wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 08:13 pm BST

PDB ID	:	6ZCE / pdb_00006zce
EMDB ID	:	EMD-11160
Title	:	Structure of a yeast ABCE1-bound 43S pre-initiation complex
Authors	:	Kratzat, H.; Mackens-Kiani, T.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on	:	2020-06-10
Resolution	:	5.30 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

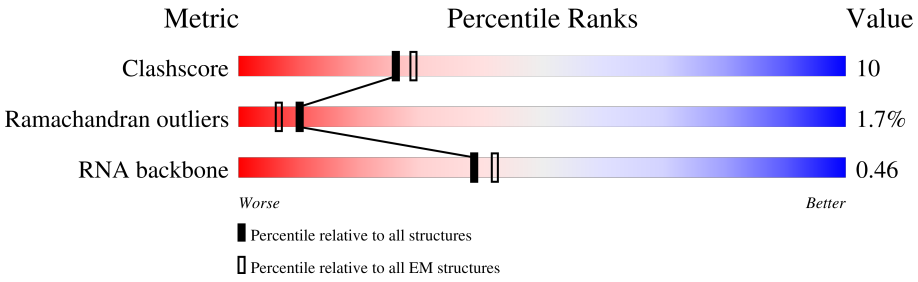
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 5.30 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.



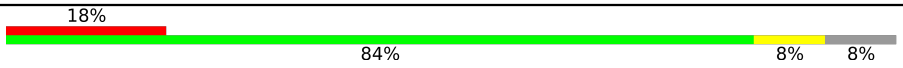
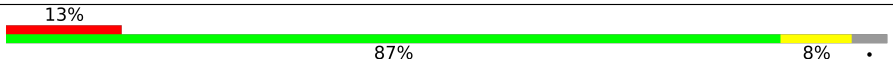
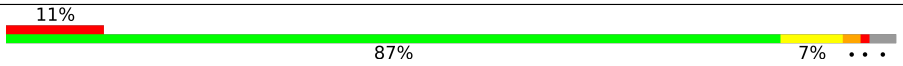
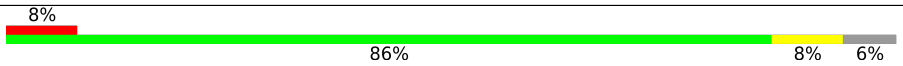
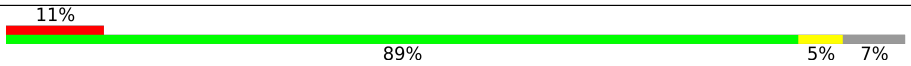
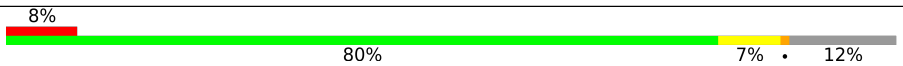
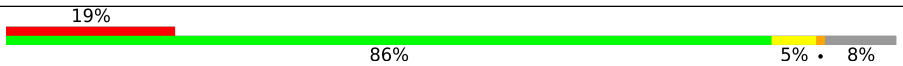
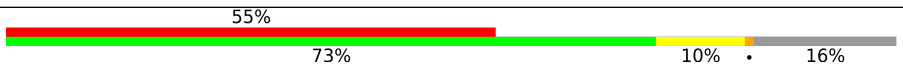
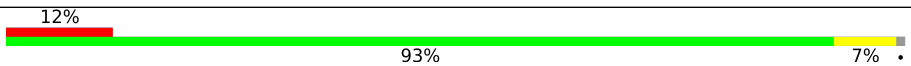
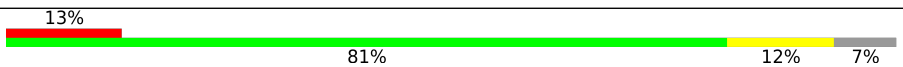
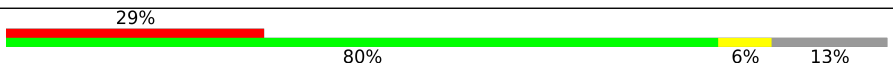
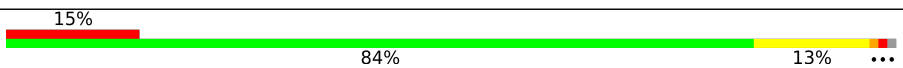
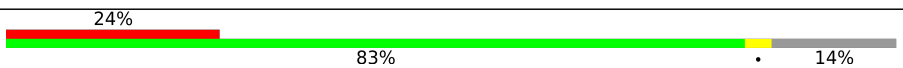
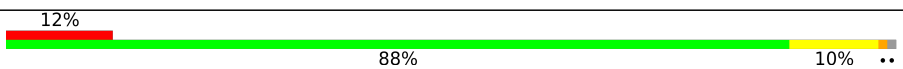
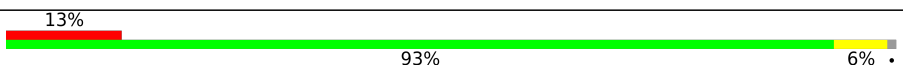
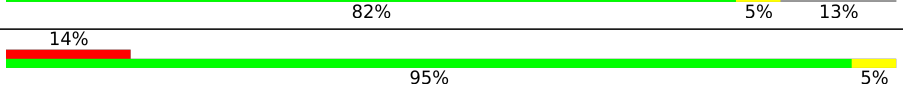
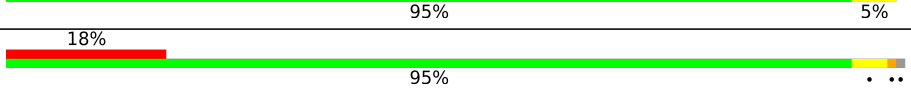
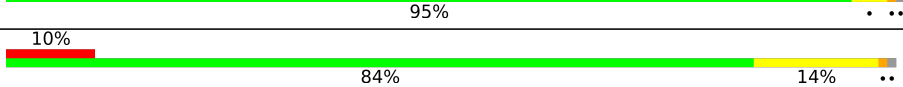
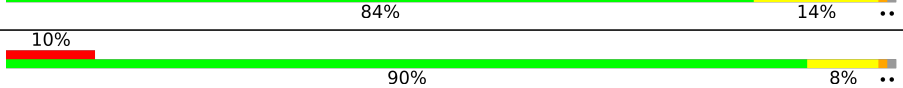
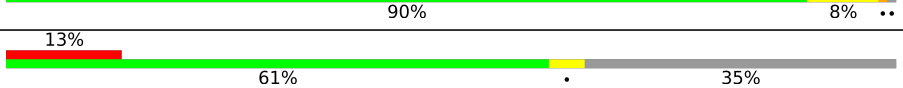
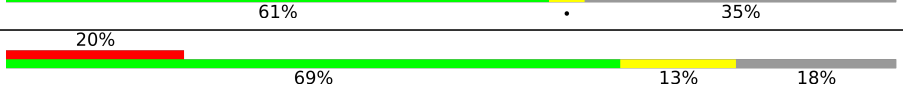
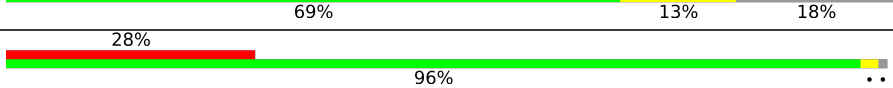
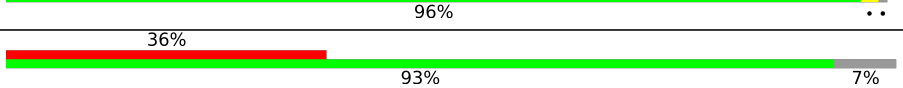
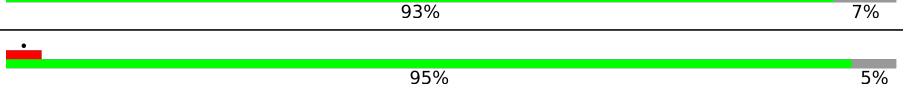
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
RNA backbone	6643	2191

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	l	347	95% 95% 5%
2	r	274	19% 19% 81%
3	A	1800	· 36% 43% 14% · ·
4	B	252	7% 77% 5% 18%
5	C	255	11% 75% 7% · 16%
6	D	254	13% 76% 9% 15%
7	E	240	30% 88% 5% 7%
8	F	261	13% 92% 7%

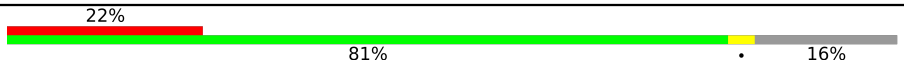
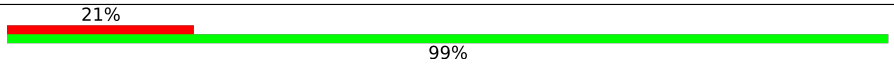
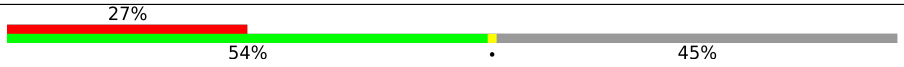
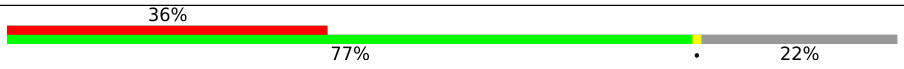
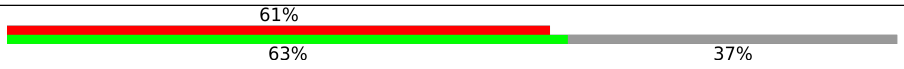
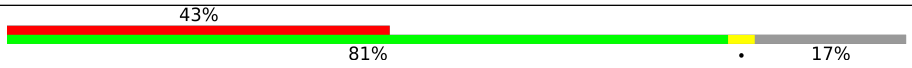
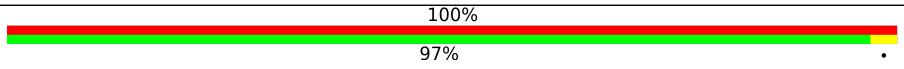
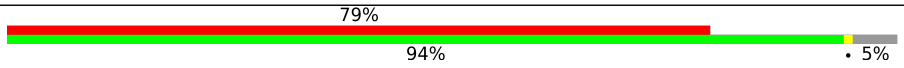
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	G	225	
10	H	236	
11	I	190	
12	J	200	
13	K	197	
14	L	105	
15	M	155	
16	N	143	
17	O	151	
18	P	136	
19	Q	141	
20	R	143	
21	S	136	
22	T	146	
23	U	144	
24	V	121	
25	W	87	
26	X	130	
27	Y	145	
28	Z	135	
29	a	108	
30	b	119	
31	c	82	
32	d	67	
33	e	56	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	f	63	
35	g	152	
36	h	319	
37	o	964	
38	p	763	
39	q	812	
40	i	153	
41	m	108	
42	s	265	
42	t	265	
43	j	77	
44	k	608	

2 Entry composition (i)

There are 49 unique types of molecules in this entry. The entry contains 76380 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 I.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	l	330	Total 1624	C 964	N 330	O 330	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	r	53	Total 261	C 155	N 53	O 53	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	139	SER	ASN	conflict	UNP Q04067

- Molecule 3 is a RNA chain called 18S ribosomal RNA (1719-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1719	Total 36643	C 16382	N 6499	O 12043	P 1719	0	0

- Molecule 4 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	B	206	Total 1020	C 608	N 206	O 206	0	0

- Molecule 5 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	C	214	Total 1061	C 633	N 214	O 214	0	0

- Molecule 6 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	D	217	Total 1063	C 629	N 217	O 217	0	0

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	E	223	Total 1098	C 652	N 223	O 223	0	0

- Molecule 8 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	F	260	Total 1276	C 756	N 260	O 260	0	0

- Molecule 9 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	G	206	Total 1020	C 608	N 206	O 206	0	0

- Molecule 10 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	H	226	Total 1113	C 661	N 226	O 226	0	0

- Molecule 11 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	I	184	Total 913	C 545	N 184	O 184	0	0

- Molecule 12 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	188	Total 924	C 548	N 188	O 188	0	0

- Molecule 13 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	K	184	Total 910	C 542	N 184	O 184	0	0

- Molecule 14 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	92	Total 456	C 272	N 92	O 92	0	0

- Molecule 15 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	M	142	Total 702	C 418	N 142	O 142	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	147	ALA	GLY	conflict	UNP P0CX47

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	N	120	Total 590	C 350	N 120	O 120	0	0

- Molecule 17 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	O	150	Total 742	C 442	N 150	O 150	0	0

- Molecule 18 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	P	127	Total 620	C 366	N 127	O 127	0	0

- Molecule 19 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	Q	122	Total 601	C 357	N 122	O 122	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	137	SER	ARG	conflict	UNP Q01855

- Molecule 20 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	141	Total 693	C 411	N 141	O 141	0	0

- Molecule 21 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	S	117	Total 579	C 345	N 117	O 117	0	0

- Molecule 22 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	T	145	Total 715	C 425	N 145	O 145	0	0

- Molecule 23 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	U	143	Total 700	C 414	N 143	O 143	0	0

- Molecule 24 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	V	105	Total 521	C 311	N 105	O 105	0	0

- Molecule 25 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	W	87	Total 429	C 255	N 87	O 87	0	0

- Molecule 26 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	X	129	Total 634	C 376	N 129	O 129	0	0

- Molecule 27 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Y	144	Total 704	C 416	N 144	O 144	0	0

- Molecule 28 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Z	134	Total 661	C 393	N 134	O 134	0	0

- Molecule 29 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	a	70	Total 347	C 207	N 70	O 70	0	0

- Molecule 30 is a protein called 40S ribosomal protein S26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	b	97	Total 482	C 288	N 97	O 97	0	0

- Molecule 31 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	c	81	Total 400	C 238	N 81	O 81	0	0

- Molecule 32 is a protein called 40S ribosomal protein S28-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	d	62	Total	C	N	O	0	0
			305	181	62	62		

- Molecule 33 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	e	53	Total	C	N	O	0	0
			260	154	53	53		

- Molecule 34 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	f	53	Total	C	N	O	0	0
			261	155	53	53		

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	g	71	Total	C	N	O	0	0
			351	209	71	71		

- Molecule 36 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	h	318	Total	C	N	O	0	0
			1568	932	318	318		

- Molecule 37 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	o	529	Total	C	N	O	0	0
			2631	1573	529	529		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	p	646	Total	C	N	O	0	0
			3201	1909	646	646		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	q	636	Total	C	N	O	0	0
			3169	1897	636	636		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	i	97	Total	C	N	O	0	0
			476	282	97	97		

- Molecule 41 is a protein called Eukaryotic translation initiation factor eIF-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	m	90	Total	C	N	O	0	0
			443	263	90	90		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 3 subunit J.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	t	84	Total	C	N	O	0	0
			418	251	84	83		
42	s	95	Total	C	N	O	0	0
			470	280	95	95		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t	254	ALA	PRO	conflict	UNP Q05775
s	254	ALA	PRO	conflict	UNP Q05775

- Molecule 43 is a protein called RNA recognition motif (unknown).

Mol	Chain	Residues	Atoms				AltConf	Trace
43	j	77	Total	C	N	O	0	0
			385	231	77	77		

- Molecule 44 is a protein called Translation initiation factor RLI1.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	k	579	Total	C	N	O	0	0
			2860	1702	579	579		

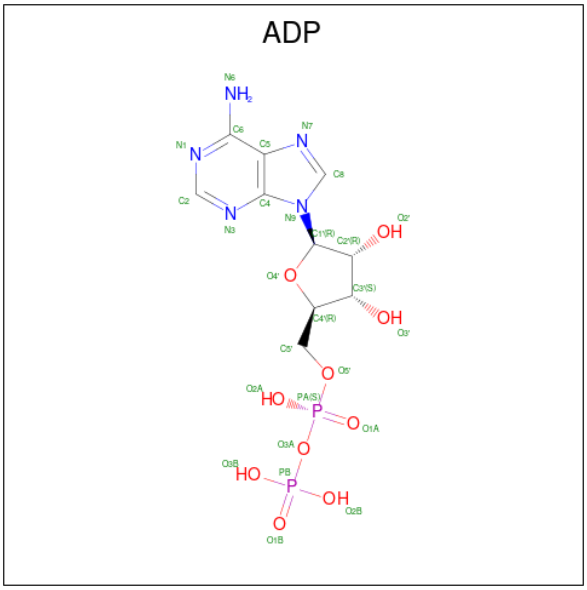
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	350	VAL	ALA	conflict	UNP Q03195

- Molecule 45 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
45	A	1	Total Zn 1 1	0
45	b	1	Total Zn 1 1	0
45	c	1	Total Zn 1 1	0
45	g	1	Total Zn 1 1	0

- Molecule 46 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

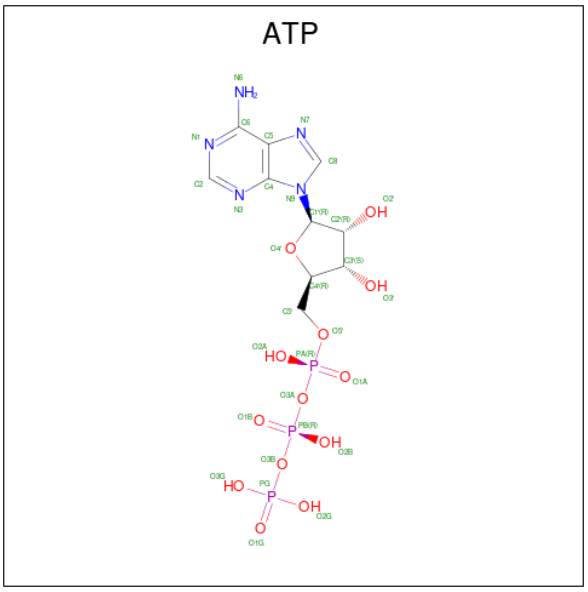


Mol	Chain	Residues	Atoms	AltConf
46	k	1	Total C N O P 27 10 5 10 2	0

- Molecule 47 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

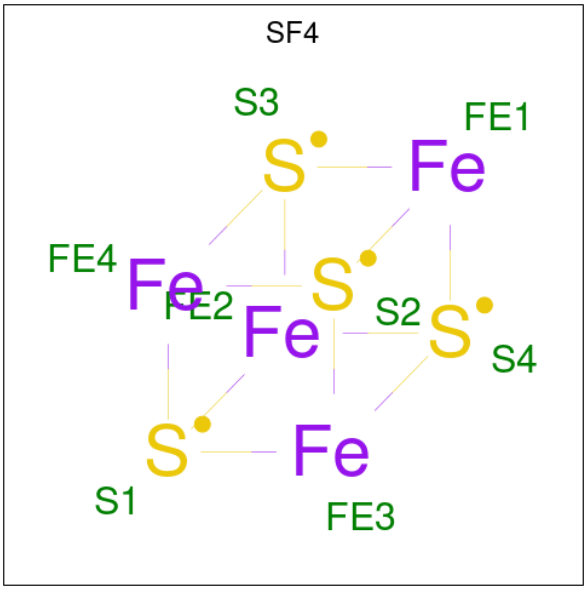
Mol	Chain	Residues	Atoms	AltConf
47	k	2	Total Mg 2 2	0

