR ARG ASP ARG TYR ASP SER ASP ARG TYR ARG ASP GLY TYR ARG ASP GLY TYR ARG ASP GLY PRO ARG ARG ASP MET ASP ARG TYR GLY GLY ARG ASP ARG TYR ASP ASP ARG

- Molecule 50: Eukaryotic translation initiation factor 3 subunit B

Chain w:





G338 K339 F340 F341 A342 R343 M344 T345 L346 D347 T348 I351 Y352 E353 T354 P355 S356 L360 D361 K362 K363 S364 L365 K366 I367 S368 G369 I370 K371 D372 F373 S374 W375 S376 P377 G378 G379 N380 W385 E388 D389 K390 D391 I392 P393 A394 R395 V396 T397 L398 M399 Q400 L401 P402 S403

E406 I407 R408 V409 L412 F413 N414 V415 V416 D417 C418 K419 L420 H421 K424 N425 G426 D427 Y428 K432 T436 P437 Q441 G442 F447 E448 T449 F450 R451 M452 R453 E454 K455 Q456 D460 V461 K465 E466 T467 I468 I469 A470 F471 A472 W473 E474 P475 N476 G477 A481 V482

L483 H484 G485 E486 A487 P488 R489 I490 S491 V492 S493 F494 Y495 H496 V497 K498 S499 N500 G501 K502 I503 E504 L505 S506 K507 M508 F509 D510 K511 Q512 Q513 A514 N515 W519 S520 P521 Q522 G523 Q524 F525 V526 A529 G530 L531 R532 S533 G536 A537 L538 A539 F540 V541 D542 T543 S544 D545 C546

T547 V548 M549 N550 I551 A552 E553 H554 Y555 M556 A557 S558 D559 V560 E561 W562 D563 P564 T565 G566 R567 Y568 S572 V573 S574 S577 H578 K579 V580 D581 N582 A583 Y584 W585 L586 W587 T588 F589 Q590 G591 R592 L593 L594 Q595 K596 N597 N598 K599 D600 R601 F602 C603 W607 R608 P609 R610 PRO

PRO THR LEU LEU SER GLN GLU GLN ILE LYS GLN ILE LYS LYS ASP LEU LYS LYS TYR SER LYS ILE PHE GLU GLN LYS ASP ARG LEU SER GLN SER LYS ALA SER LYS GLU LEU VAL GLU ARG ARG ARG ALA MET MET GLU ASP PHE ARG LYS TYR GLY LYS ALA ALA GLN GLU LEU TYR

VAL GLY GLN LYS ASN GLU ARG LEU GLU LEU ARG GLY GLY VAL ASP THR ASP GLU LEU ASP SER ASN VAL ASP ASP TRP GLU GLU GLU THR ILE GLU PHE PHE VAL THR GLU GLU VAL ILE PRO LEU GLY SER GLN GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50604	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	112000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.544	Depositor
Minimum map value	-0.322	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	520.0, 520.0, 520.0	wwPDB
Map dimensions	208, 208, 208	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.5, 2.5, 2.5	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	1	0.35	0/5021	0.63	1/6781 (0.0%)
2	2	0.34	0/4608	0.57	1/6219 (0.0%)
3	3	0.35	0/3539	0.70	8/4788 (0.2%)
4	4	0.33	0/2149	0.66	0/2920
5	5	0.33	0/2675	0.65	2/3609 (0.1%)
6	6	0.33	0/1773	0.60	0/2398
7	7	0.31	0/3186	0.63	3/4298 (0.1%)
8	8	0.32	0/2964	0.71	5/4000 (0.1%)
9	9	0.29	0/2921	0.54	0/3957
10	A	0.56	1/42353 (0.0%)	1.31	441/66010 (0.7%)
11	F	0.31	0/606	0.95	0/941
12	G	0.36	0/1319	0.65	0/1761
13	H	0.32	0/1142	0.63	0/1528
14	I	0.33	0/2125	0.64	1/2856 (0.0%)
15	J	0.35	0/455	0.58	0/603
16	K	0.32	0/1523	0.60	0/2031
17	L	0.33	0/1158	0.63	0/1548
18	N	0.46	0/1795	1.13	6/2798 (0.2%)
19	P	0.33	0/2178	0.68	0/2935
20	Q	0.32	0/1125	0.60	1/1500 (0.1%)
21	R	0.35	0/1133	0.59	1/1517 (0.1%)
22	S	0.30	0/3267	0.60	1/4415 (0.0%)
23	U	0.31	0/1531	0.56	0/2059
24	V	0.30	0/478	0.69	0/628
25	W	0.36	0/605	0.67	0/810
26	X	0.35	0/1553	0.74	4/2079 (0.2%)
27	Y	0.35	0/673	0.65	1/902 (0.1%)
28	Z	0.31	0/1232	0.54	0/1656
29	a	0.28	0/1051	0.55	0/1406
30	b	0.32	0/627	0.64	0/839
31	c	0.34	0/1779	0.57	0/2399
32	d	0.24	0/149	0.49	0/197
33	e	0.32	0/1032	0.60	0/1383
34	f	0.36	0/1680	0.68	1/2283 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	g	0.32	0/1793	0.60	1/2412 (0.0%)
36	h	0.29	0/832	0.59	0/1117
37	i	0.35	0/1770	0.65	1/2367 (0.0%)
38	j	0.31	0/1029	0.65	0/1380
39	k	0.30	0/803	0.58	0/1076
40	l	0.35	0/509	0.60	0/680
41	m	0.38	0/2494	0.68	1/3394 (0.0%)
42	n	0.36	0/1080	0.68	0/1437
43	o	0.40	0/1709	0.70	1/2278 (0.0%)
44	p	0.44	0/594	0.78	1/786 (0.1%)
45	q	0.35	0/1947	0.64	0/2590
46	r	0.36	0/968	0.66	0/1296
47	s	0.37	0/1083	0.66	1/1437 (0.1%)
48	t	0.34	0/852	0.73	2/1147 (0.2%)
49	u	0.35	0/619	0.83	2/836 (0.2%)
50	w	0.27	0/3407	0.59	1/4620 (0.0%)
All	All	0.43	1/122894 (0.0%)	0.96	488/174907 (0.3%)

