wwPDB EM Validation Summary Report (i)

Apr 29, 2024 – 01:53 am BST

PDB ID	:	4UER
EMDB ID	:	EMD-2845
Title	:	40S-eIF1-eIF1A-eIF3-eIF3j translation initiation complex from Lachancea kluyveri
Authors	:	Aylett, C.H.S.; Boehringer, D.; Erzberger, J.P.; Schaefer, T.; Ban, N.
Deposited on	:	2014-12-18
Resolution	:	6.47 Å(reported)
Based on initial model	:	3U5B

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:

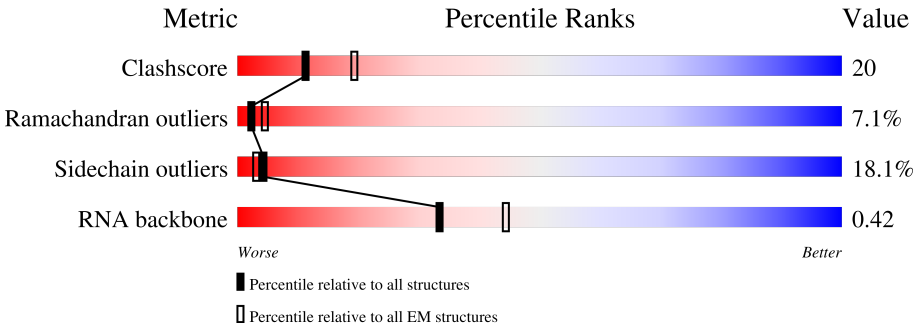
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 6.47 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	0	100	15%, 42%, 51%, 6%
2	1	63	27%, 49%, 24%
3	2	188	56%, 31%, 12%
4	3	184	40%, 38%, 19%
5	4	214	32%, 40%, 21%, 7%
6	5	97	42%, 39%, 13%, 5%
7	6	81	58%, 35%, 6%

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Mol	Chain	Length	Quality of chain
8	7	96	42% 39% 18%
9	8	70	31% 39% 24% 6%
10	9	71	41% 41% 14%
11	A	1781	33% 38% 23% 6%
12	B	206	36% 41% 19%
13	C	223	53% 33% 13%
14	D	185	51% 33% 15%
15	E	217	52% 36% 11%
16	F	83	11% 46% 46% 7%
17	G	206	50% 38% 10%
18	H	129	47% 39% 12%
19	I	141	43% 39% 16%
20	J	107	42% 39% 19%
21	K	127	49% 36% 10% 5%
22	L	144	49% 38% 10%
23	M	145	39% 43% 15%
24	N	53	47% 42% 8%
25	O	150	53% 33% 12%
26	P	134	55% 30% 12%
27	Q	155	52% 38% 8%
28	R	318	58% 36% 6%
29	S	124	6% 50% 38% 9%
30	T	143	39% 45% 15%
31	U	124	31% 48% 16% 5%
32	V	120	49% 36% 11%

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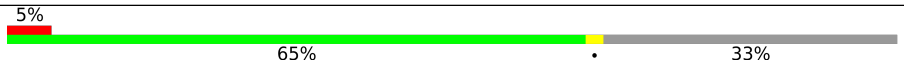
Mol	Chain	Length	Quality of chain
33	W	260	
34	X	60	
35	Y	226	
36	Z	87	
37	a	964	
38	b	763	
39	c	812	

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 89319 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 EIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	100	805	495	148	157	5	0	0

- Molecule 2 is a protein called ES28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	63	497	306	99	91	1	0	0

- Molecule 3 is a protein called ES8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	188	1489	925	298	264	2	0	0

- Molecule 4 is a protein called ES7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	3	184	1481	951	265	265	0	0

- Molecule 5 is a protein called ES1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	214	1709	1084	310	311	4	0	0

- Molecule 6 is a protein called ES26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	97	769	475	160	129	5	0	0