- Molecule 48 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 49 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



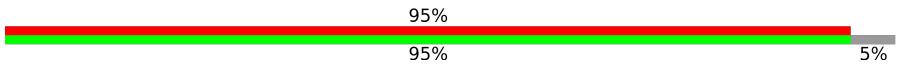
Mol	Chain	Residues	Atoms			AltConf
49	k	1	Total	Fe	S	0
			8	4	4	
49	k	1	Total	Fe	S	0
			8	4	4	

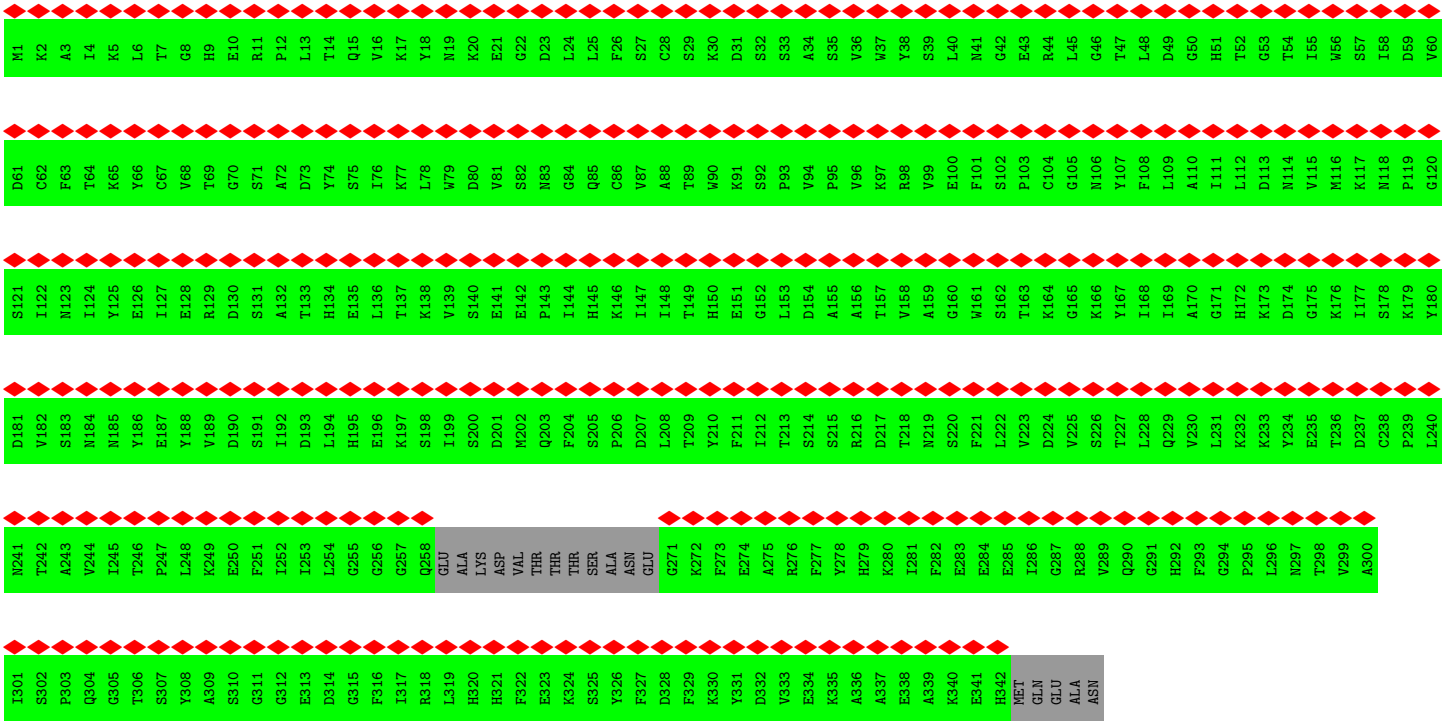
3 Residue-property plots (i)

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 I

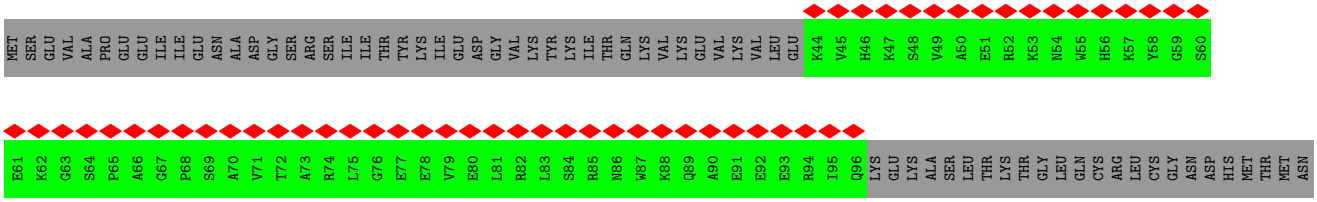
Chain l:

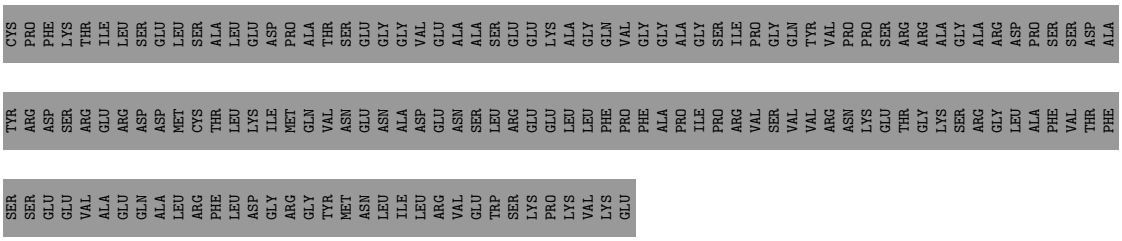




• Molecule 2: Eukaryotic translation initiation factor 3 subunit G

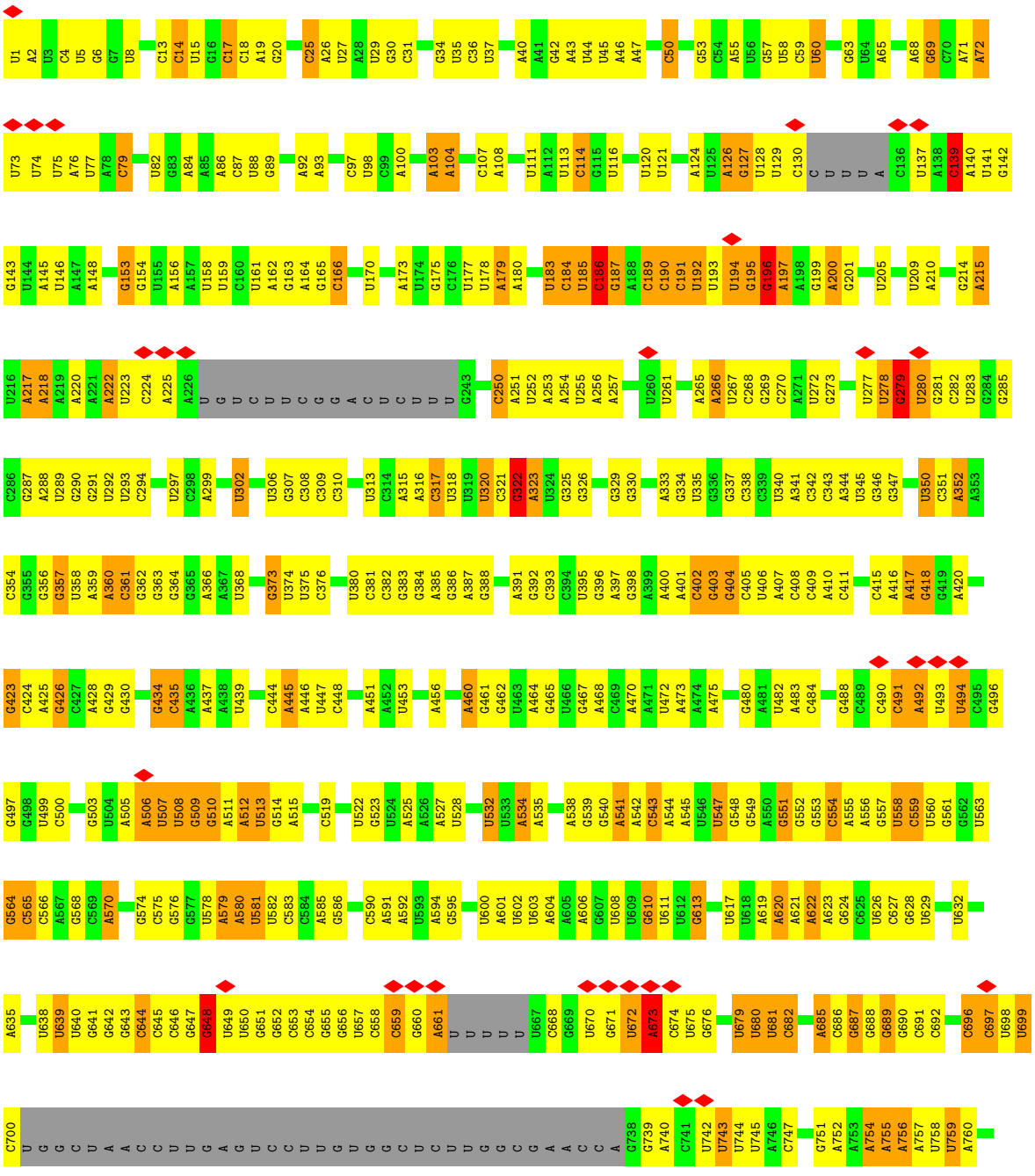
Chain r:

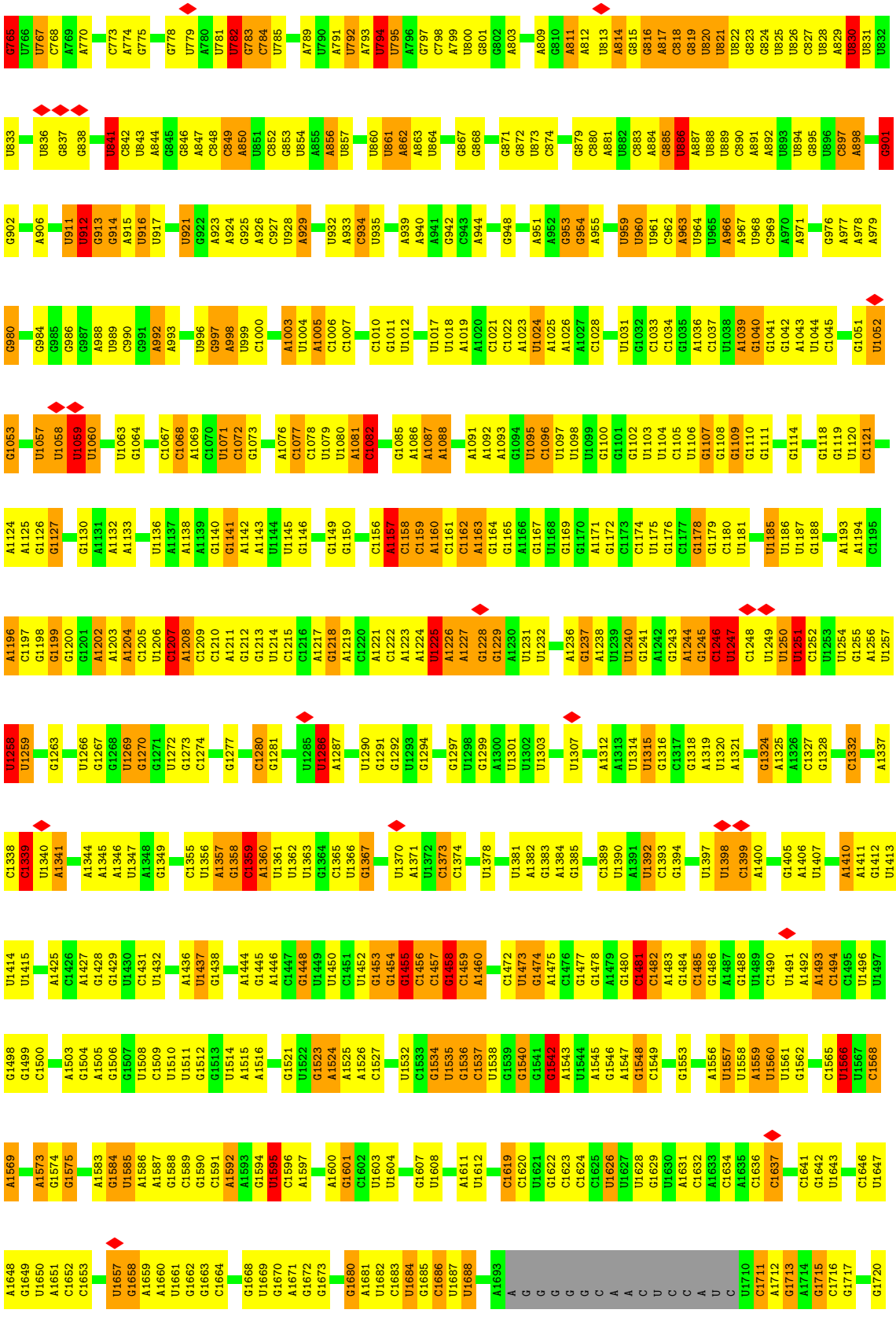


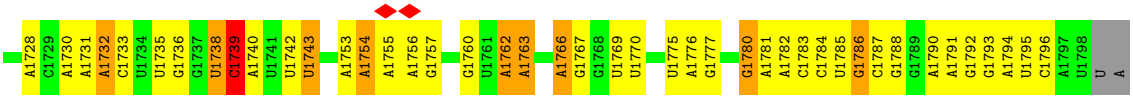


• Molecule 3: 18S ribosomal RNA (1719-MER)

Chain A:

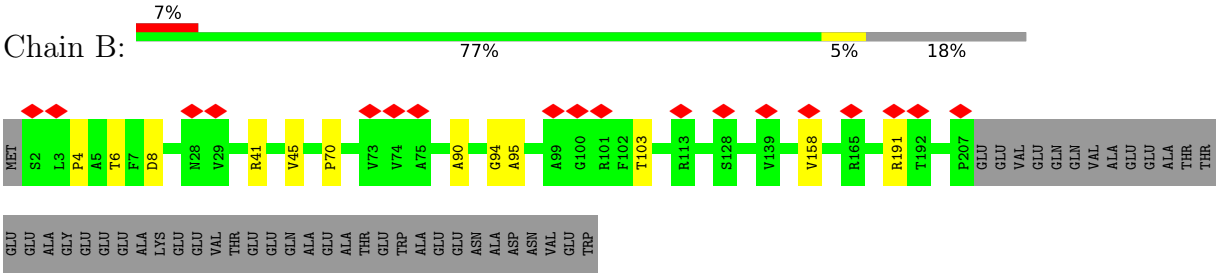






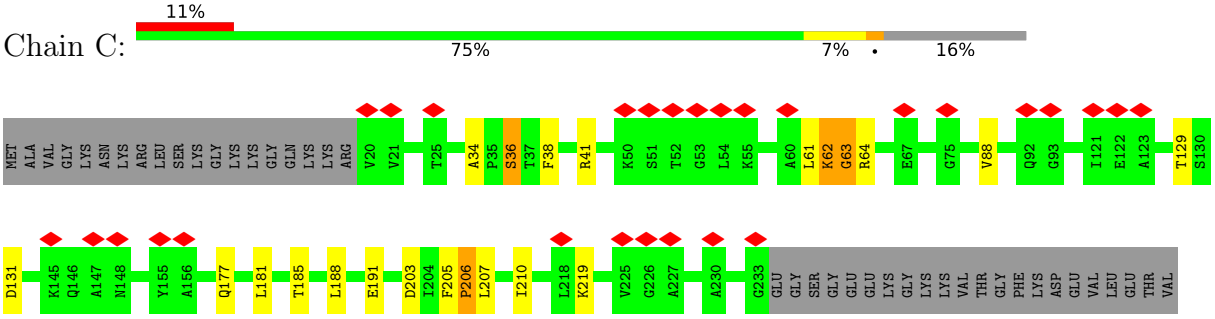
• Molecule 4: 40S ribosomal protein S0-A

Chain B:



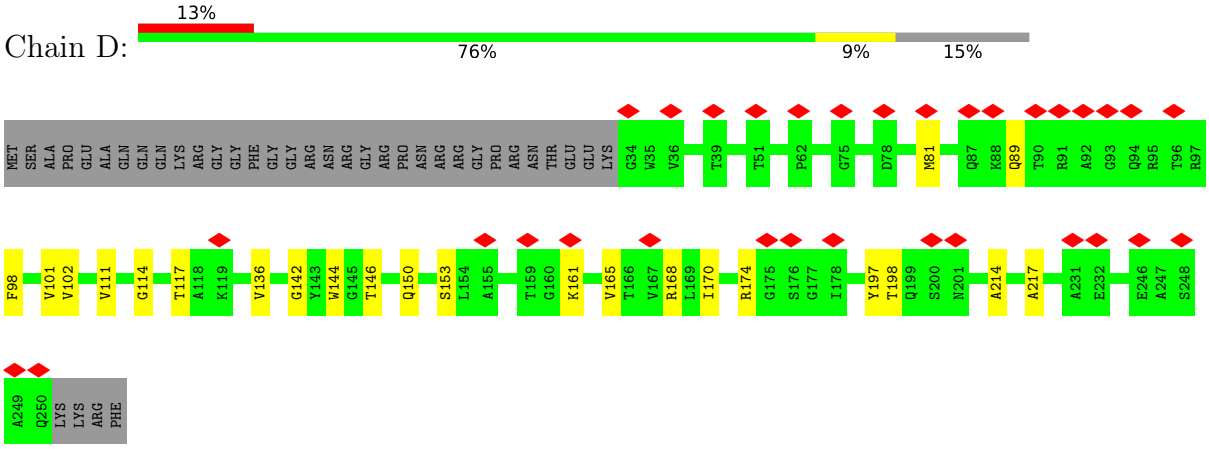
• Molecule 5: 40S ribosomal protein S1-A

Chain C:



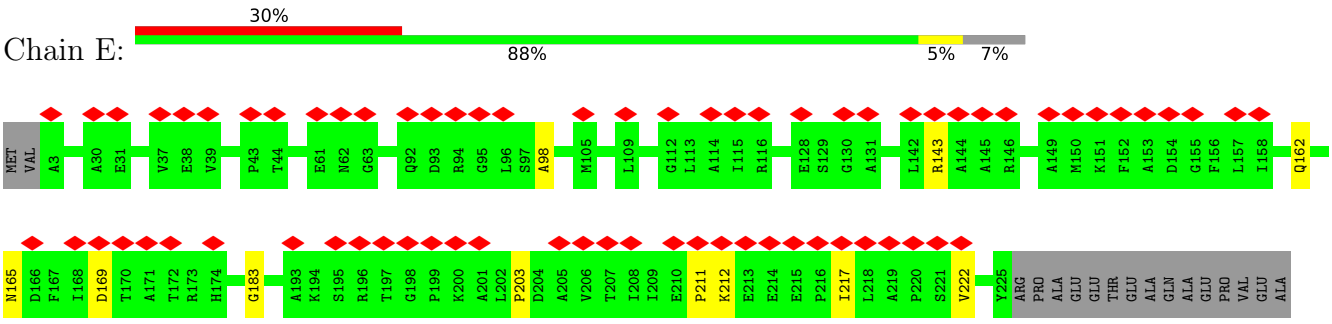
• Molecule 6: 40S ribosomal protein S2

Chain D:



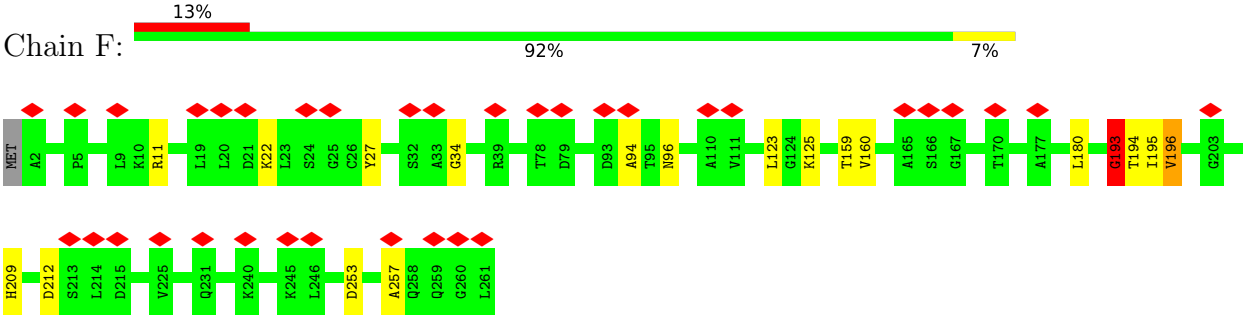
• Molecule 7: 40S ribosomal protein S3

Chain E:



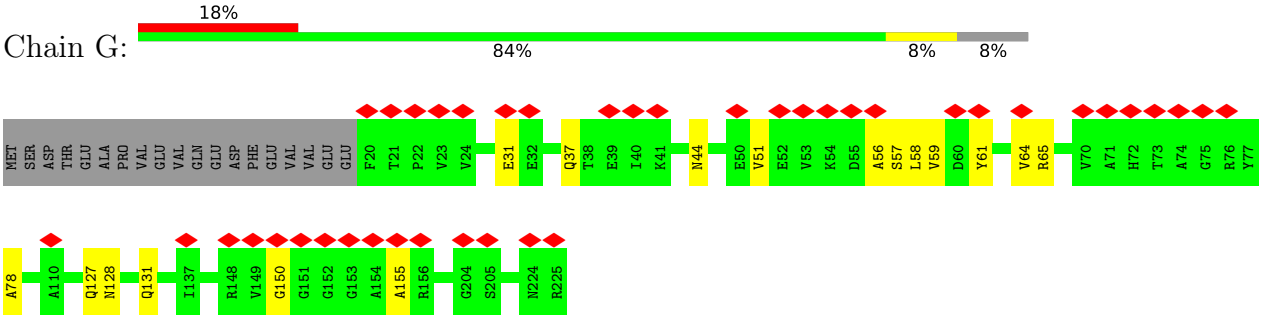
• Molecule 8: 40S ribosomal protein S4-A

Chain F:



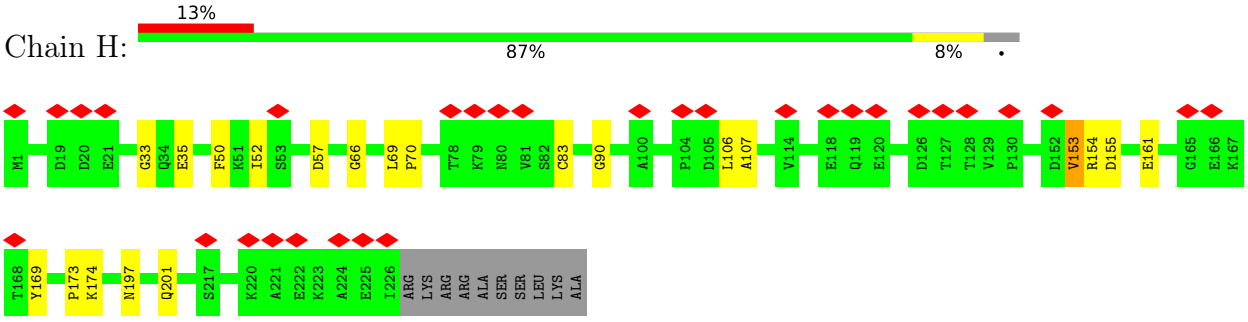
• Molecule 9: 40S ribosomal protein S5

Chain G:



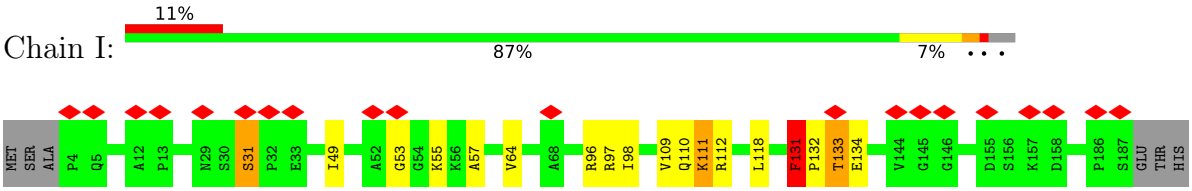
• Molecule 10: 40S ribosomal protein S6-A

Chain H:



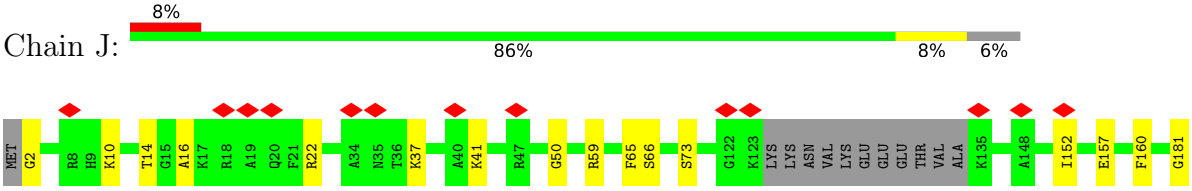
• Molecule 11: 40S ribosomal protein S7-A

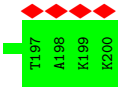
Chain I:



• Molecule 12: 40S ribosomal protein S8-A

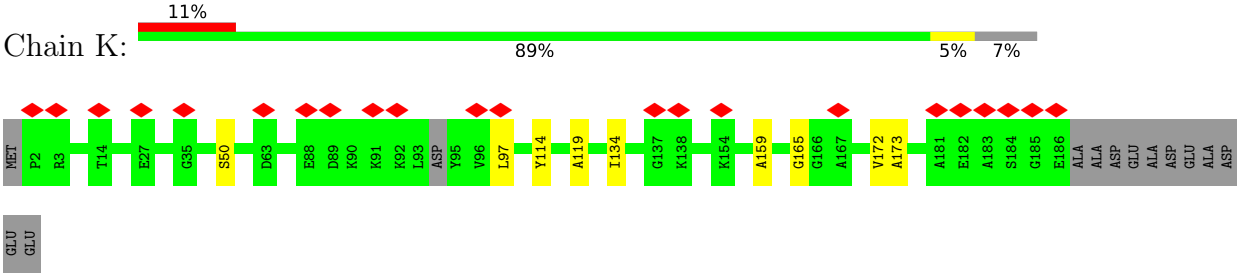
Chain J:





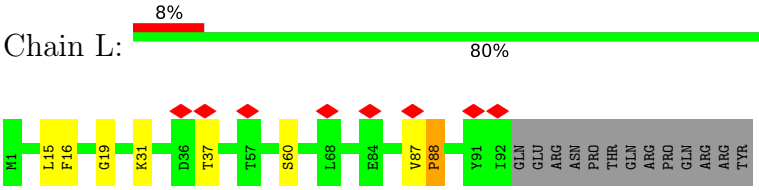
• Molecule 13: 40S ribosomal protein S9-A

Chain K:



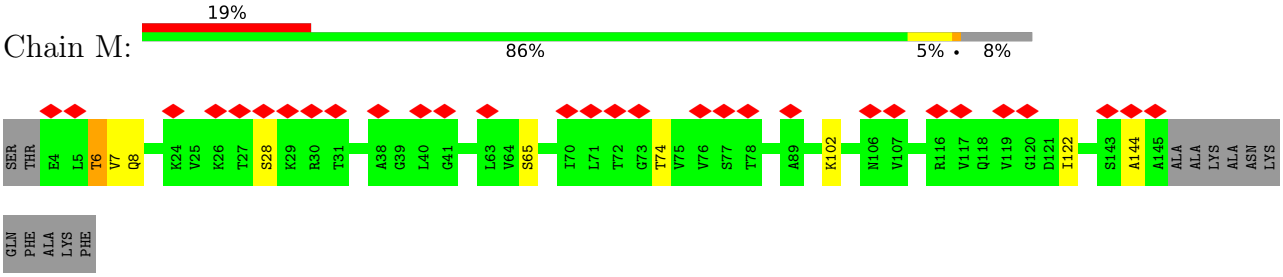
• Molecule 14: 40S ribosomal protein S10-A

Chain L:



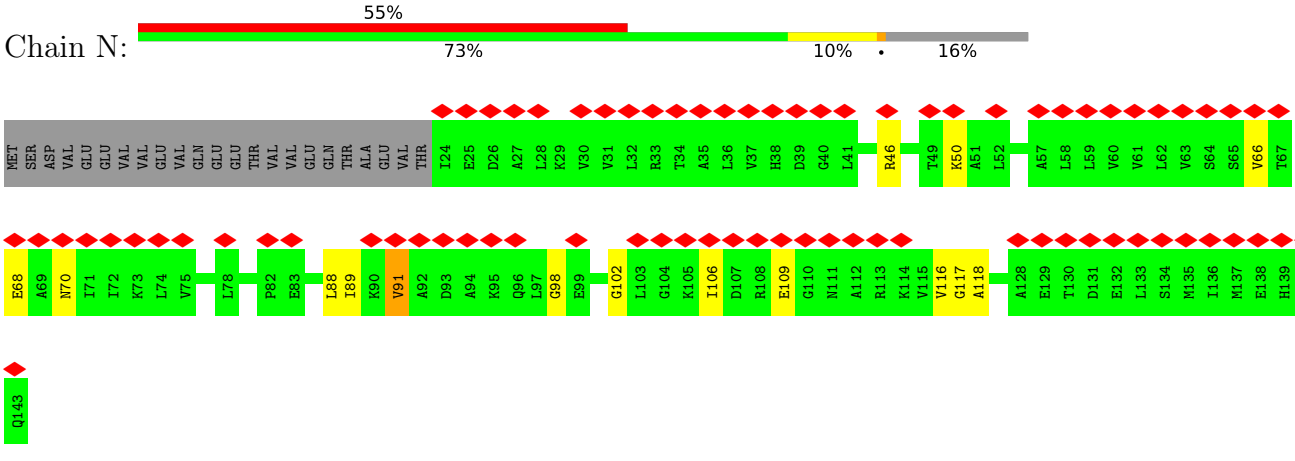
• Molecule 15: 40S ribosomal protein S11-A

Chain M:



• Molecule 16: 40S ribosomal protein S12

Chain N:

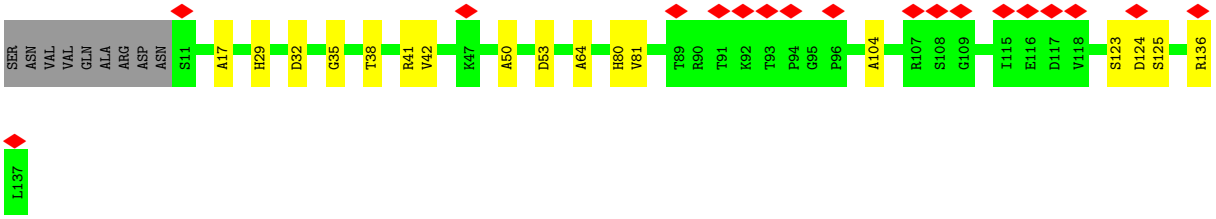


• Molecule 17: 40S ribosomal protein S13

Chain O:

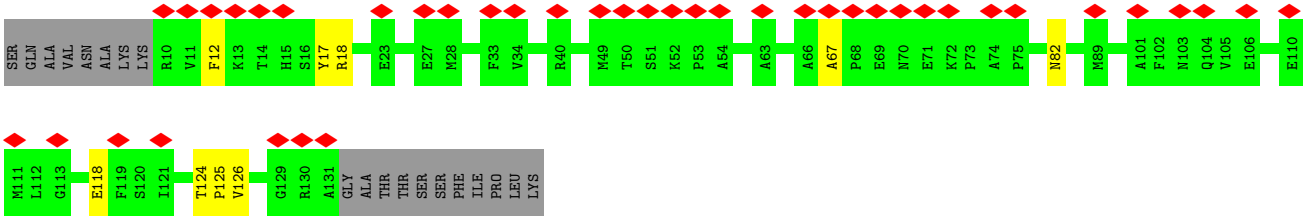
• Molecule 18: 40S ribosomal protein S14-A

Chain P:



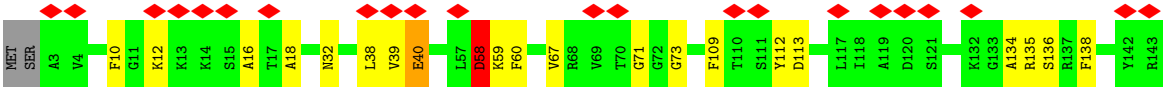
• Molecule 19: 40S ribosomal protein S15

Chain Q:



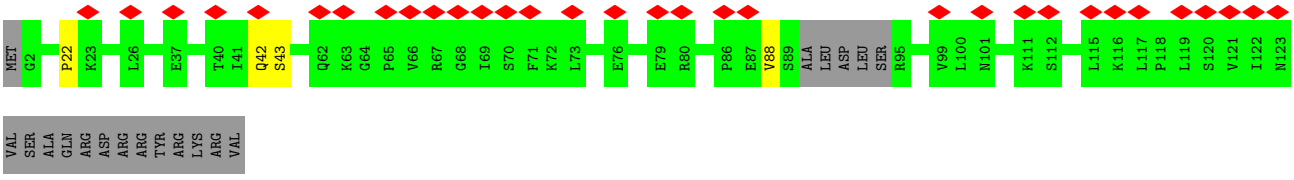
• Molecule 20: 40S ribosomal protein S16-A

Chain R:



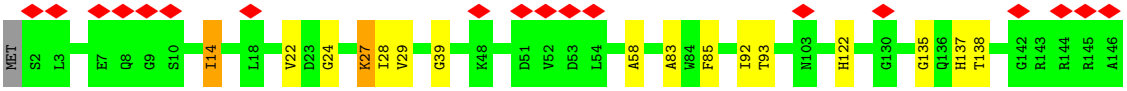
• Molecule 21: 40S ribosomal protein S17-A

Chain S:

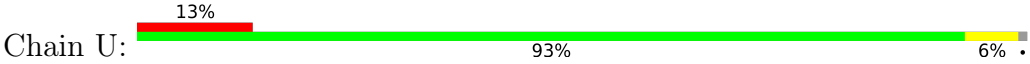


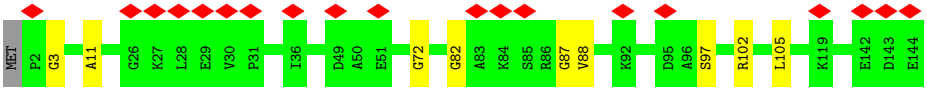
• Molecule 22: 40S ribosomal protein S18-A

Chain T:

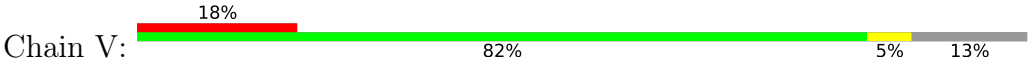


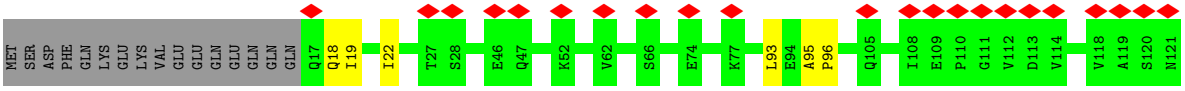
• Molecule 23: 40S ribosomal protein S19-A



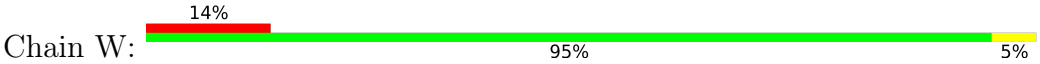


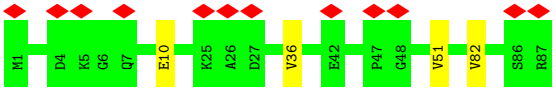
• Molecule 24: 40S ribosomal protein S20



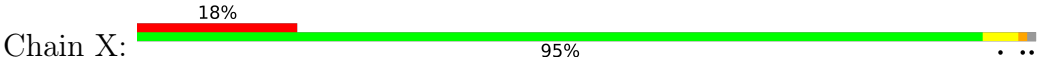


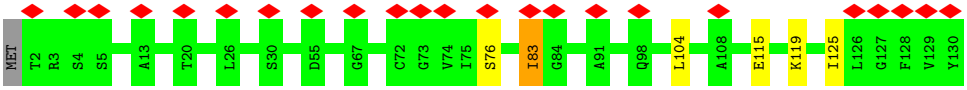
• Molecule 25: 40S ribosomal protein S21-A



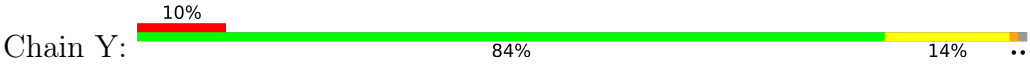


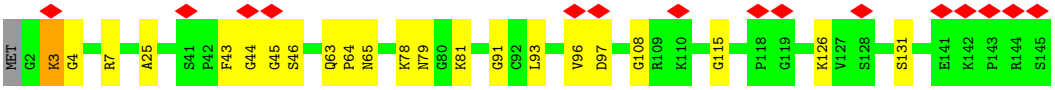
• Molecule 26: 40S ribosomal protein S22-A



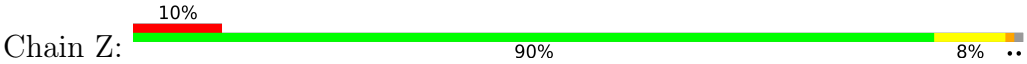


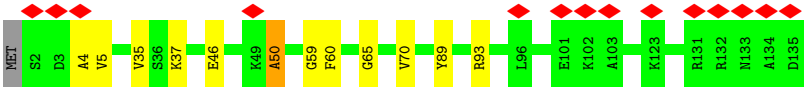
• Molecule 27: 40S ribosomal protein S23-A