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	1	0	6
2	2	0	8
3	3	0	12
4	4	0	8
5	5	0	4
7	7	0	4
8	8	0	8
9	9	0	3
12	G	0	1
13	H	0	2
14	I	0	2
16	K	0	1
17	L	0	3
19	P	0	11
22	S	0	1
23	U	0	2
24	V	0	1
25	W	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	X	0	5
27	Y	0	1
30	b	0	2
31	c	0	1
33	e	0	1
34	f	0	4
35	g	0	2
36	h	0	2
37	i	0	6
38	j	0	1
41	m	0	3
42	n	0	4
43	o	0	2
44	p	0	6
45	q	0	4
46	r	0	4
48	t	0	3
49	u	0	1
50	w	0	1
All	All	0	132

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1311	U	N3-C4	-5.60	1.33	1.38

The worst 5 of 488 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1311	U	N3-C2-O2	-13.33	112.87	122.20
10	A	835	C	N1-C2-O2	11.55	125.83	118.90
10	A	1549	C	N1-C2-O2	11.46	125.77	118.90
10	A	1311	U	N1-C2-O2	11.31	130.72	122.80
10	A	491	C	N1-C2-O2	11.29	125.67	118.90

There are no chirality outliers.

5 of 132 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	264	LYS	Peptide
1	1	330	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	1	384	VAL	Peptide
1	1	417	GLN	Peptide
1	1	7	ARG	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	1	4935	0	5017	227	0
2	2	4529	0	4533	158	0
3	3	3466	0	3446	121	0
4	4	2111	0	2105	116	0
5	5	2624	0	2592	104	0
6	6	1738	0	1706	81	0
7	7	3110	0	3084	101	0
8	8	2919	0	2950	137	0
9	9	2867	0	2838	108	0
10	A	37881	0	19144	0	0
11	F	544	0	283	0	0
12	G	1296	0	1374	0	0
13	H	1124	0	1193	0	0
14	I	2083	0	2189	0	0
15	J	445	0	442	0	0
16	K	1499	0	1608	0	0
17	L	1140	0	1191	0	0
18	N	1604	0	816	0	0
19	P	2147	0	2191	0	0
20	Q	1107	0	1179	0	0
21	R	1113	0	1149	0	0
22	S	3214	0	3354	0	0
23	U	1509	0	1563	0	0
24	V	473	0	524	0	0
25	W	599	0	656	0	0
26	X	1530	0	1627	0	0
27	Y	659	0	683	0	0
28	Z	1208	0	1294	0	0
29	a	1034	0	1080	0	0
30	b	620	0	622	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	c	1743	0	1836	0	0
32	d	147	0	146	0	0
33	e	1020	0	1075	0	0
34	f	1643	0	1646	0	0
35	g	1765	0	1863	0	0
36	h	822	0	887	0	0
37	i	1742	0	1815	0	0
38	j	1016	0	1039	0	0
39	k	790	0	839	0	0
40	l	507	0	536	0	0
41	m	2437	0	2393	0	0
42	n	1061	0	1120	0	0
43	o	1680	0	1762	0	0
44	p	582	0	599	0	0
45	q	1924	0	2089	0	0
46	r	958	0	993	0	0
47	s	1065	0	1137	0	0
48	t	828	0	854	0	0
49	u	608	0	598	0	0
50	w	3308	0	3235	0	0
51	1	1	0	0	0	0
51	9	376	0	0	27	0
51	A	6	0	0	1	0
51	H	5	0	0	0	0
51	U	13	0	0	1	0
51	j	1	0	0	0	0
51	l	8	0	0	0	0
51	m	5	0	0	0	0
All	All	117189	0	98895	1032	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 17.

The worst 5 of 1032 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:396:ASP:OD2	7:7:400:ARG:NH1	1.86	1.08
6:6:20:ARG:NH1	6:6:45:GLU:OE2	1.90	1.05
3:3:136:LYS:NZ	3:3:140:GLU:OE2	1.89	1.04
5:5:36:VAL:HG11	5:5:168:ARG:HH12	1.29	0.94
3:3:266:ASP:OD1	3:3:269:LYS:NZ	2.03	0.91