- Molecule 7 is a protein called ES27.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 8 is a protein called ES10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	96	Total	C	N	O	S	0	0
			772	499	126	145	2		

- Molecule 9 is a protein called ES25.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	8	70	Total	C	N	O	0	0
			563	360	104	99		

- Molecule 10 is a protein called ES31.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	71	Total	C	N	O	S	0	0
			516	328	93	91	4		

- Molecule 11 is a RNA chain called 18S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1781	Total	C	N	O	P	1	0
			37835	16910	6661	12482	1782		

- Molecule 12 is a protein called US2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	206	Total	C	N	O	S	0	0
			1577	1014	278	283	2		

- Molecule 13 is a protein called US3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 14 is a protein called US4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 15 is a protein called US5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 16 is a protein called EIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	83	Total	C	N	O	S	0	0
			671	423	124	120	4		

- Molecule 17 is a protein called US7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 18 is a protein called US8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 19 is a protein called US9.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	I	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 20 is a protein called US10.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 21 is a protein called US11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 22 is a protein called US12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 23 is a protein called US13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 24 is a protein called US14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 25 is a protein called US15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 26 is a protein called ES24.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	P	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 27 is a protein called US17.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	155	Total	C	N	O	S	0	0
			1213	774	230	206	3		

- Molecule 28 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	R	318	Total	C	N	O	S	0	0
			2437	1541	418	470	8		

- Molecule 29 is a protein called US19.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S	124	Total	C	N	O	S	0	0
			977	622	182	166	7		

- Molecule 30 is a protein called ES19.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 31 is a protein called ES12.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	U	124	Total	C	N	O	S	0	0
			890	560	156	172	2		

- Molecule 32 is a protein called ES17.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	V	120	Total	C	N	O	S	0	0
			926	577	177	170	2		

- Molecule 33 is a protein called ES4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	W	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 34 is a protein called ES30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	X	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 35 is a protein called ES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Y	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 36 is a protein called ES21.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Z	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 37 is a protein called EIF3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	449	Total	C	N	O	S	0	0
			3656	2350	616	683	7		

- Molecule 38 is a protein called EIF3B.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	572	Total	C	N	O	S	0	92
			3978	2578	667	720	13		

- Molecule 39 is a protein called EIF3C.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	544	Total	C	N	O	S	0	0
			4442	2845	736	849	12		

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

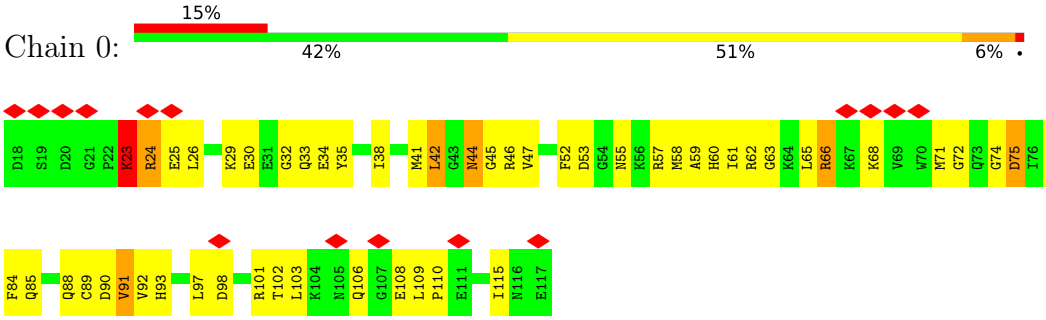
Mol	Chain	Residues	Atoms		AltConf
40	5	1	Total	Zn	0
			1	1	
40	6	1	Total	Zn	0
			1	1	
40	9	1	Total	Zn	0
			1	1	
40	N	1	Total	Zn	0
			1	1	

3 Residue-property plots

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.