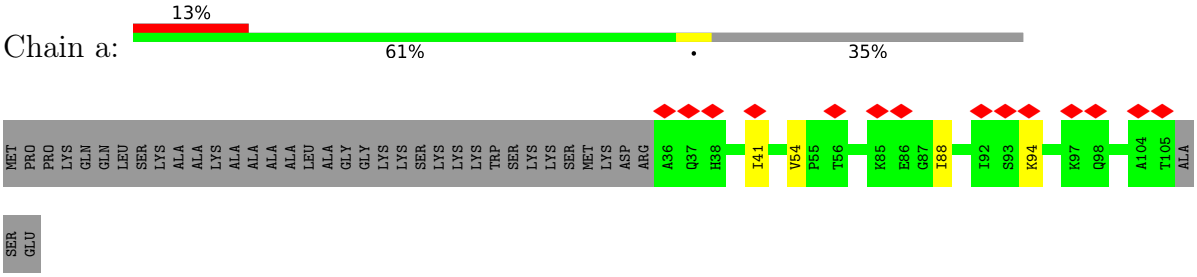
• Molecule 28: 40S ribosomal protein S24-A





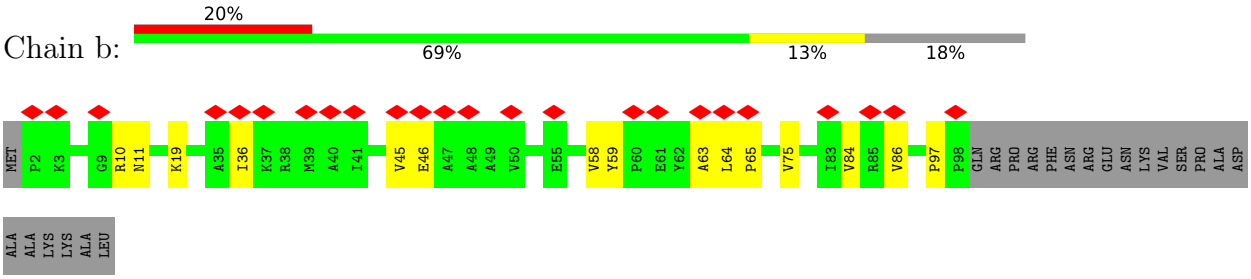
• Molecule 29: 40S ribosomal protein S25-A

Chain a:



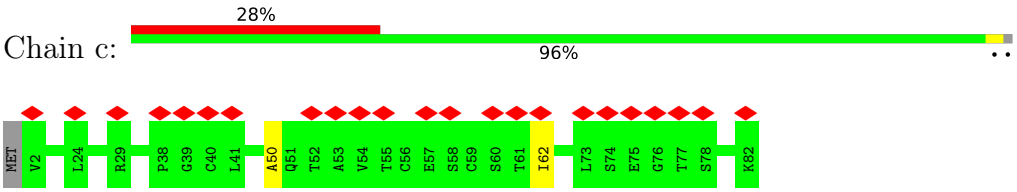
• Molecule 30: 40S ribosomal protein S26-A

Chain b:



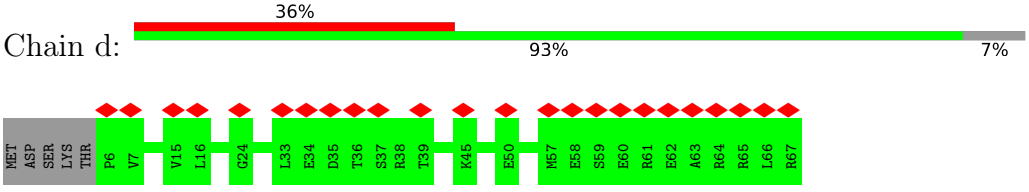
• Molecule 31: 40S ribosomal protein S27-A

Chain c:



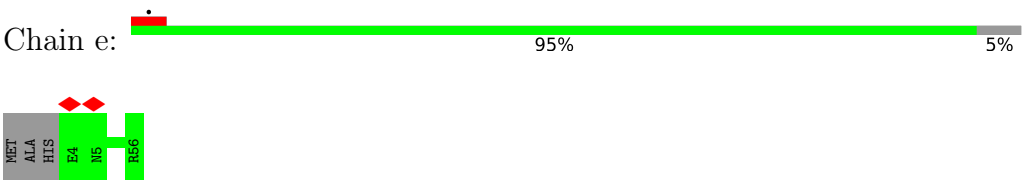
• Molecule 32: 40S ribosomal protein S28-B

Chain d:



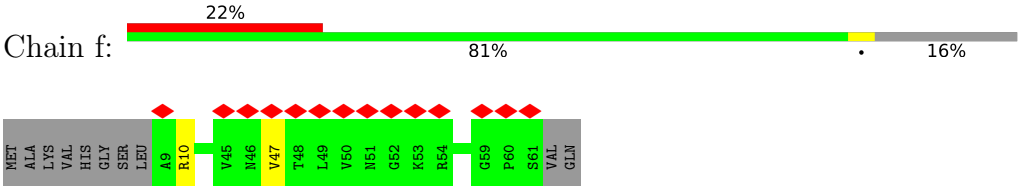
• Molecule 33: 40S ribosomal protein S29-A

Chain e:



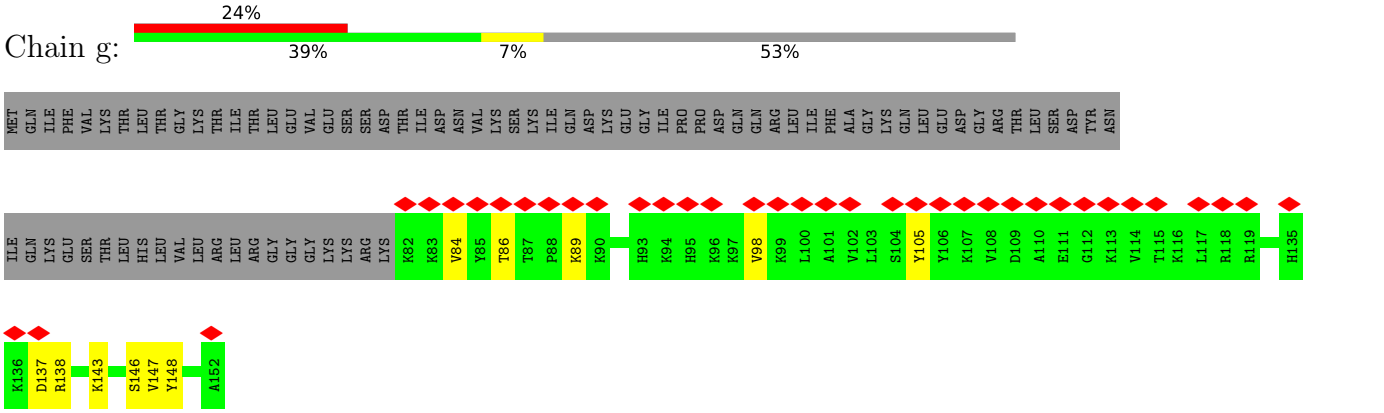
• Molecule 34: 40S ribosomal protein S30-A

Chain f:



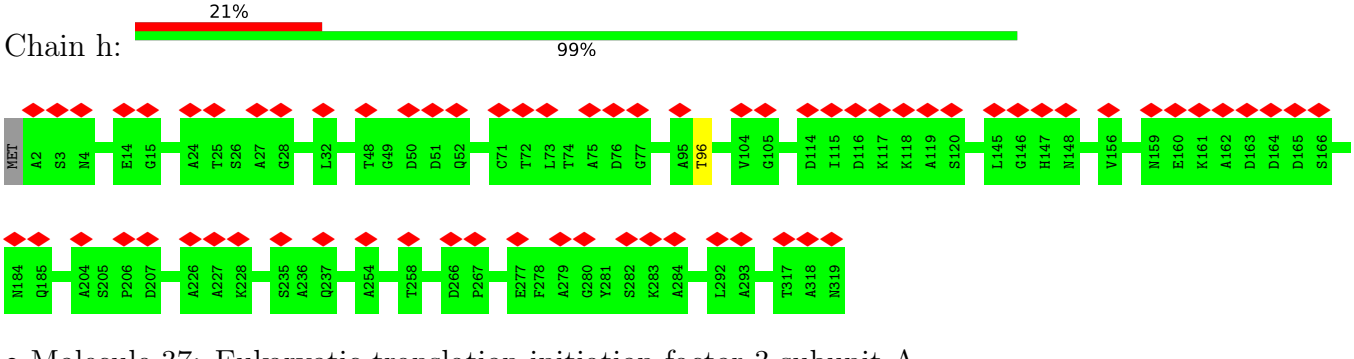
• Molecule 35: Ubiquitin-40S ribosomal protein S31

Chain g:



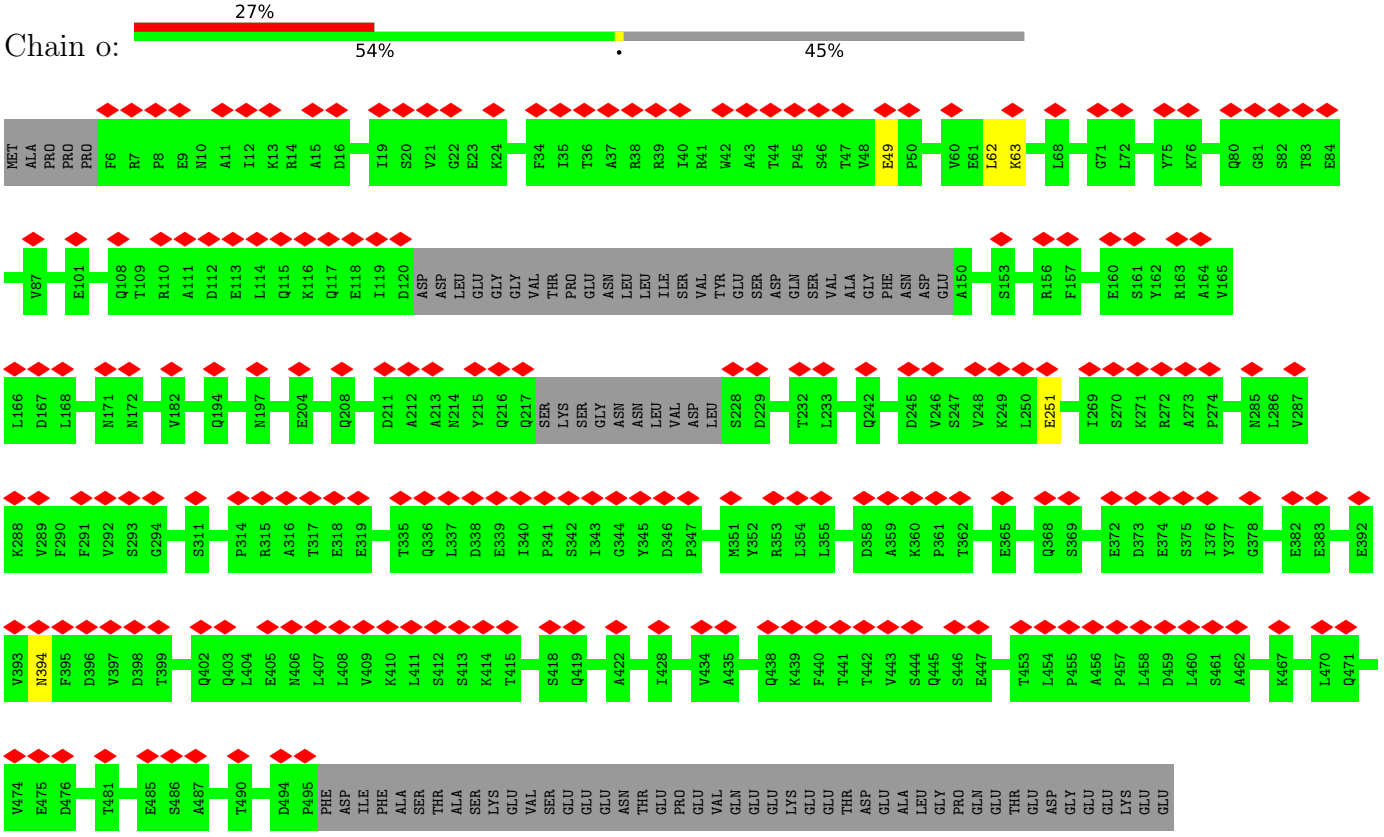
• Molecule 36: Guanine nucleotide-binding protein subunit beta-like protein

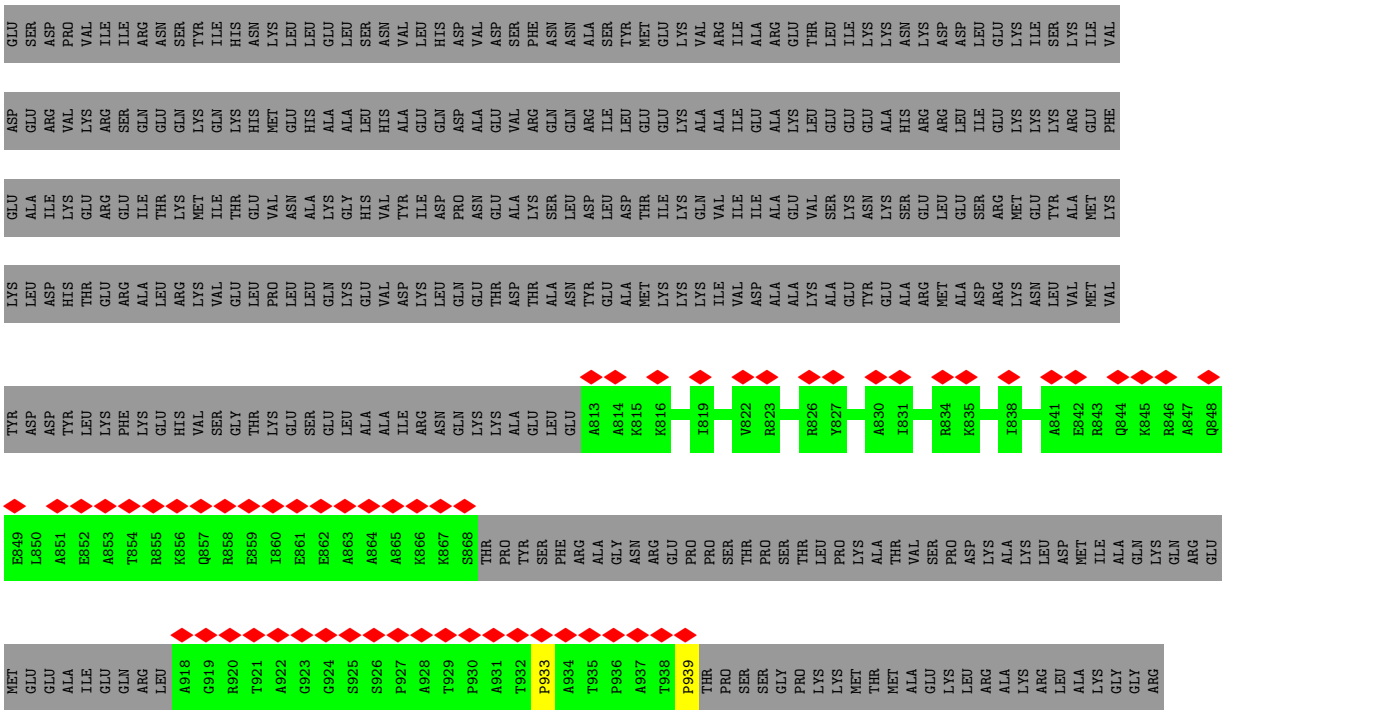
Chain h:



• Molecule 37: Eukaryotic translation initiation factor 3 subunit A

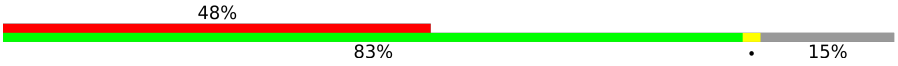
Chain o:

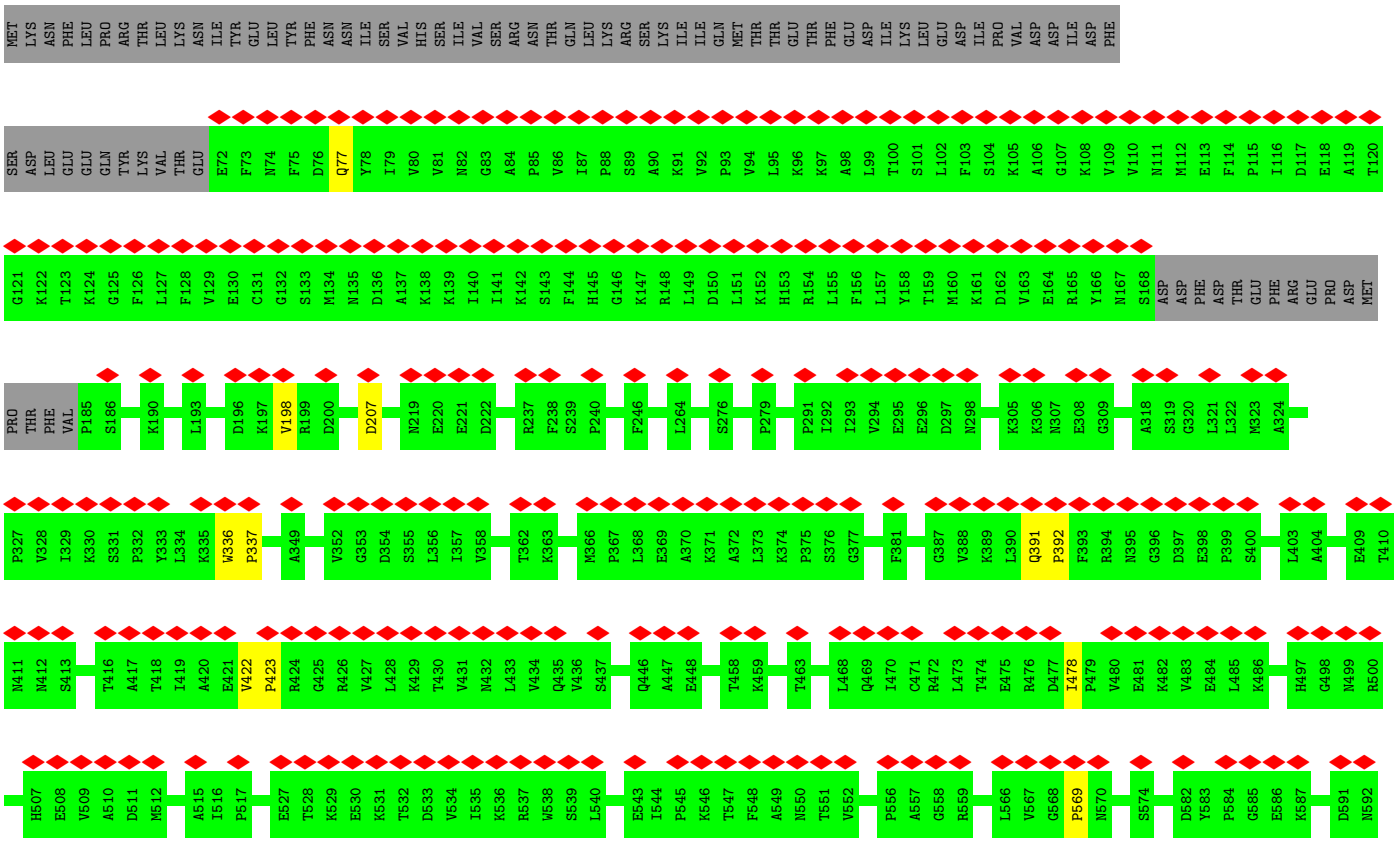


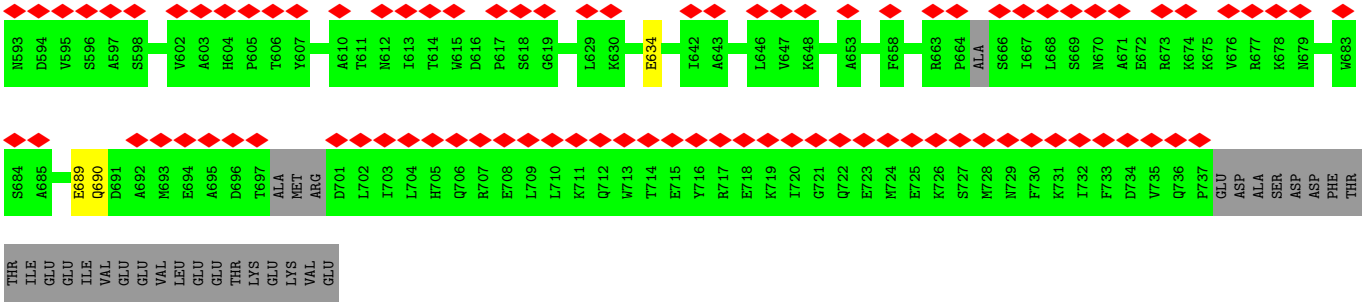


• Molecule 38: Eukaryotic translation initiation factor 3 subunit B

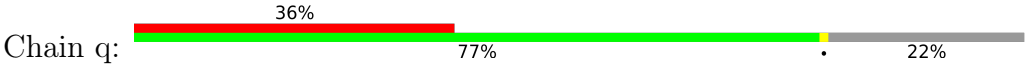
Chain p:

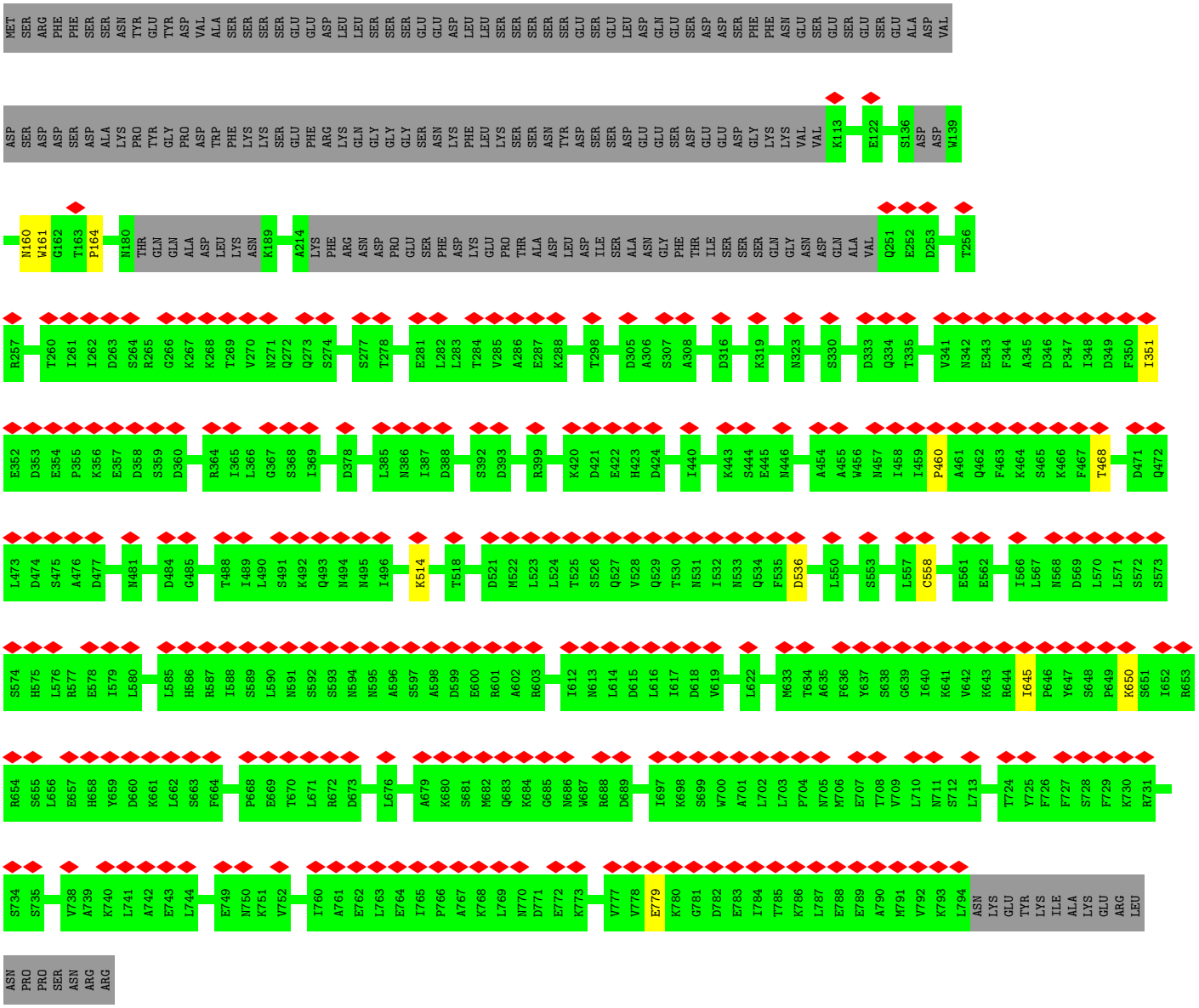






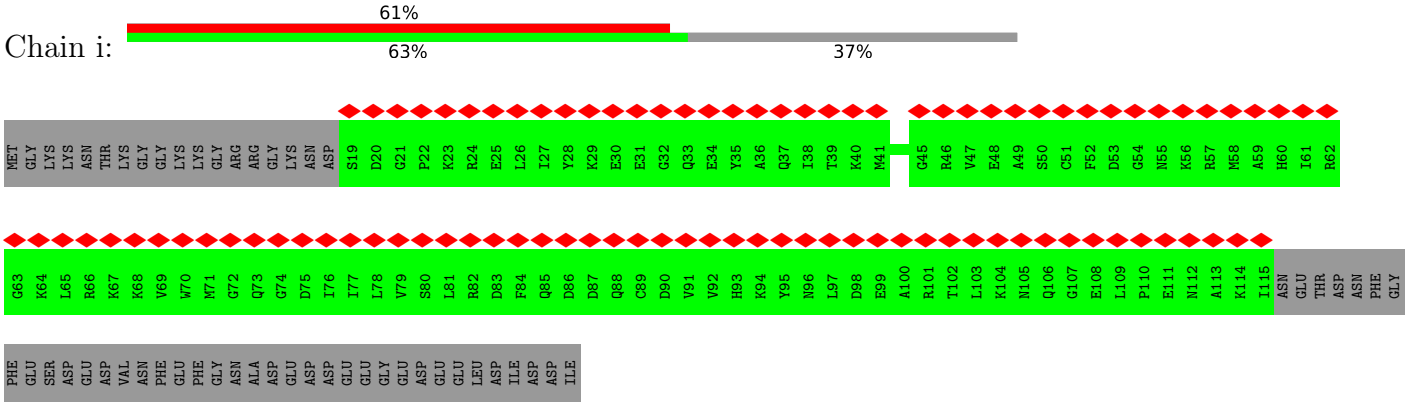
• Molecule 39: Eukaryotic translation initiation factor 3 subunit C





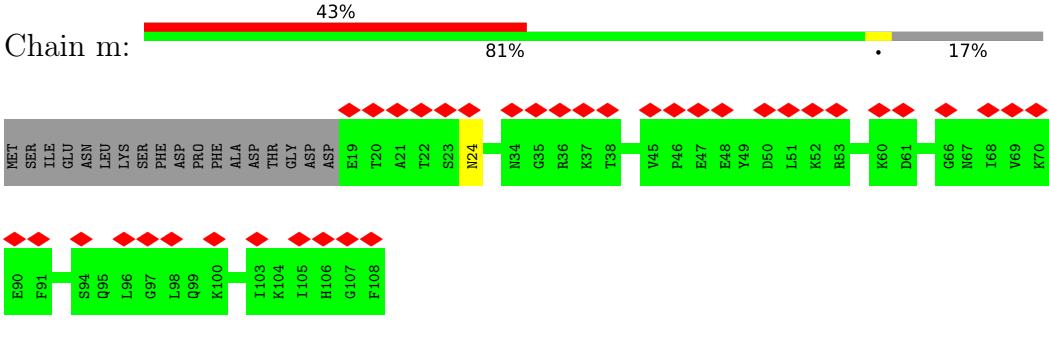
• Molecule 40: Eukaryotic translation initiation factor 1A

Chain i:



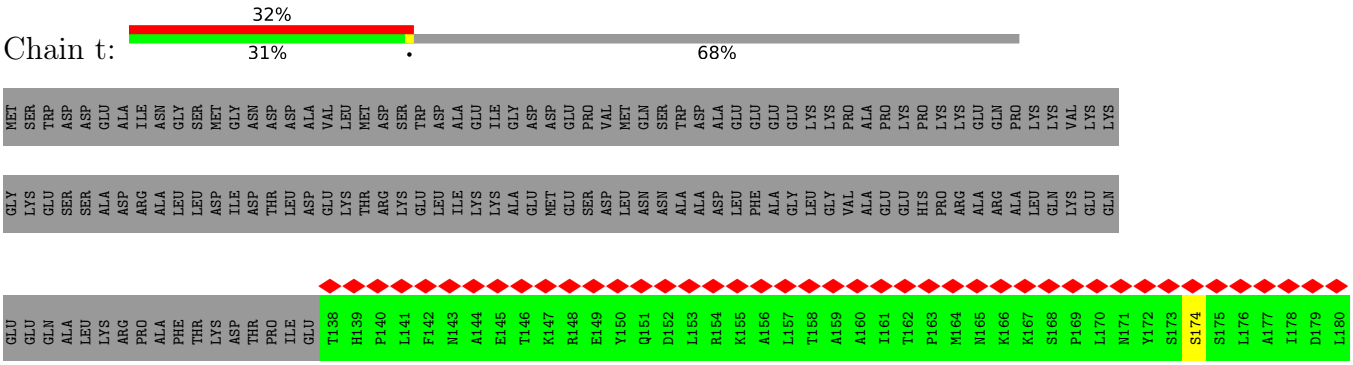
• Molecule 41: Eukaryotic translation initiation factor eIF-1

Chain m:



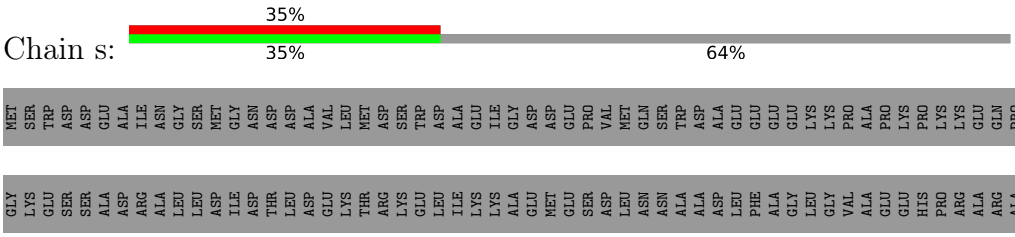
• Molecule 42: Eukaryotic translation initiation factor 3 subunit J

Chain t:



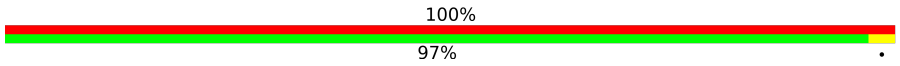
• Molecule 42: Eukaryotic translation initiation factor 3 subunit J

Chain s:



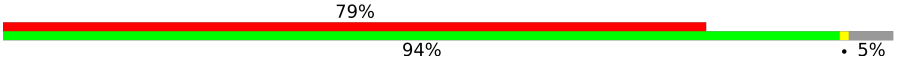
• Molecule 43: RNA recognition motif (unknown)

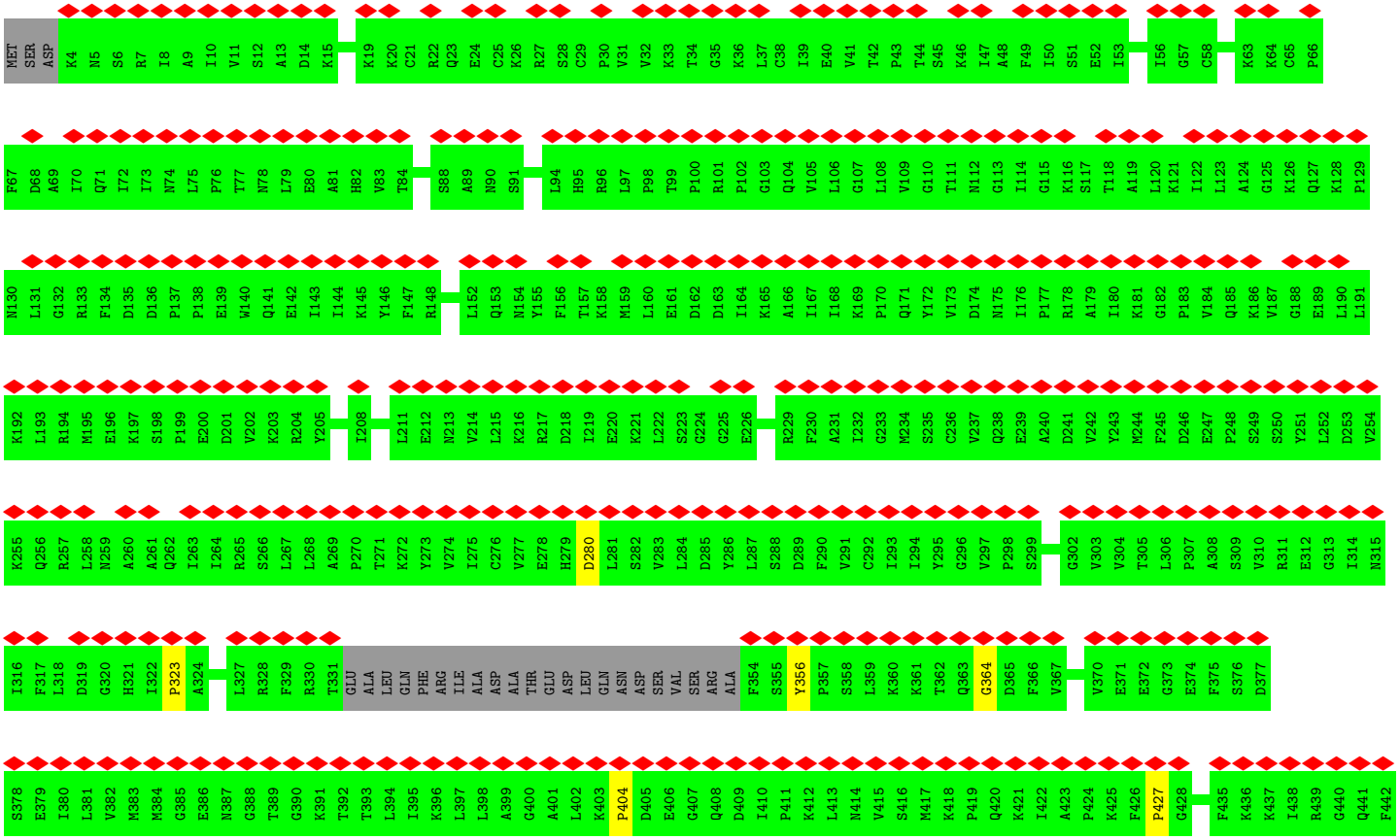
Chain j:

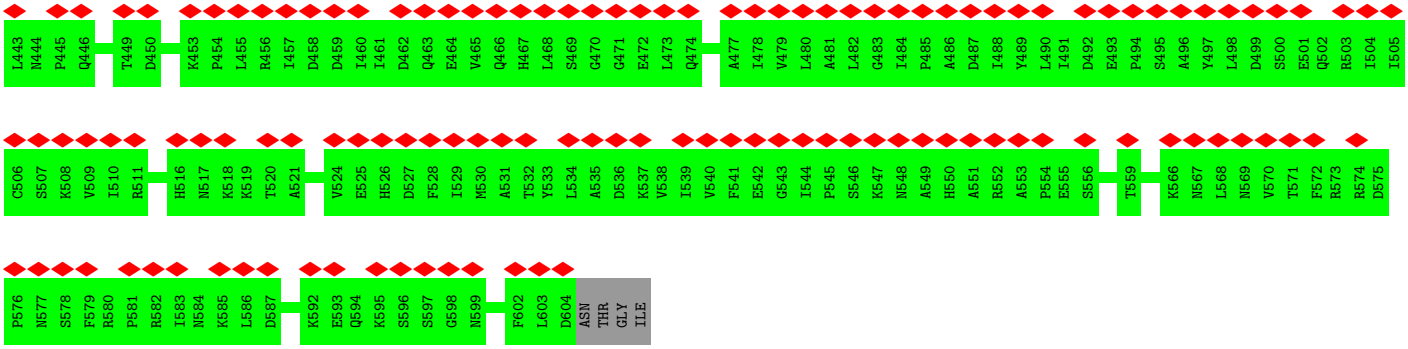


• Molecule 44: Translation initiation factor RLI1

Chain k:






L443 N444 P445 Q446 T449 D450 K453 P454 L455 R456 I457 D458 D459 I460 I461 D462 Q463 E464 V465 Q466 H467 L468 S469 G470 G471 E472 L473 Q474 A477 I478 V479 L480 A481 L482 G483 I484 P485 A486 D487 I488 Y489 L490 I491 D492 E493 P494 S495 A496 Y497 L498 D499 S500 E501 Q502 R503 I504 I505
C506 S507 K508 V509 I510 R511 H516 N517 K518 K519 T520 A521 V524 E525 H526 D527 F528 I529 M530 A531 T532 Y533 L534 A535 D536 K537 V538 I539 V540 F541 E542 G543 I544 P545 S546 K547 N548 A549 H550 A551 R552 A553 P554 E555 S556 T559 K566 N567 L568 N569 V570 T571 F572 R573 R574 D575
P576 N577 S578 F579 R580 P581 R582 I583 N584 K585 L586 D587 K592 E593 Q594 K595 S596 S597 G598 N599 F602 L603 D604 ASN THR GLY ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20618	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, SF4, ATP, ADP