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	1	598/1362 (44%)	530 (89%)	67 (11%)	1 (0%)	47	81
2	2	556/843 (66%)	507 (91%)	48 (9%)	1 (0%)	47	81
3	3	418/445 (94%)	348 (83%)	64 (15%)	6 (1%)	11	46
4	4	270/364 (74%)	230 (85%)	40 (15%)	0	100	100
5	5	322/352 (92%)	272 (84%)	50 (16%)	0	100	100
6	6	214/218 (98%)	193 (90%)	21 (10%)	0	100	100
7	7	371/564 (66%)	329 (89%)	41 (11%)	1 (0%)	41	76
8	8	364/374 (97%)	301 (83%)	63 (17%)	0	100	100
9	9	350/368 (95%)	325 (93%)	23 (7%)	2 (1%)	25	66
12	G	156/158 (99%)	139 (89%)	17 (11%)	0	100	100
13	H	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	11	46
14	I	261/263 (99%)	227 (87%)	31 (12%)	3 (1%)	14	52
15	J	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
16	K	180/182 (99%)	165 (92%)	14 (8%)	1 (1%)	25	66
17	L	135/137 (98%)	114 (84%)	21 (16%)	0	100	100
19	P	264/266 (99%)	212 (80%)	48 (18%)	4 (2%)	10	45
20	Q	140/142 (99%)	124 (89%)	16 (11%)	0	100	100
21	R	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
22	S	420/422 (100%)	366 (87%)	54 (13%)	0	100	100
23	U	189/191 (99%)	173 (92%)	15 (8%)	1 (0%)	29	69
24	V	57/59 (97%)	49 (86%)	8 (14%)	0	100	100
25	W	73/75 (97%)	65 (89%)	8 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	X	188/190 (99%)	166 (88%)	17 (9%)	5 (3%)	5	31
27	Y	82/84 (98%)	74 (90%)	8 (10%)	0	100	100
28	Z	148/150 (99%)	143 (97%)	5 (3%)	0	100	100
29	a	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
30	b	80/82 (98%)	69 (86%)	9 (11%)	2 (2%)	5	32
31	c	224/226 (99%)	205 (92%)	19 (8%)	0	100	100
32	d	15/17 (88%)	15 (100%)	0	0	100	100
33	e	124/126 (98%)	111 (90%)	12 (10%)	1 (1%)	19	60
34	f	206/208 (99%)	177 (86%)	27 (13%)	2 (1%)	15	54
35	g	225/227 (99%)	203 (90%)	20 (9%)	2 (1%)	17	56
36	h	102/104 (98%)	94 (92%)	8 (8%)	0	100	100
37	i	213/215 (99%)	188 (88%)	25 (12%)	0	100	100
38	j	134/136 (98%)	117 (87%)	16 (12%)	1 (1%)	22	63
39	k	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
40	l	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
41	m	311/313 (99%)	271 (87%)	40 (13%)	0	100	100
42	n	125/127 (98%)	106 (85%)	17 (14%)	2 (2%)	9	44
43	o	204/206 (99%)	173 (85%)	29 (14%)	2 (1%)	15	54
44	p	69/71 (97%)	48 (70%)	21 (30%)	0	100	100
45	q	235/237 (99%)	211 (90%)	22 (9%)	2 (1%)	17	56
46	r	122/124 (98%)	97 (80%)	23 (19%)	2 (2%)	9	44
47	s	129/131 (98%)	110 (85%)	18 (14%)	1 (1%)	19	60
48	t	96/98 (98%)	76 (79%)	19 (20%)	1 (1%)	15	54
49	u	74/636 (12%)	61 (82%)	12 (16%)	1 (1%)	11	46
50	w	401/1121 (36%)	335 (84%)	66 (16%)	0	100	100
All	All	9460/12241 (77%)	8286 (88%)	1128 (12%)	46 (0%)	32	69

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	51	VAL
13	H	42	ILE
14	I	12	VAL

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Mol	Chain	Res	Type
26	X	17	ASP
30	b	42	VAL

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	1	551/1245 (44%)	542 (98%)	9 (2%)	62	79
2	2	503/750 (67%)	497 (99%)	6 (1%)	71	83
3	3	384/406 (95%)	371 (97%)	13 (3%)	37	60
4	4	239/282 (85%)	234 (98%)	5 (2%)	53	72
5	5	293/311 (94%)	287 (98%)	6 (2%)	55	74
6	6	190/193 (98%)	189 (100%)	1 (0%)	88	93
7	7	342/516 (66%)	340 (99%)	2 (1%)	86	92
8	8	327/335 (98%)	327 (100%)	0	100	100
9	9	320/331 (97%)	317 (99%)	3 (1%)	78	87
12	G	142/142 (100%)	137 (96%)	5 (4%)	36	59
13	H	117/117 (100%)	114 (97%)	3 (3%)	46	66
14	I	225/225 (100%)	222 (99%)	3 (1%)	69	82
15	J	47/47 (100%)	47 (100%)	0	100	100
16	K	157/157 (100%)	156 (99%)	1 (1%)	86	92
17	L	119/119 (100%)	118 (99%)	1 (1%)	81	89
19	P	238/238 (100%)	231 (97%)	7 (3%)	42	64
20	Q	114/114 (100%)	113 (99%)	1 (1%)	78	87
21	R	113/113 (100%)	111 (98%)	2 (2%)	59	77
22	S	354/354 (100%)	349 (99%)	5 (1%)	67	80
23	U	161/161 (100%)	157 (98%)	4 (2%)	47	68
24	V	49/49 (100%)	48 (98%)	1 (2%)	55	74
25	W	66/66 (100%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	X	170/170 (100%)	168 (99%)	2 (1%)	71	83
27	Y	76/76 (100%)	75 (99%)	1 (1%)	69	82
28	Z	130/130 (100%)	130 (100%)	0	100	100
29	a	112/112 (100%)	111 (99%)	1 (1%)	78	87
30	b	67/67 (100%)	65 (97%)	2 (3%)	41	63
31	c	187/187 (100%)	186 (100%)	1 (0%)	88	93
32	d	17/17 (100%)	17 (100%)	0	100	100
33	e	114/114 (100%)	112 (98%)	2 (2%)	59	77
34	f	174/174 (100%)	170 (98%)	4 (2%)	50	70
35	g	190/190 (100%)	188 (99%)	2 (1%)	73	84
36	h	94/94 (100%)	94 (100%)	0	100	100
37	i	196/196 (100%)	195 (100%)	1 (0%)	88	93
38	j	106/106 (100%)	105 (99%)	1 (1%)	78	87
39	k	87/87 (100%)	84 (97%)	3 (3%)	37	60
40	l	57/57 (100%)	56 (98%)	1 (2%)	59	77
41	m	272/272 (100%)	270 (99%)	2 (1%)	84	90
42	n	116/116 (100%)	112 (97%)	4 (3%)	37	60
43	o	177/177 (100%)	174 (98%)	3 (2%)	60	78
44	p	64/64 (100%)	64 (100%)	0	100	100
45	q	207/207 (100%)	205 (99%)	2 (1%)	76	86
46	r	104/104 (100%)	104 (100%)	0	100	100
47	s	113/113 (100%)	112 (99%)	1 (1%)	78	87
48	t	89/89 (100%)	88 (99%)	1 (1%)	73	84
49	u	66/548 (12%)	61 (92%)	5 (8%)	13	37
50	w	360/928 (39%)	358 (99%)	2 (1%)	86	92
All	All	8396/10666 (79%)	8277 (99%)	119 (1%)	68	80

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	L	118	ARG
47	s	61	ARG
22	S	284	VAL

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Mol	Chain	Res	Type
45	q	131	ARG
50	w	500	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
5	5	345	GLN
7	7	453	GLN
6	6	10	ASN
7	7	229	ASN
8	8	270	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1771/1776 (99%)	707 (39%)	51 (2%)
11	F	25/26 (96%)	14 (56%)	1 (4%)
18	N	74/75 (98%)	21 (28%)	2 (2%)
All	All	1870/1877 (99%)	742 (39%)	54 (2%)

5 of 742 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	3	C
10	A	4	C
10	A	9	U
10	A	17	C
10	A	20	G

5 of 54 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	865	A
10	A	1391	C
10	A	1819	A
10	A	876	G
10	A	1279	C

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	736:C	O3'	744:C	P	27.46
1	A	761:G	O3'	774:U	P	18.00
1	A	679:U	O3'	683:G	P	15.42
1	A	687:G	O3'	730:C	P	13.04
1	A	243:C	O3'	267:G	P	13.01

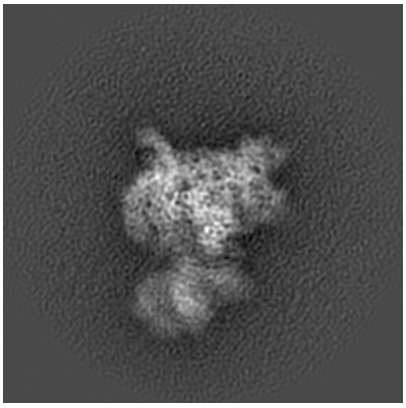
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4242. These allow visual inspection of the internal detail of the map and identification of artifacts.

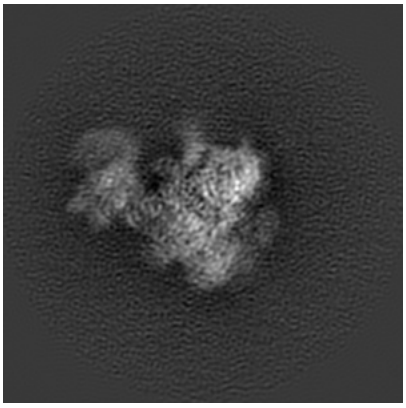
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

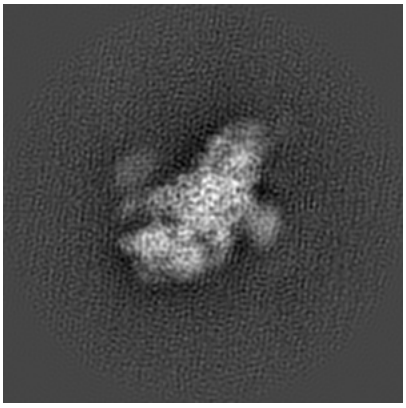
6.1.1 Primary map



X



Y

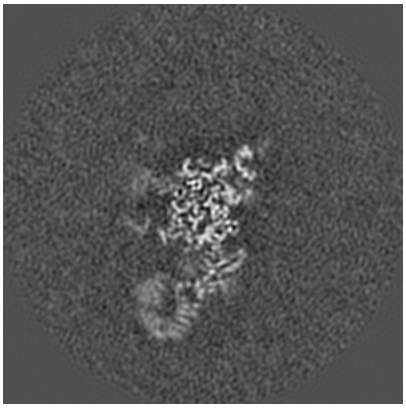


Z

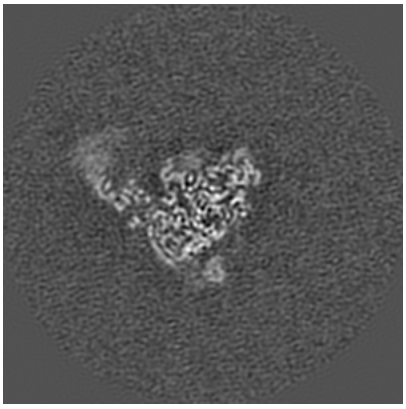
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

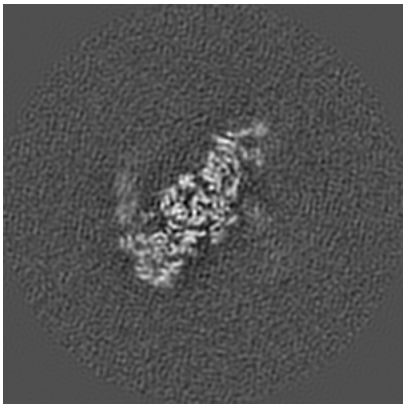
6.2.1 Primary map



X Index: 104



Y Index: 104

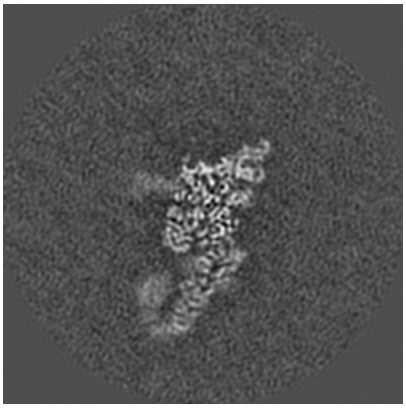


Z Index: 104

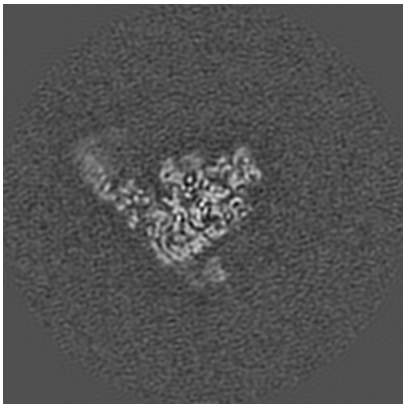
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