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	l	0.31	0/1622	0.52	0/2252
2	r	0.26	0/260	0.47	0/360
3	A	0.78	8/40986 (0.0%)	1.17	307/63859 (0.5%)
4	B	0.30	0/1019	0.62	0/1419
5	C	0.28	0/1060	0.64	1/1477 (0.1%)
6	D	0.30	0/1062	0.63	0/1472
7	E	0.30	0/1097	0.58	0/1524
8	F	0.30	0/1275	0.67	1/1769 (0.1%)
9	G	0.27	0/1019	0.58	0/1419
10	H	0.28	0/1112	0.55	0/1545
11	I	0.31	0/912	0.63	0/1271
12	J	0.30	0/922	0.60	0/1278
13	K	0.28	0/908	0.59	0/1262
14	L	0.28	0/455	0.69	0/633
15	M	0.33	0/701	0.70	0/975
16	N	0.29	0/589	0.66	0/817
17	O	0.31	0/741	0.58	0/1031
18	P	0.33	0/619	0.61	0/856
19	Q	0.52	1/600 (0.2%)	0.63	0/833
20	R	0.34	0/692	0.65	0/960
21	S	0.29	0/577	0.56	0/801
22	T	0.31	0/714	0.62	0/992
23	U	0.31	0/699	0.58	0/968
24	V	0.32	0/520	0.62	0/724
25	W	0.29	0/428	0.61	0/594
26	X	0.31	0/633	0.65	0/878
27	Y	0.32	0/703	0.70	0/973
28	Z	0.26	0/660	0.62	1/917 (0.1%)
29	a	0.30	0/346	0.65	0/481
30	b	0.81	1/481 (0.2%)	0.72	1/670 (0.1%)
31	c	0.28	0/399	0.64	0/554
32	d	0.29	0/304	0.60	0/421

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.34	0/259	0.76	0/358
34	f	0.28	0/260	0.55	0/360
35	g	0.38	0/350	0.90	0/486
36	h	0.27	0/1567	0.57	0/2179
37	o	0.41	0/2626	0.56	1/3660 (0.0%)
38	p	0.40	0/3197	0.57	0/4452
39	q	0.49	0/3165	0.58	0/4418
40	i	0.34	0/475	0.55	0/658
41	m	0.40	0/442	0.55	0/613
42	s	0.56	0/469	1.09	2/652 (0.3%)
42	t	0.58	0/417	1.12	1/581 (0.2%)
43	j	0.16	0/384	0.29	0/536
44	k	0.57	0/2858	0.98	0/3977
All	All	0.62	10/80584 (0.0%)	0.97	315/118915 (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
4	B	0	1
5	C	0	4
6	D	0	1
8	F	0	1
9	G	0	3
11	I	0	3
15	M	0	1
16	N	0	3
18	P	0	1
19	Q	0	2
20	R	0	3
21	S	0	1
22	T	0	2
26	X	0	1
27	Y	0	1
28	Z	0	2
29	a	0	2
30	b	0	2
31	c	0	1
35	g	0	4
36	h	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
38	p	0	2
All	All	0	42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	59	TYR	C-N	16.37	1.65	1.34
19	Q	67	ALA	C-N	9.85	1.52	1.34
3	A	649	U	O3'-P	7.34	1.70	1.61
3	A	652	G	O3'-P	6.58	1.69	1.61
3	A	685	A	O3'-P	6.01	1.68	1.61

The worst 5 of 315 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	190	C	N3-C2-O2	-11.94	113.54	121.90
3	A	543	C	N1-C2-O2	11.31	125.68	118.90
3	A	190	C	N1-C2-O2	10.57	125.24	118.90
3	A	873	U	N3-C2-O2	-10.21	115.05	122.20
3	A	638	U	N1-C2-O2	9.97	129.78	122.80

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	94	GLY	Peptide
5	C	131	ASP	Peptide
5	C	205	PHE	Peptide
5	C	206	PRO	Peptide
5	C	36	SER	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	l	1624	0	727	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	r	261	0	122	0	0
3	A	36643	0	18433	736	0
4	B	1020	0	474	5	0
5	C	1061	0	473	10	0
6	D	1063	0	499	11	0
7	E	1098	0	525	8	0
8	F	1276	0	576	11	0
9	G	1020	0	482	9	0
10	H	1113	0	510	11	0
11	I	913	0	400	14	0
12	J	924	0	452	12	0
13	K	910	0	419	6	0
14	L	456	0	196	3	0
15	M	702	0	304	6	0
16	N	590	0	286	7	0
17	O	742	0	345	7	0
18	P	620	0	311	13	0
19	Q	601	0	277	6	0
20	R	693	0	323	11	0
21	S	579	0	246	2	0
22	T	715	0	318	18	0
23	U	700	0	334	10	0
24	V	521	0	217	3	0
25	W	429	0	201	1	0
26	X	634	0	289	3	0
27	Y	704	0	324	21	0
28	Z	661	0	312	5	0
29	a	347	0	158	0	0
30	b	482	0	223	0	0
31	c	400	0	180	0	0
32	d	305	0	133	0	0
33	e	260	0	112	0	0
34	f	261	0	113	0	0
35	g	351	0	158	0	0
36	h	1568	0	754	0	0
37	o	2631	0	1207	0	0
38	p	3201	0	1397	0	0
39	q	3169	0	1372	0	0
40	i	476	0	215	0	0
41	m	443	0	193	0	0
42	s	470	0	223	0	0
42	t	418	0	191	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	j	385	0	387	0	0
44	k	2860	0	1246	0	0
45	A	1	0	0	0	0
45	b	1	0	0	0	0
45	c	1	0	0	0	0
45	g	1	0	0	0	0
46	k	27	0	12	0	0
47	k	2	0	0	0	0
48	k	31	0	12	0	0
49	k	16	0	0	0	0
All	All	76380	0	36661	844	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 10.

The worst 5 of 844 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)
3:A:1103:U:OP2	27:Y:7:ARG:N	1.84	1.10
3:A:1179:G:H21	3:A:1460:A:N6	1.49	1.09
3:A:1525:A:OP1	23:U:82:GLY:HA2	1.53	1.07
3:A:1646:C:N4	3:A:1754:A:H61	1.53	1.05
3:A:856:A:H62	11:I:97:ARG:H	1.05	1.03

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	l	326/347 (94%)	318 (98%)	8 (2%)	0	100	100
2	r	51/274 (19%)	48 (94%)	3 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	B	204/252 (81%)	174 (85%)	26 (13%)	4 (2%)	6 30
5	C	212/255 (83%)	162 (76%)	45 (21%)	5 (2%)	5 26
6	D	215/254 (85%)	194 (90%)	19 (9%)	2 (1%)	14 51
7	E	221/240 (92%)	202 (91%)	15 (7%)	4 (2%)	7 33
8	F	258/261 (99%)	226 (88%)	30 (12%)	2 (1%)	16 54
9	G	204/225 (91%)	178 (87%)	21 (10%)	5 (2%)	4 26
10	H	224/236 (95%)	209 (93%)	9 (4%)	6 (3%)	4 25
11	I	182/190 (96%)	153 (84%)	20 (11%)	9 (5%)	2 16
12	J	184/200 (92%)	160 (87%)	23 (12%)	1 (0%)	25 64
13	K	180/197 (91%)	160 (89%)	19 (11%)	1 (1%)	22 60
14	L	90/105 (86%)	77 (86%)	10 (11%)	3 (3%)	3 20
15	M	140/155 (90%)	128 (91%)	10 (7%)	2 (1%)	9 39
16	N	118/143 (82%)	85 (72%)	29 (25%)	4 (3%)	3 20
17	O	148/151 (98%)	134 (90%)	12 (8%)	2 (1%)	9 39
18	P	125/136 (92%)	112 (90%)	12 (10%)	1 (1%)	16 54
19	Q	120/141 (85%)	100 (83%)	17 (14%)	3 (2%)	4 26
20	R	139/143 (97%)	121 (87%)	14 (10%)	4 (3%)	3 23
21	S	113/136 (83%)	100 (88%)	12 (11%)	1 (1%)	14 51
22	T	143/146 (98%)	122 (85%)	18 (13%)	3 (2%)	5 29
23	U	141/144 (98%)	125 (89%)	16 (11%)	0	100 100
24	V	103/121 (85%)	98 (95%)	5 (5%)	0	100 100
25	W	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	5 26
26	X	127/130 (98%)	115 (91%)	11 (9%)	1 (1%)	16 54
27	Y	142/145 (98%)	119 (84%)	19 (13%)	4 (3%)	4 24
28	Z	132/135 (98%)	121 (92%)	8 (6%)	3 (2%)	5 27
29	a	68/108 (63%)	52 (76%)	14 (21%)	2 (3%)	3 23
30	b	95/119 (80%)	67 (70%)	17 (18%)	11 (12%)	0 5
31	c	79/82 (96%)	70 (89%)	8 (10%)	1 (1%)	10 41
32	d	60/67 (90%)	51 (85%)	9 (15%)	0	100 100
33	e	51/56 (91%)	49 (96%)	2 (4%)	0	100 100
34	f	51/63 (81%)	47 (92%)	2 (4%)	2 (4%)	2 18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	g	69/152 (45%)	44 (64%)	18 (26%)	7 (10%)	0 7
36	h	316/319 (99%)	298 (94%)	18 (6%)	0	100 100
37	o	519/964 (54%)	483 (93%)	30 (6%)	6 (1%)	11 43
38	p	638/763 (84%)	583 (91%)	43 (7%)	12 (2%)	6 31
39	q	628/812 (77%)	568 (90%)	48 (8%)	12 (2%)	6 31
40	i	95/153 (62%)	82 (86%)	13 (14%)	0	100 100
41	m	88/108 (82%)	77 (88%)	8 (9%)	3 (3%)	3 20
42	s	93/265 (35%)	87 (94%)	5 (5%)	1 (1%)	12 46
42	t	82/265 (31%)	74 (90%)	7 (8%)	1 (1%)	11 43
43	j	75/77 (97%)	68 (91%)	5 (7%)	2 (3%)	4 25
44	k	575/608 (95%)	522 (91%)	47 (8%)	6 (1%)	13 49
All	All	7909/9930 (80%)	7035 (89%)	736 (9%)	138 (2%)	10 35

5 of 138 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	C	207	LEU
10	H	153	VAL
11	I	109	VAL
14	L	87	VAL
14	L	88	PRO

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	A	1713/1800 (95%)	500 (29%)	35 (2%)

5 of 500 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	A	2	A
3	A	4	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	17	C
3	A	25	C
3	A	26	A

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	1250	U
3	A	1339	C
3	A	1493	A
3	A	507	U
3	A	417	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
49	SF4	k	705	-	0,12,12	-	-	-		
46	ADP	k	701	47	24,29,29	0.95	1 (4%)	29,45,45	1.46	4 (13%)
49	SF4	k	706	-	0,12,12	-	-	-		
48	ATP	k	703	44,47	26,33,33	0.93	1 (3%)	31,52,52	1.60	5 (16%)

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
49	SF4	k	705	-	-	-	0/6/5/5
46	ADP	k	701	47	-	5/12/32/32	0/3/3/3
49	SF4	k	706	-	-	-	0/6/5/5
48	ATP	k	703	44,47	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	k	703	ATP	C5-C4	2.50	1.47	1.40
46	k	701	ADP	C5-C4	2.47	1.47	1.40

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	k	701	ADP	PA-O3A-PB	-3.70	120.12	132.83
48	k	703	ATP	PB-O3B-PG	-3.64	120.35	132.83
48	k	703	ATP	PA-O3A-PB	-3.49	120.84	132.83
48	k	703	ATP	C3'-C2'-C1'	3.43	106.14	100.98
48	k	703	ATP	N3-C2-N1	-3.19	123.69	128.68

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	k	701	ADP	C5'-O5'-PA-O1A
46	k	701	ADP	C5'-O5'-PA-O2A
48	k	703	ATP	O4'-C4'-C5'-O5'
46	k	701	ADP	PA-O3A-PB-O2B
46	k	701	ADP	C5'-O5'-PA-O3A

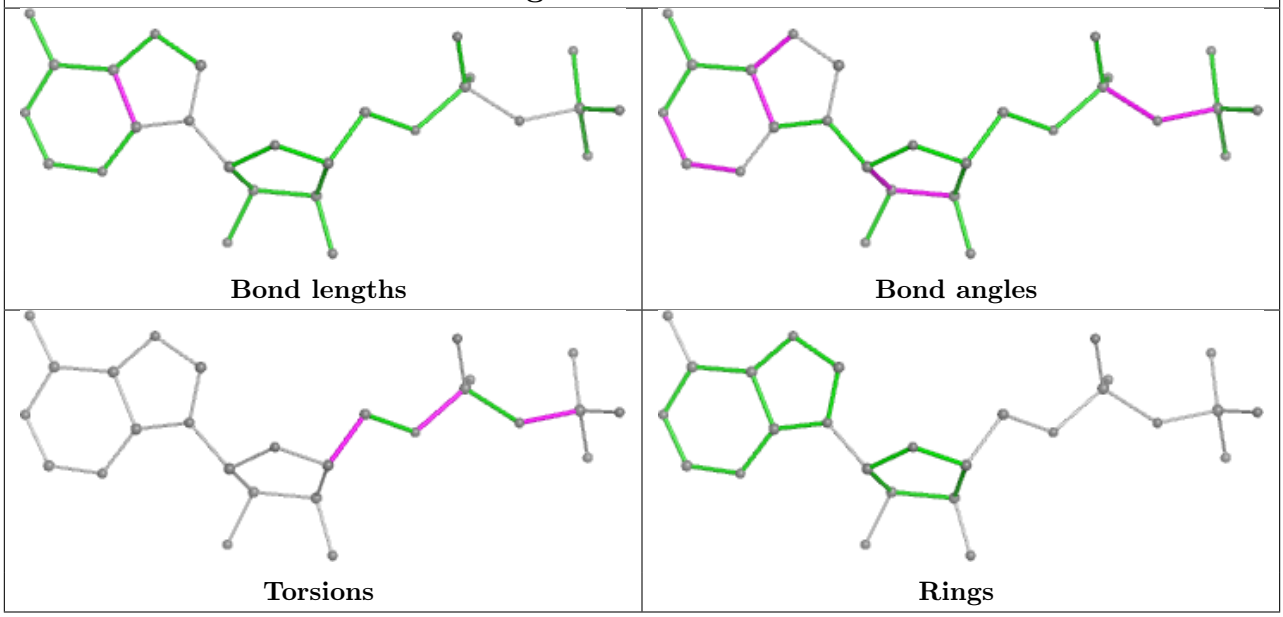
There are no ring outliers.

No monomer is involved in short contacts.

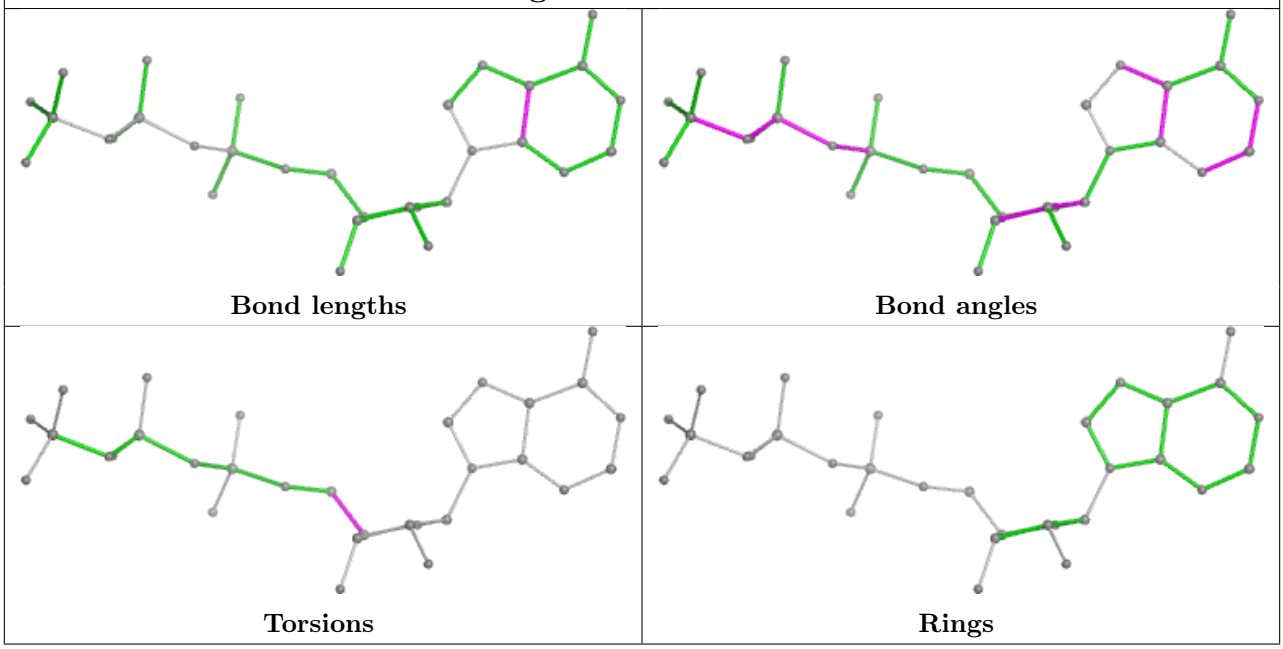
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ADP k 701



Ligand ATP k 703



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	b	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	59:TYR	C	60:PRO	N	1.65

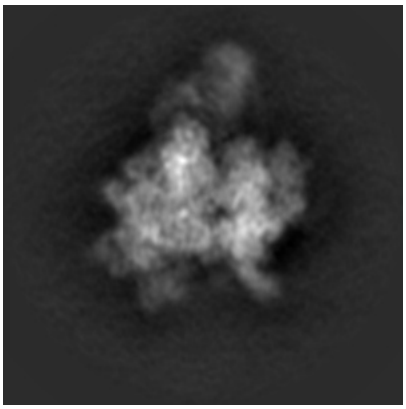
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11160. These allow visual inspection of the internal detail of the map and identification of artifacts.