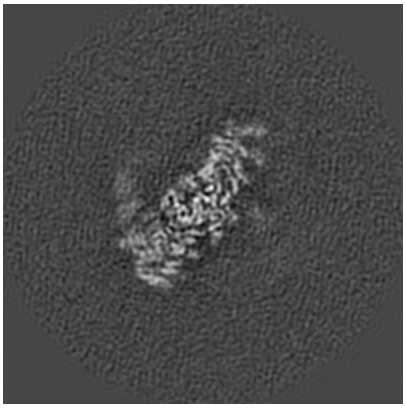
6.3.1 Primary map



X Index: 106



Y Index: 105

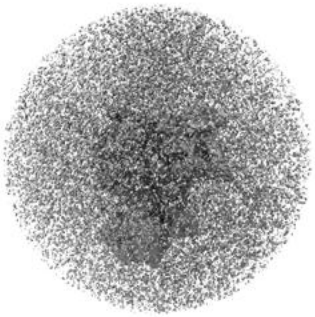


Z Index: 105

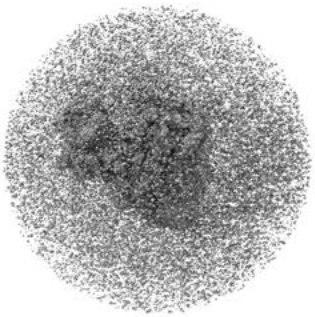
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

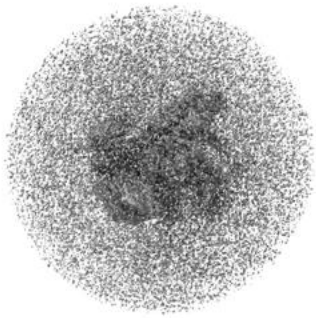
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

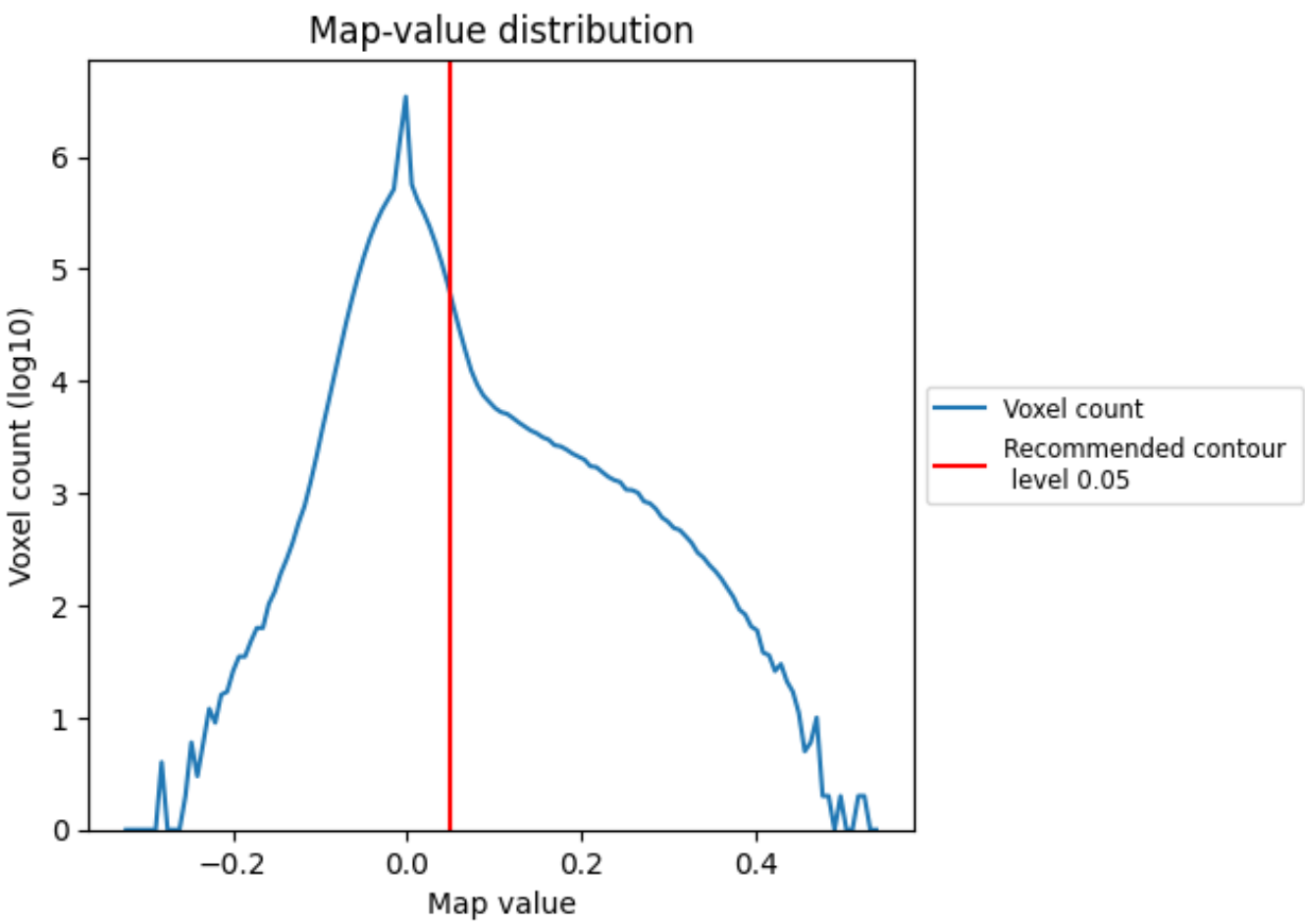
6.5 Mask visualisation (i)