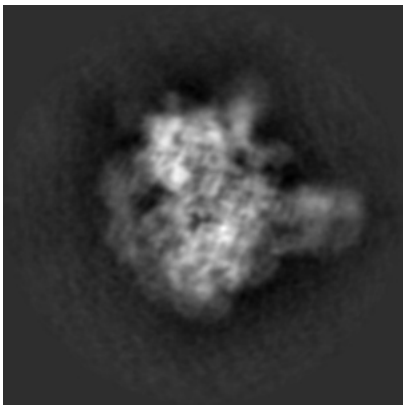
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

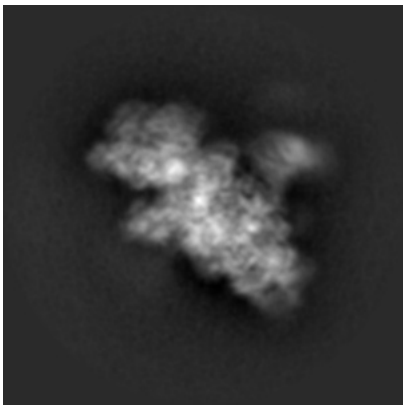
6.1.1 Primary map



X

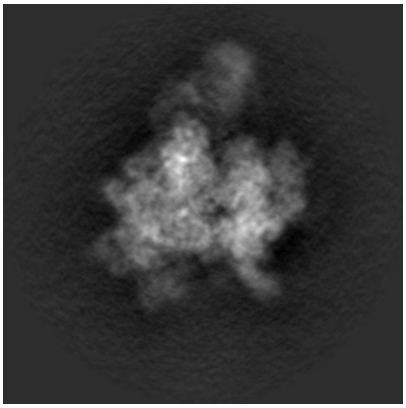


Y

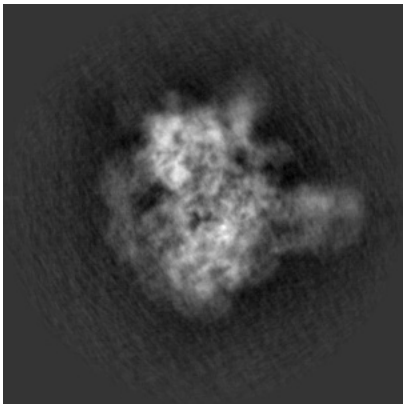


Z

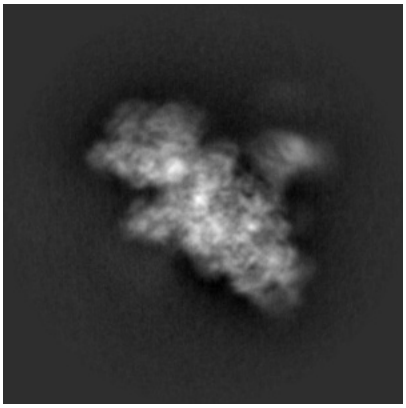
6.1.2 Raw map



X



Y

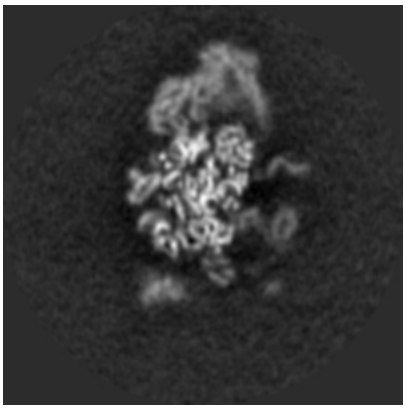


Z

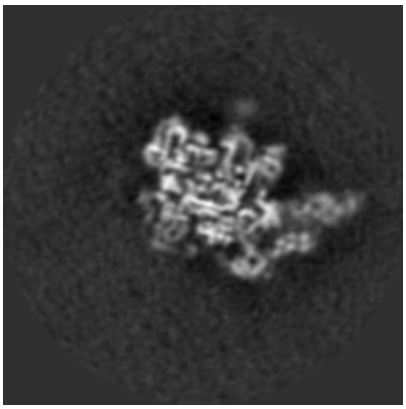
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

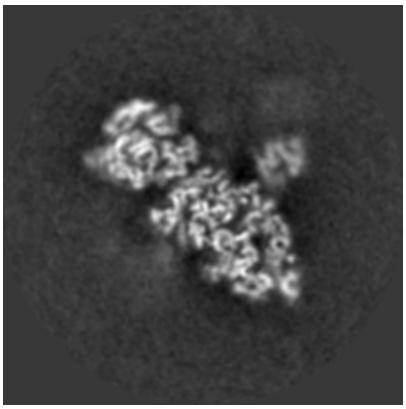
6.2.1 Primary map



X Index: 180

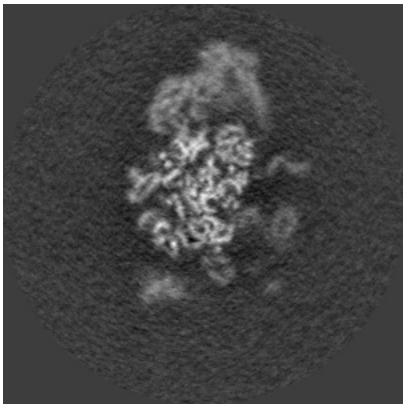


Y Index: 180

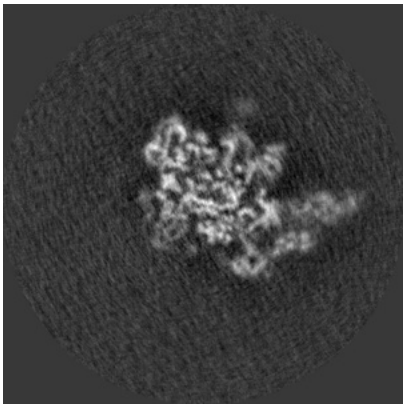


Z Index: 180

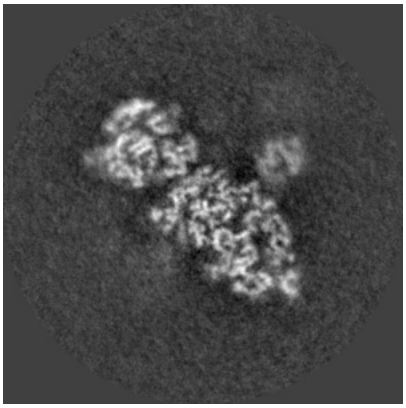
6.2.2 Raw map



X Index: 180



Y Index: 180

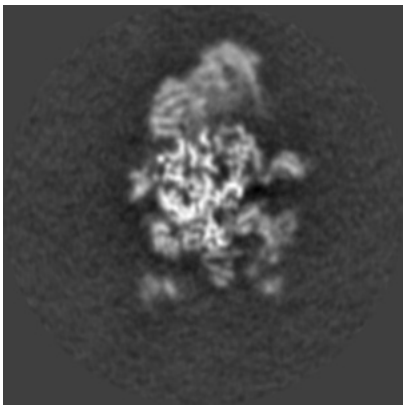


Z Index: 180

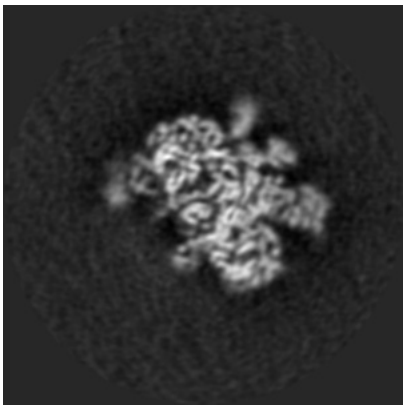
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

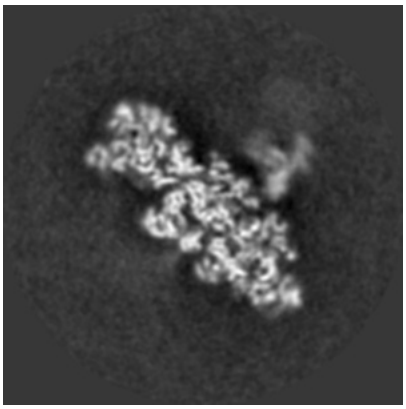
6.3.1 Primary map



X Index: 175

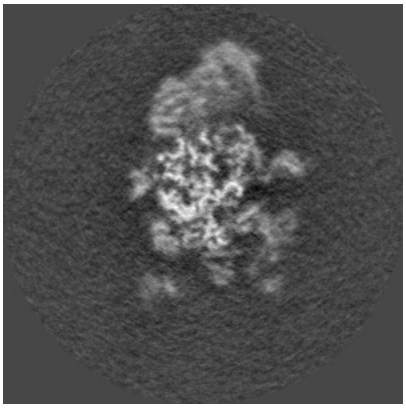


Y Index: 159

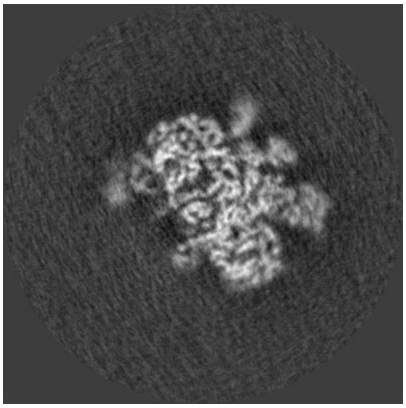


Z Index: 189

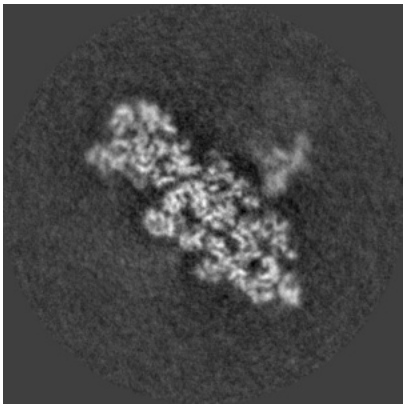
6.3.2 Raw map



X Index: 175



Y Index: 159

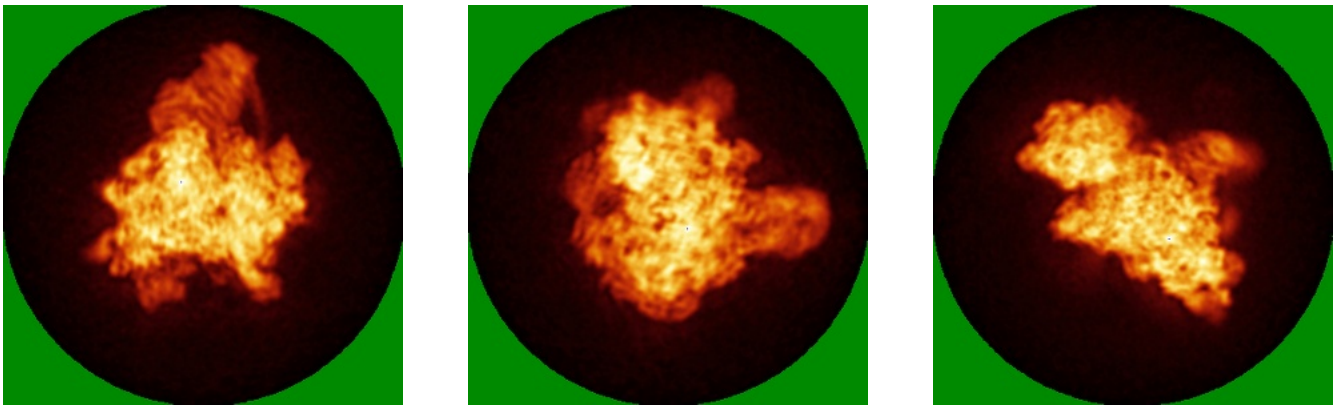


Z Index: 187

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

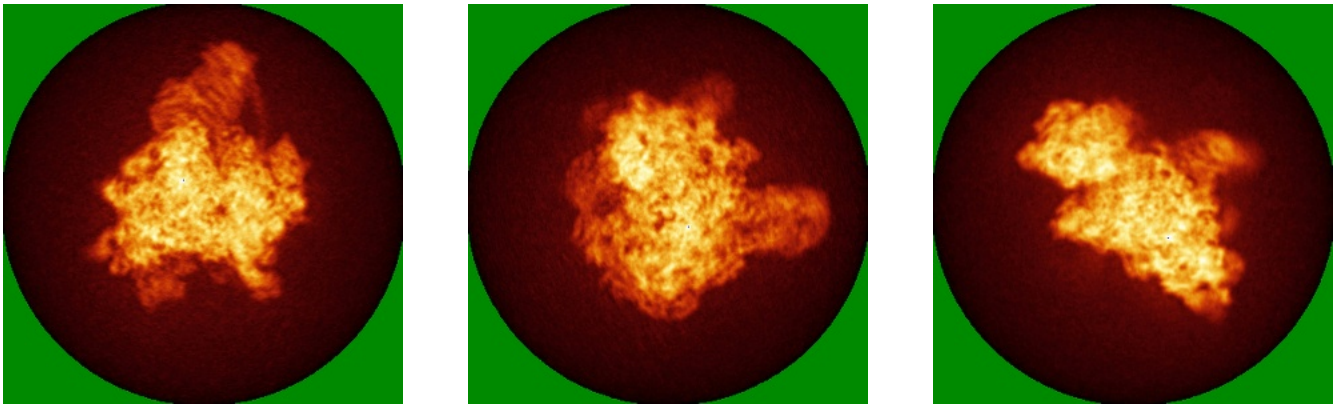
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

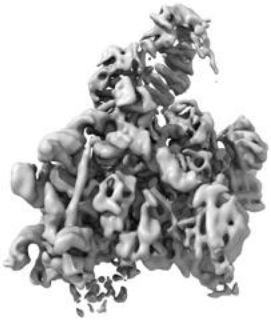


X Y Z

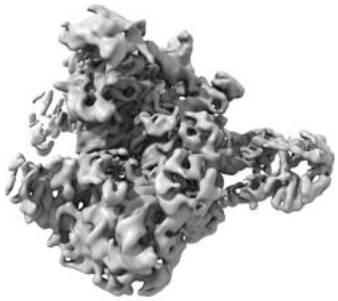
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

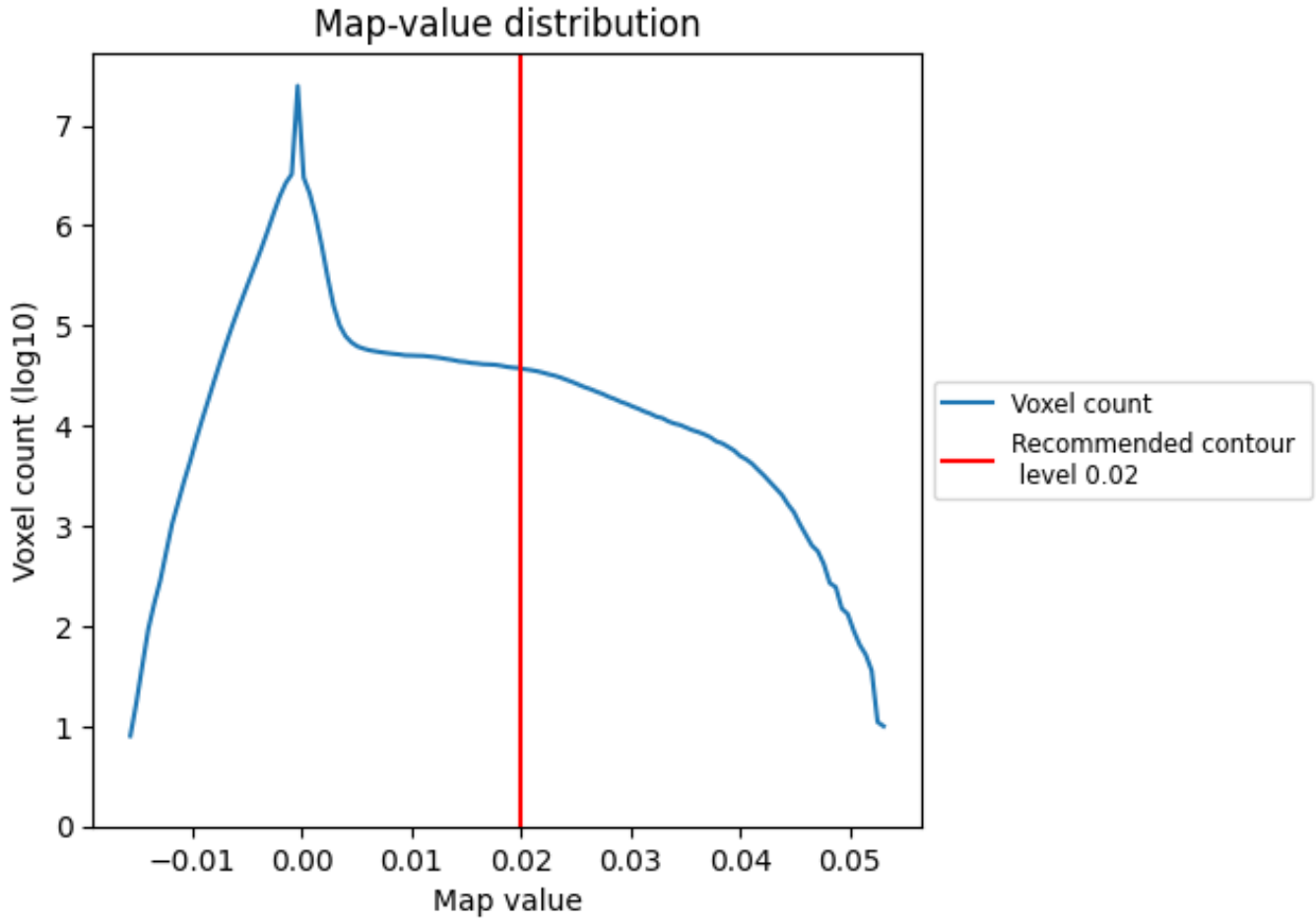
6.6 Mask visualisation (i)

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

7 Map analysis

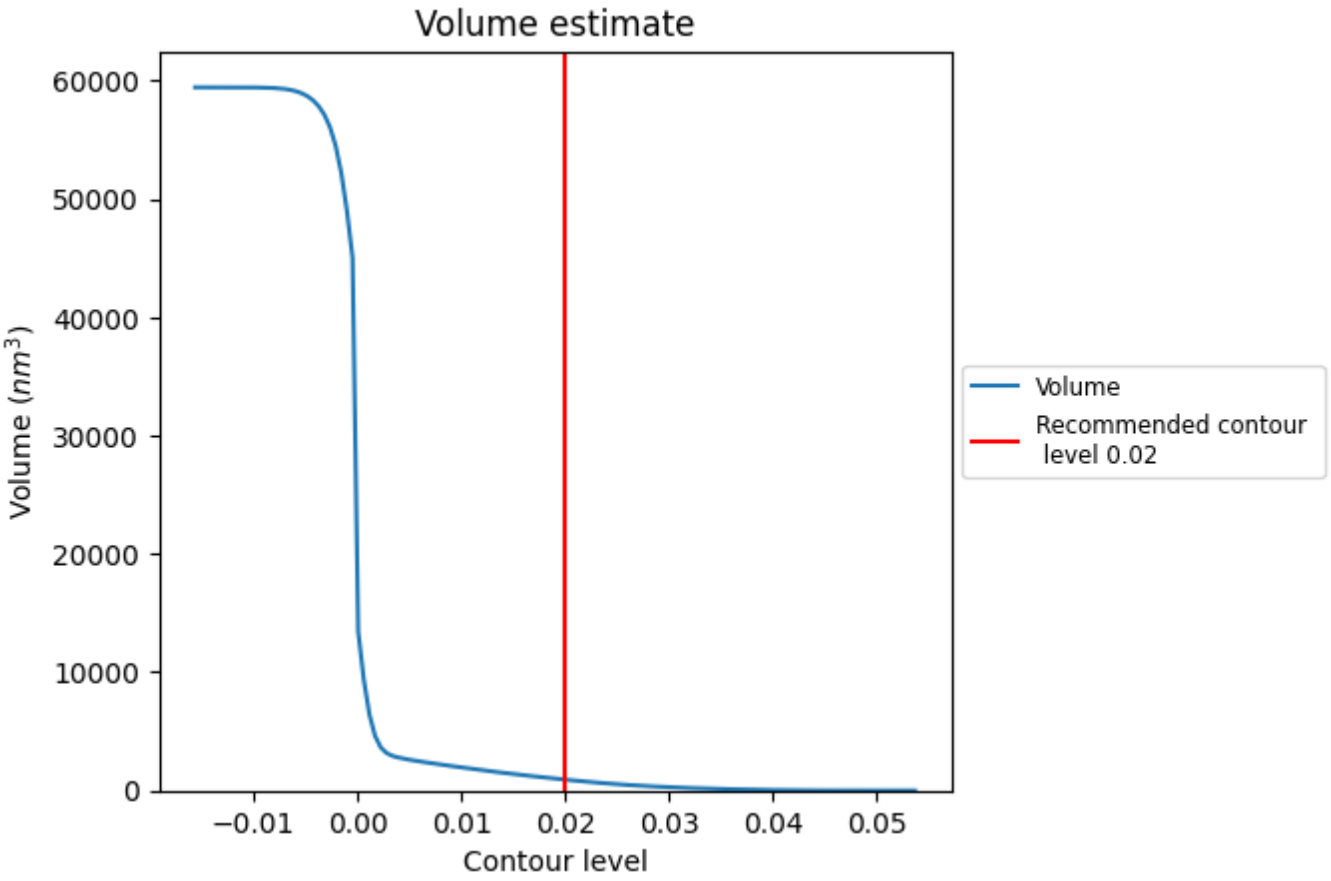
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