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

7 Map analysis (i)

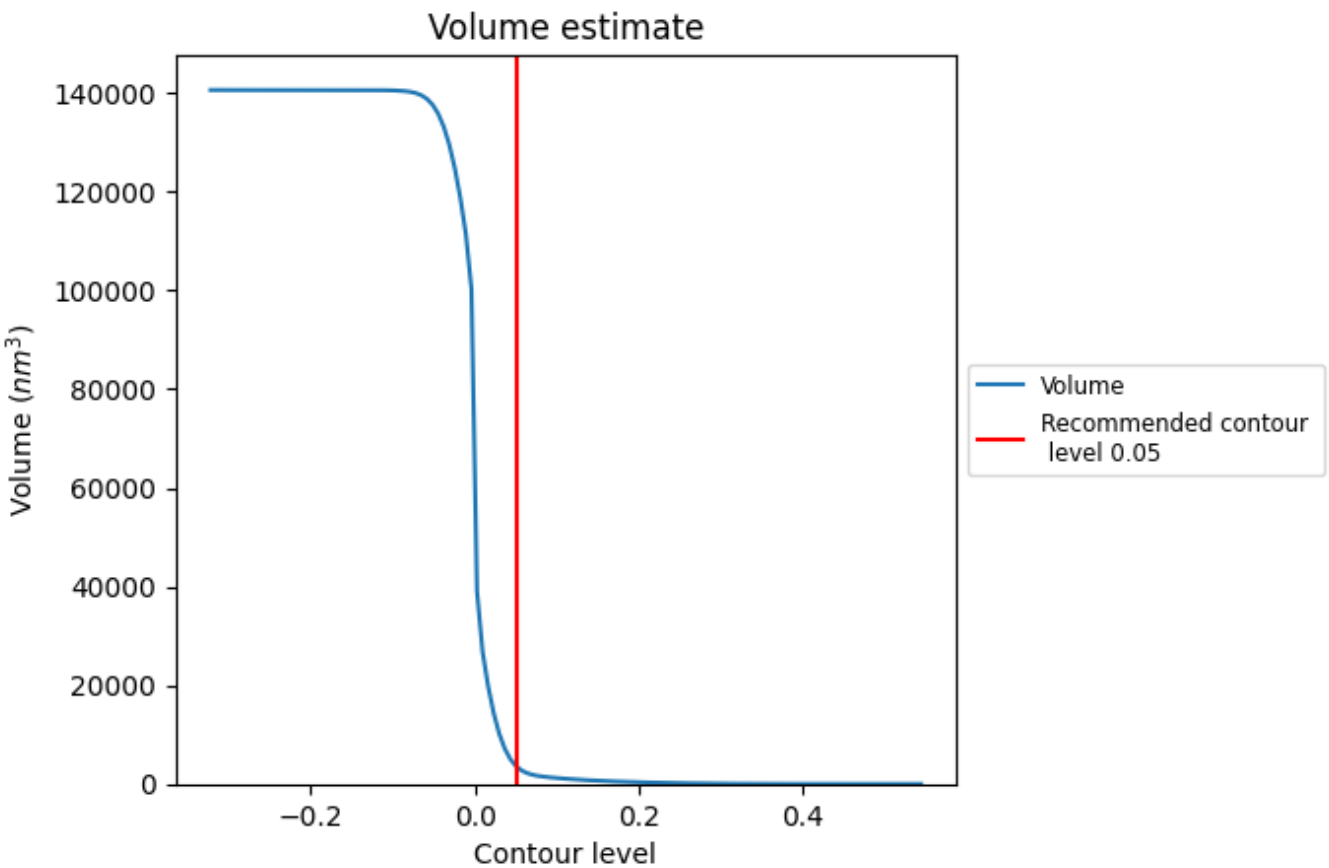
This section contains the results of statistical analysis of the map.

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.

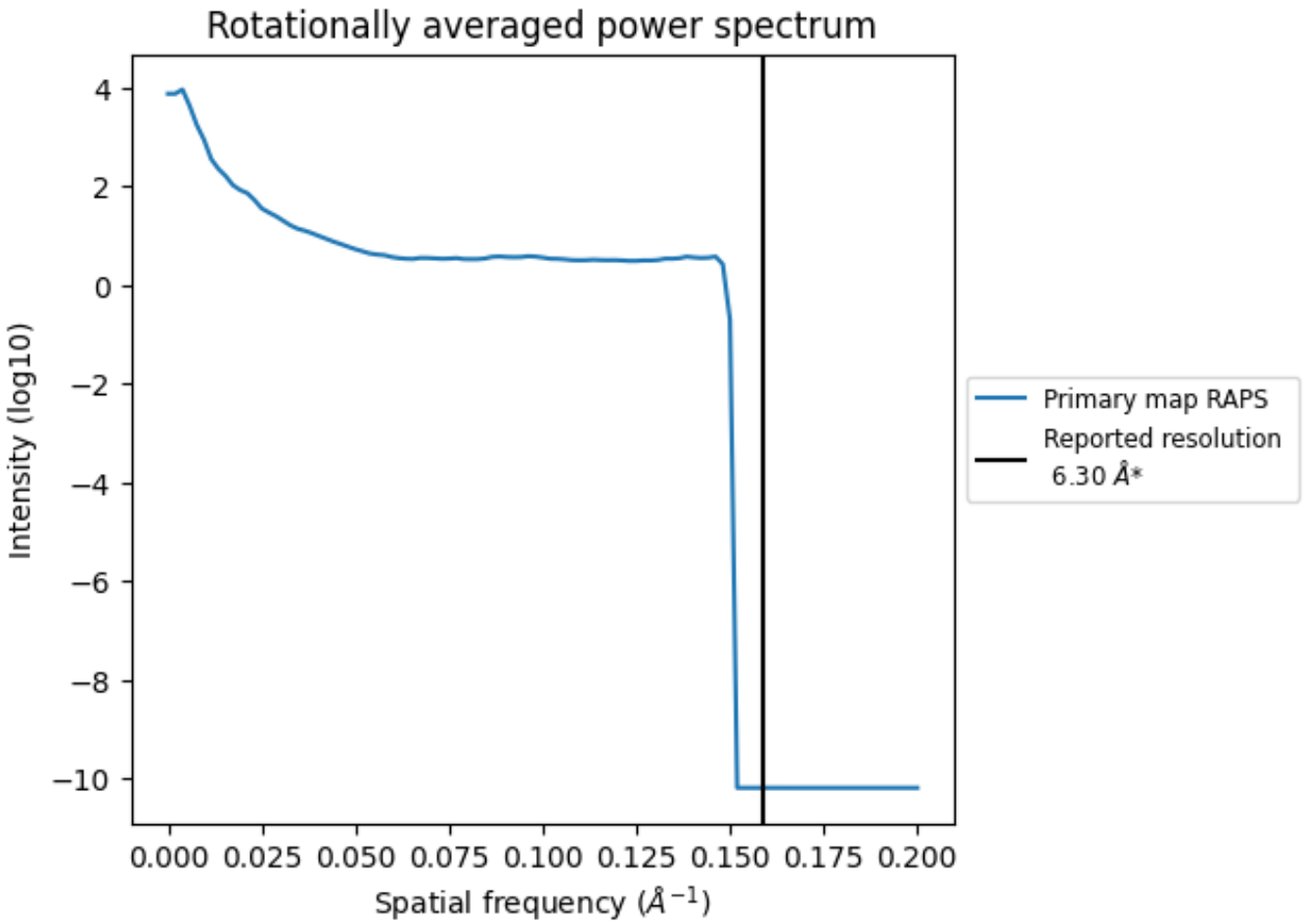
7.2 Volume estimate (i)



The volume at the recommended contour level is 3639 nm^3; this corresponds to an approximate mass of 3287 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 0.159 Å^{-1}

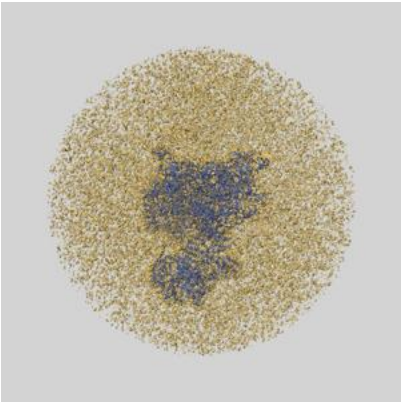
8 Fourier-Shell correlation (i)

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

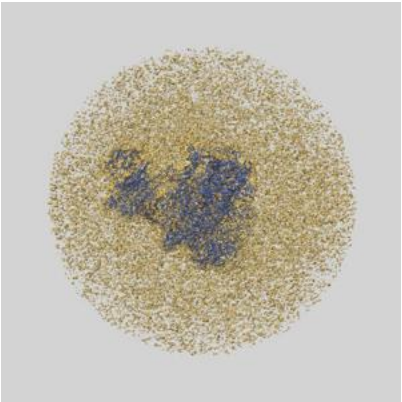
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4242 and PDB model 6FEC. Per-residue inclusion information can be found in section 3 on page 15.

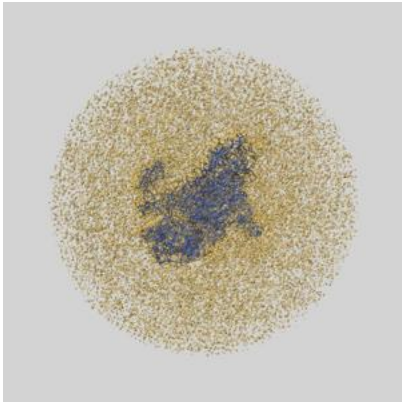
9.1 Map-model overlay (i)



X



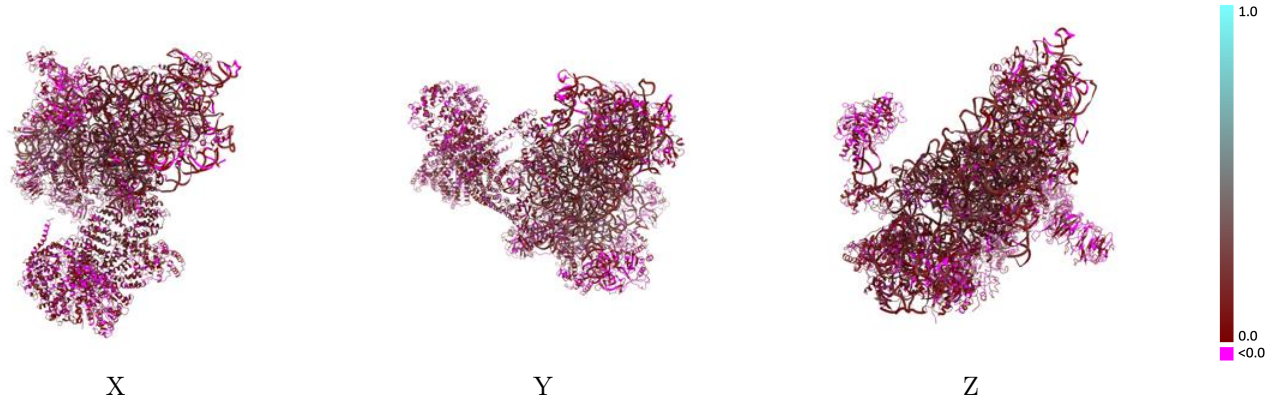
Y



Z

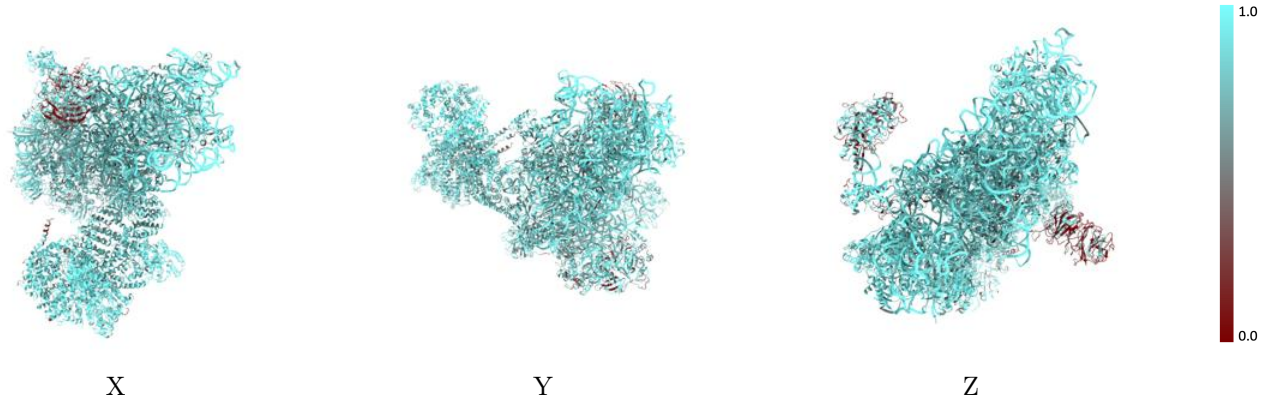
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