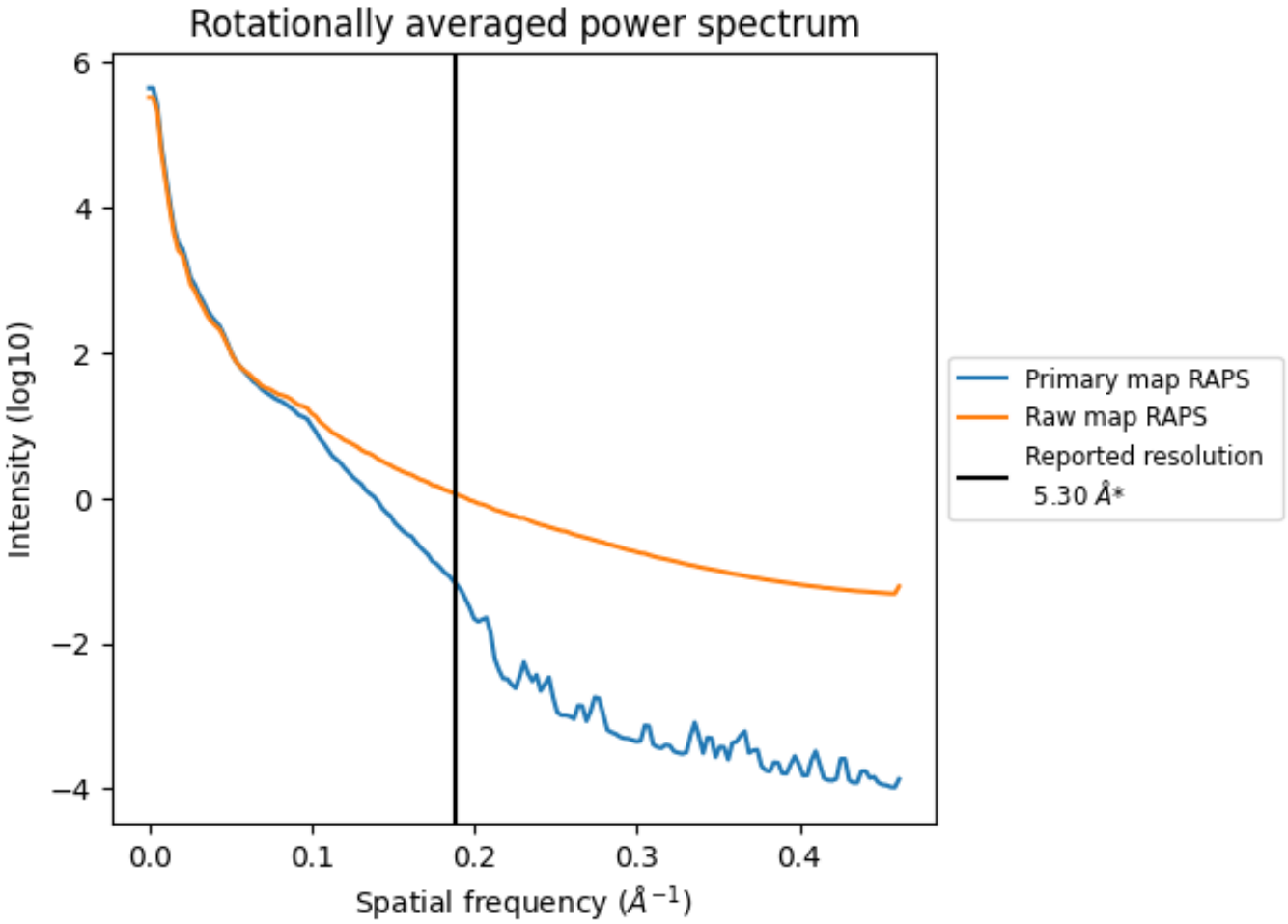
7.2 Volume estimate (i)



The volume at the recommended contour level is 925 nm^3; this corresponds to an approximate mass of 836 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)

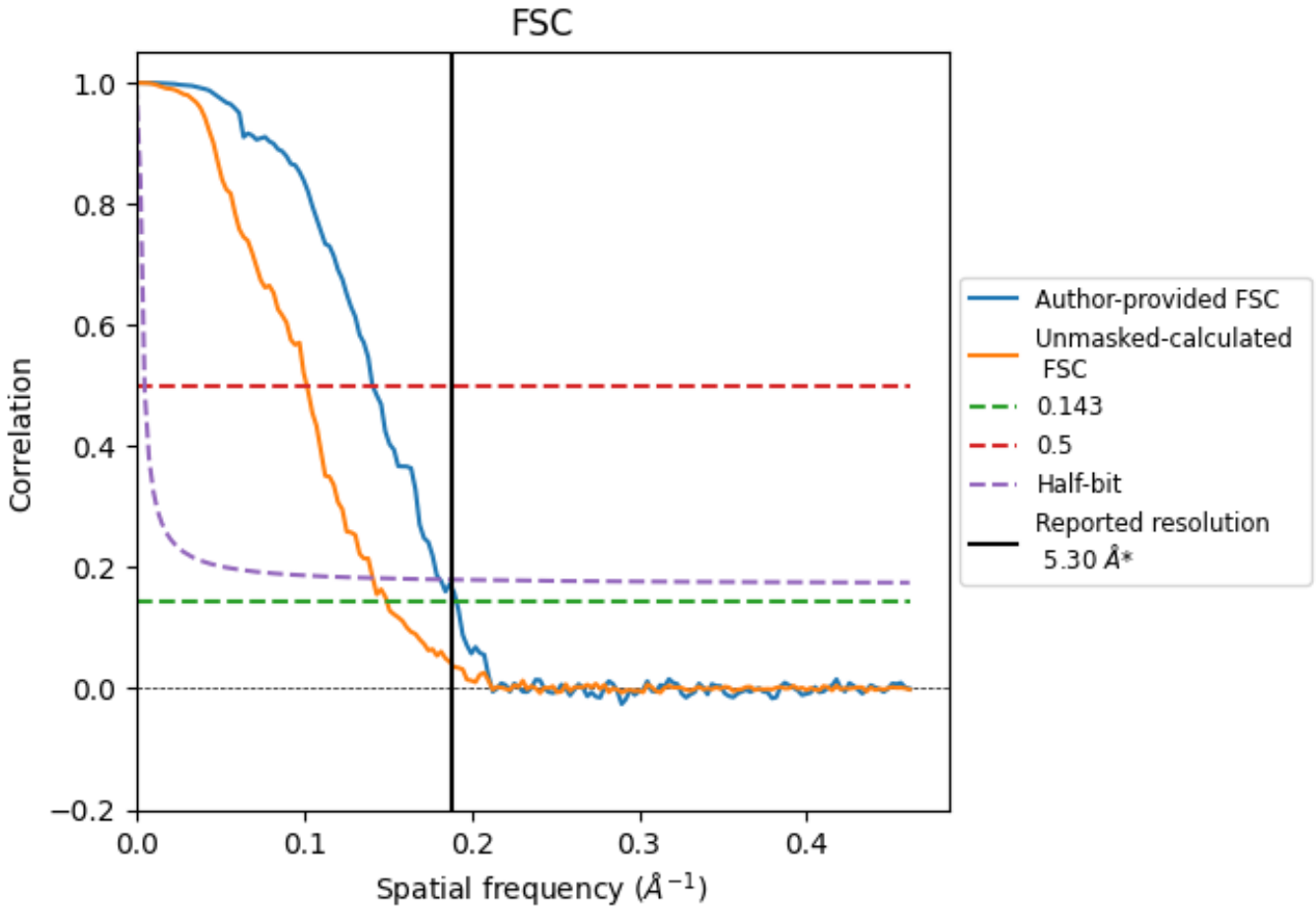


*Reported resolution corresponds to spatial frequency of 0.189 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.189 Å^{-1}

8.2 Resolution estimates (i)

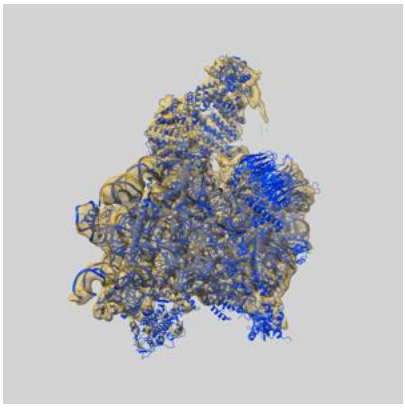
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	5.23	7.09	5.52
Unmasked-calculated*	6.68	9.82	7.08

*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 6.68 differs from the reported value 5.3 by more than 10 %

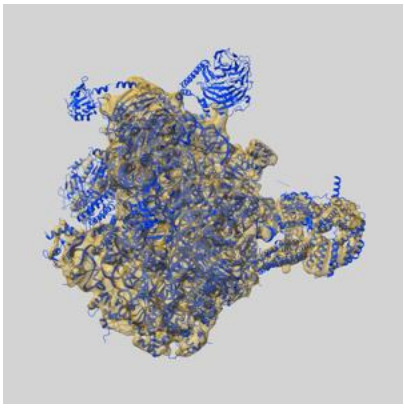
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11160 and PDB model 6ZCE. Per-residue inclusion information can be found in section 3 on page 14.

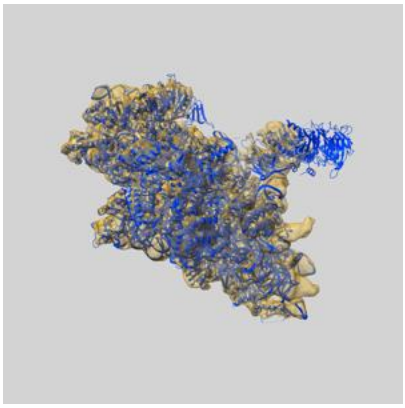
9.1 Map-model overlay



X



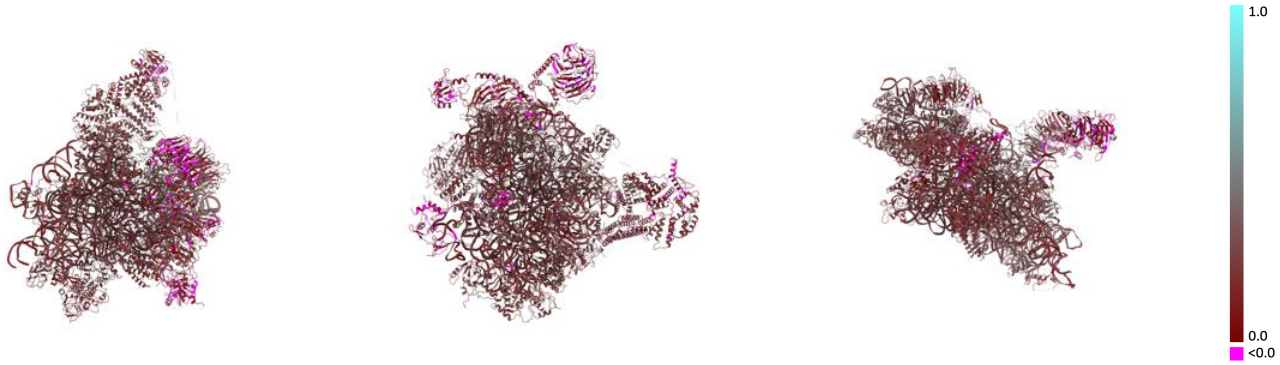
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

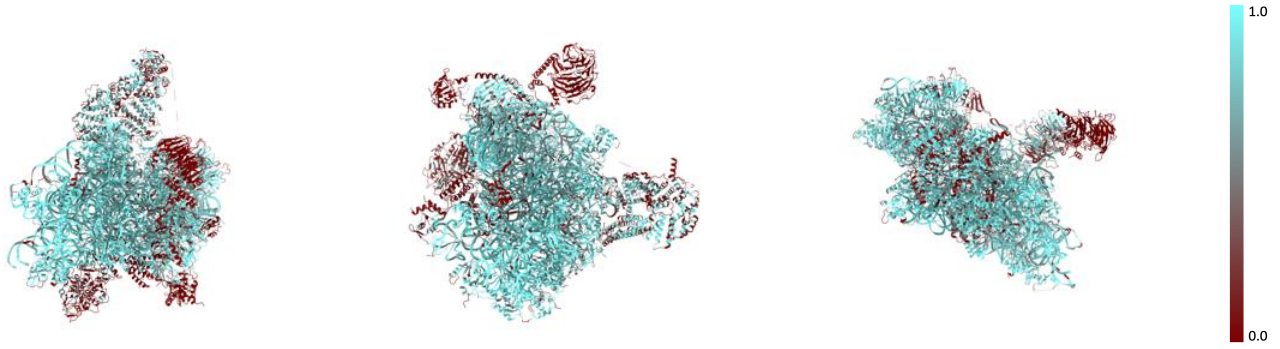
9.2 Q-score mapped to coordinate model



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.

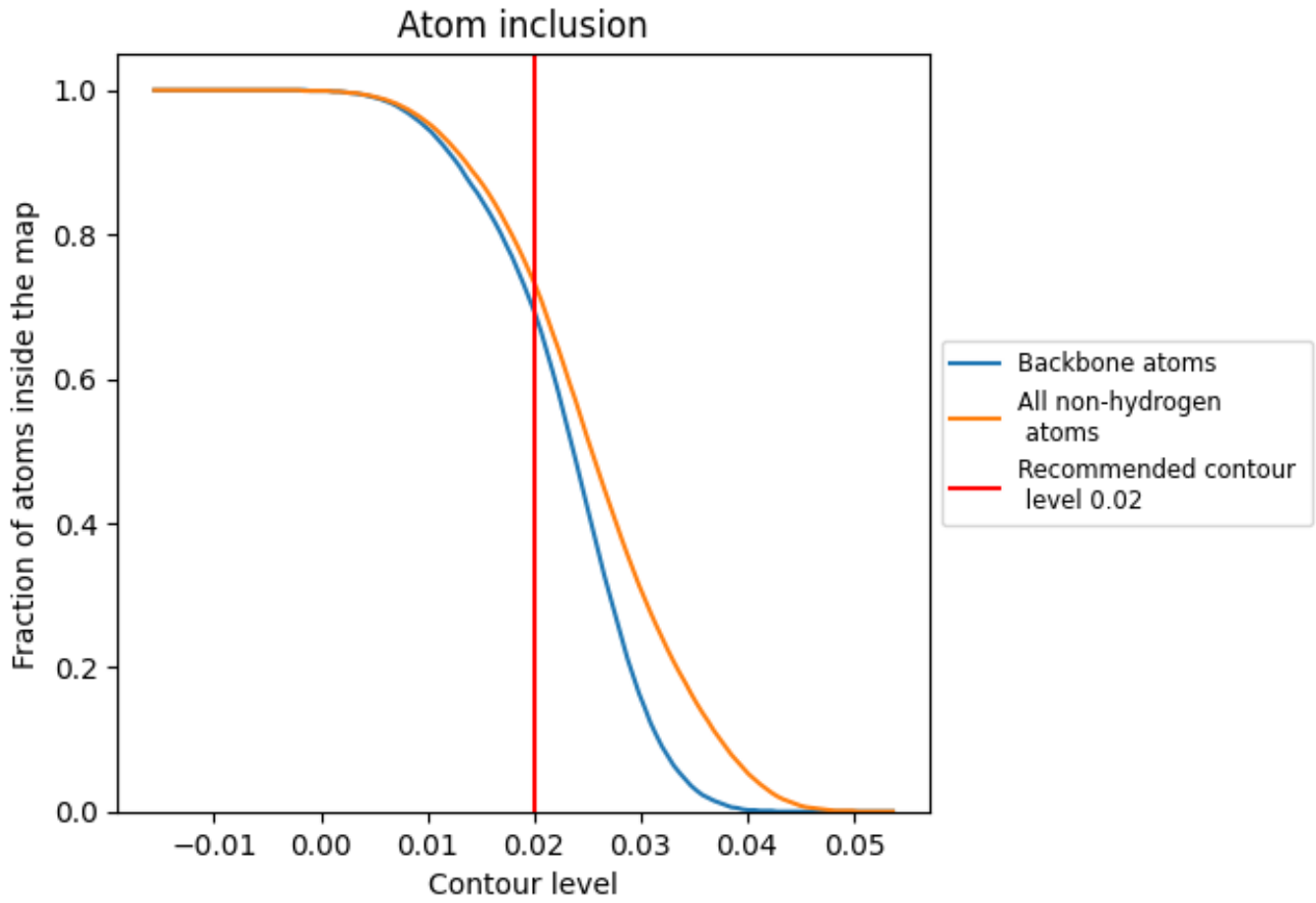
9.3 Atom inclusion mapped to coordinate model



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7340	0.2310
A	0.9030	0.2370
B	0.8190	0.2900
C	0.7970	0.2700
D	0.7250	0.2860
E	0.6370	0.2750
F	0.7910	0.2840
G	0.7530	0.2640
H	0.8110	0.2590
I	0.8170	0.2710
J	0.8620	0.2650
K	0.7820	0.2710
L	0.8580	0.2530
M	0.7410	0.2930
N	0.3360	0.0530
O	0.8050	0.2740
P	0.7740	0.2340
Q	0.6390	0.2110
R	0.7750	0.2540
S	0.6820	0.2760
T	0.8030	0.2530
U	0.8230	0.2390
V	0.7270	0.2600
W	0.7810	0.2850
X	0.7370	0.2680
Y	0.8030	0.2870
Z	0.8320	0.2640
a	0.7520	0.2380
b	0.6560	0.2730
c	0.6530	0.2650
d	0.5740	0.2590
e	0.8650	0.2460
f	0.6940	0.2870
g	0.4720	0.0900
h	0.7600	0.2200

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.0290	0.2280
j	0.0030	0.0520
k	0.1880	0.2140
l	0.0000	0.0820
m	0.4920	0.2080
o	0.5090	0.1870
p	0.4120	0.1670
q	0.5340	0.1930
r	0.0000	0.1130
s	0.0300	0.1930
t	0.0000	0.2500