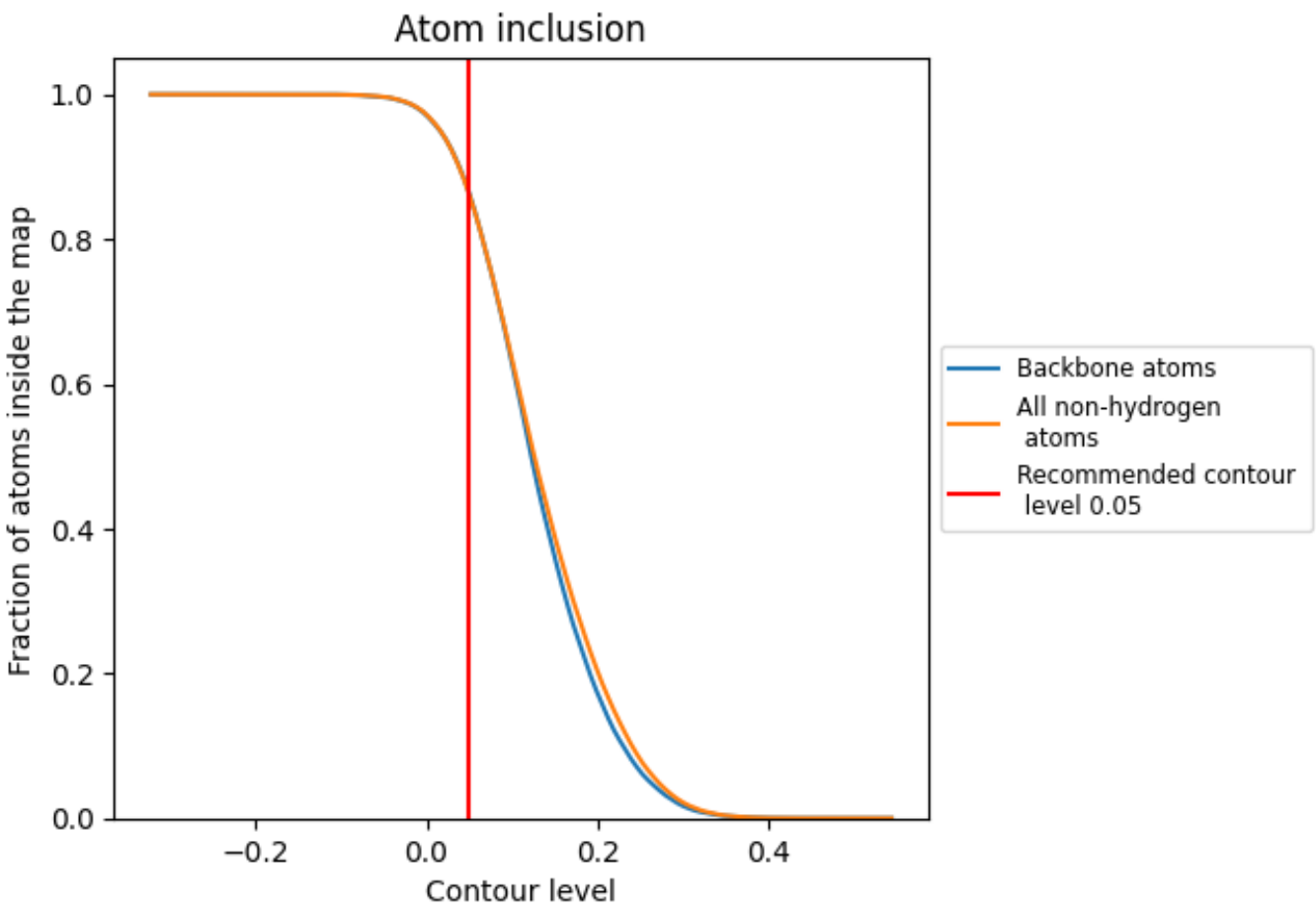
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8616	0.1160
1	0.8527	0.1170
2	0.8636	0.1310
3	0.9127	0.1020
4	0.8978	0.0660
5	0.8600	0.0680
6	0.9218	0.0560
7	0.9057	0.0550
8	0.9235	0.0780
9	0.7723	0.0900
A	0.9705	0.1650
F	0.7445	0.0990
G	0.8160	0.0920
H	0.8392	0.1000
I	0.8353	0.1160
J	0.7611	0.0440
K	0.8008	0.1050
L	0.8715	0.0990
N	0.9208	0.1350
P	0.6206	0.0750
Q	0.8130	0.1090
R	0.8919	0.0970
S	0.6428	0.0230
U	0.8018	0.1000
V	0.8465	0.0780
W	0.8801	0.1020
X	0.8274	0.1240
Y	0.8083	0.1290
Z	0.8072	0.1180
a	0.7812	0.1230
b	0.8152	0.1160
c	0.7992	0.1310
d	0.6503	0.0460
e	0.7812	0.1090
f	0.8352	0.1230

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Chain	Atom inclusion	Q-score
g	0.8240	0.1140
h	0.8402	0.0840
i	0.8432	0.1250
j	0.8156	0.0780
k	0.7792	0.1050
l	0.8090	0.1020
m	0.8980	0.1010
n	0.8481	0.0800
o	0.8737	0.0940
p	0.8519	0.0550
q	0.8847	0.0850
r	0.8962	0.0800
s	0.8592	0.0990
t	0.8499	0.1060
u	0.7868	0.0800
w	0.2675	0.0140