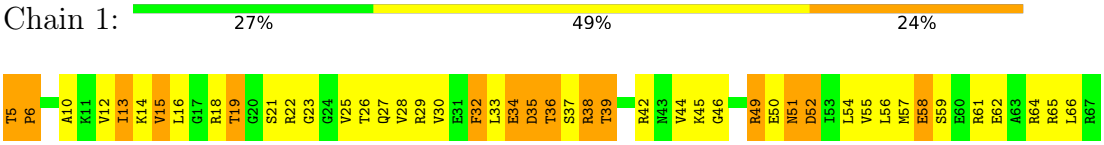
- Molecule 1: EIF1A

Chain 0:



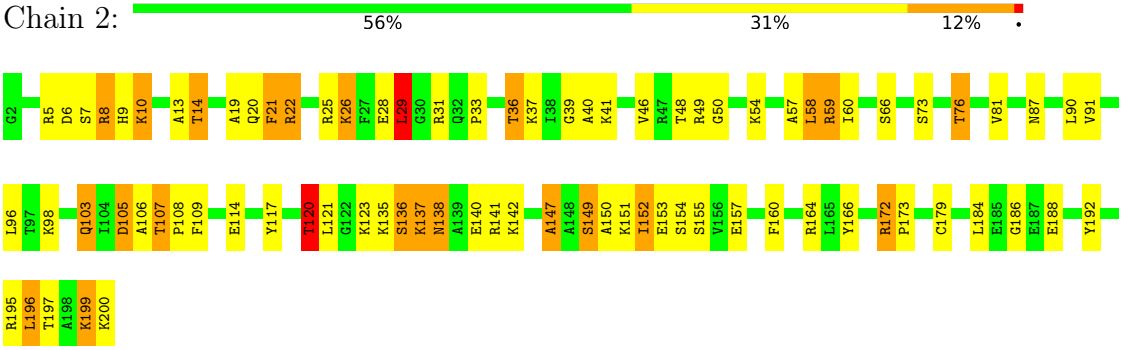
- Molecule 2: ES28

Chain 1:



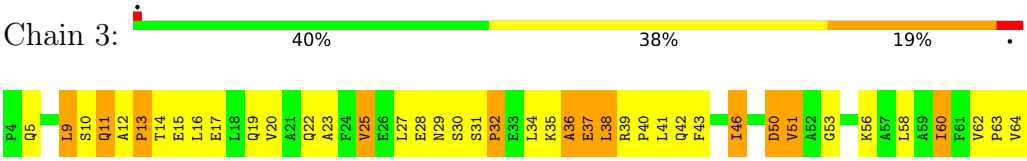
- Molecule 3: ES8

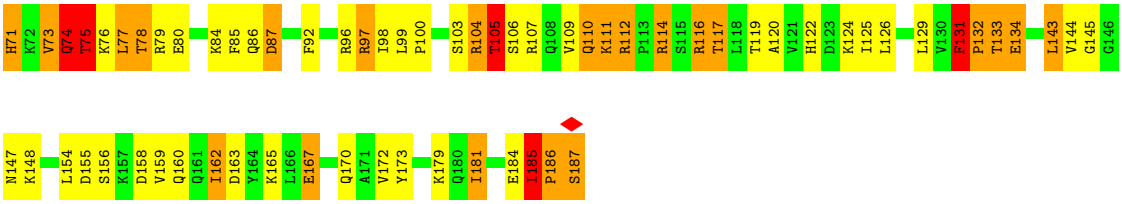
Chain 2:



- Molecule 4: ES7

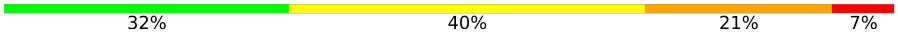
Chain 3:

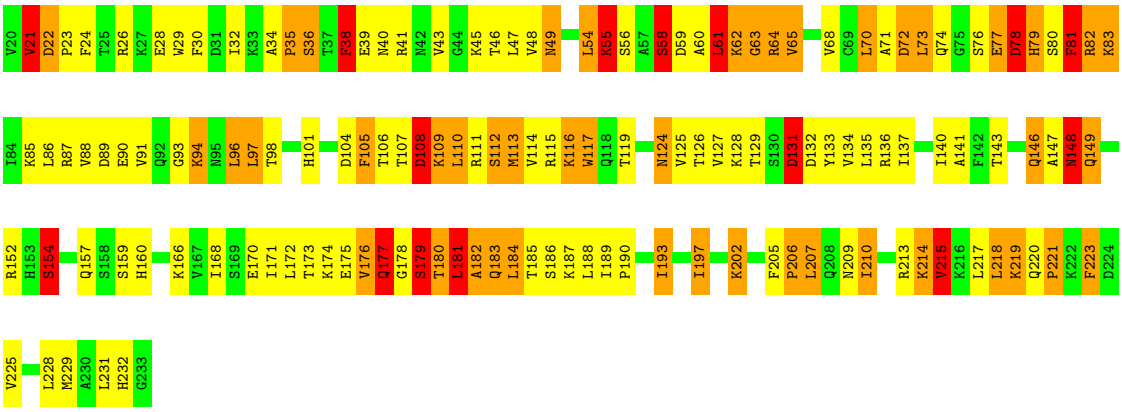




• Molecule 5: ES1

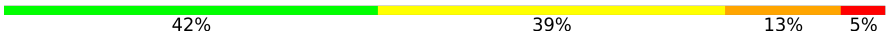
Chain 4:





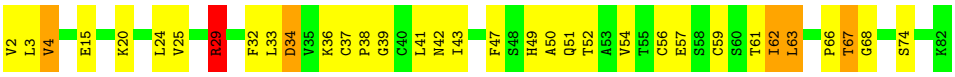
• Molecule 6: ES26

Chain 5:



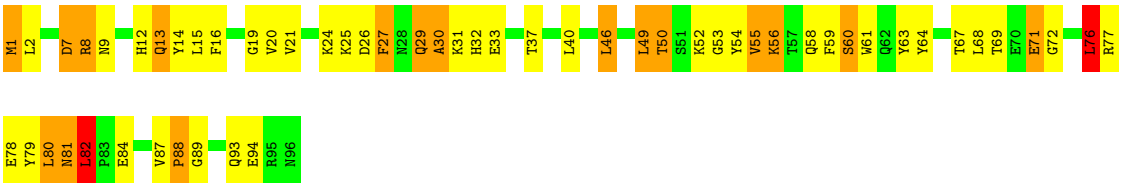
• Molecule 7: ES27

Chain 6:



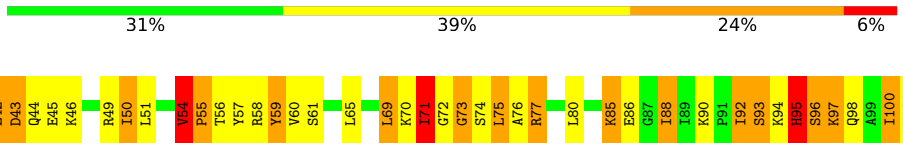
• Molecule 8: ES10

Chain 7:



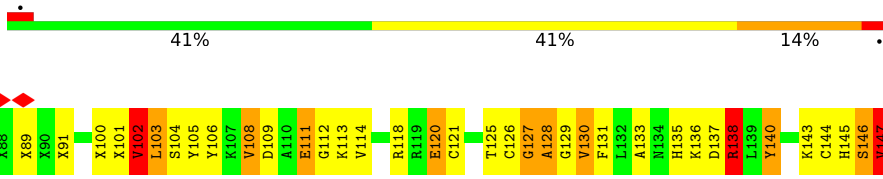
• Molecule 9: ES25

Chain 8:



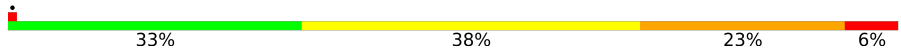
• Molecule 10: ES31

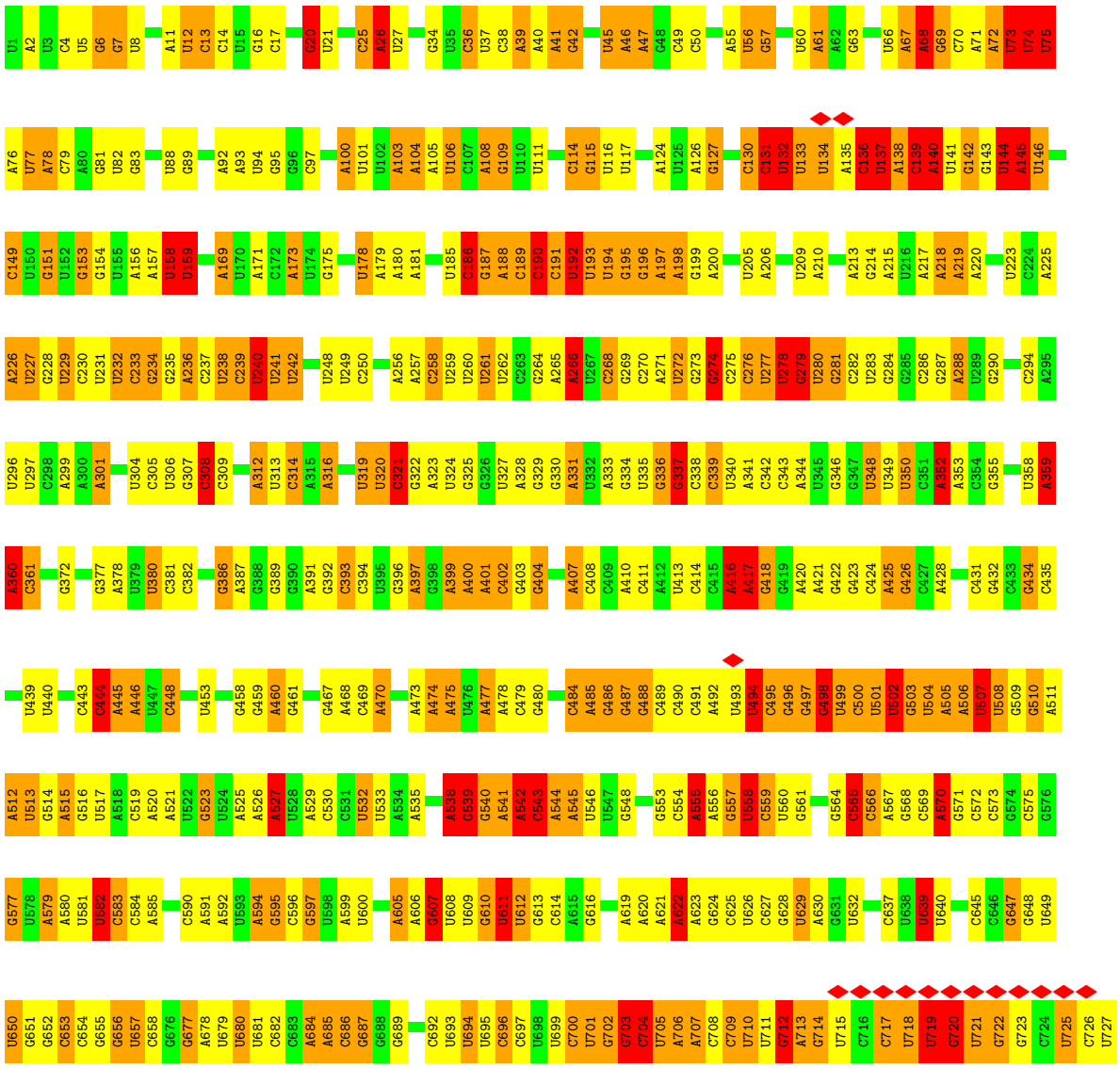
Chain 9:

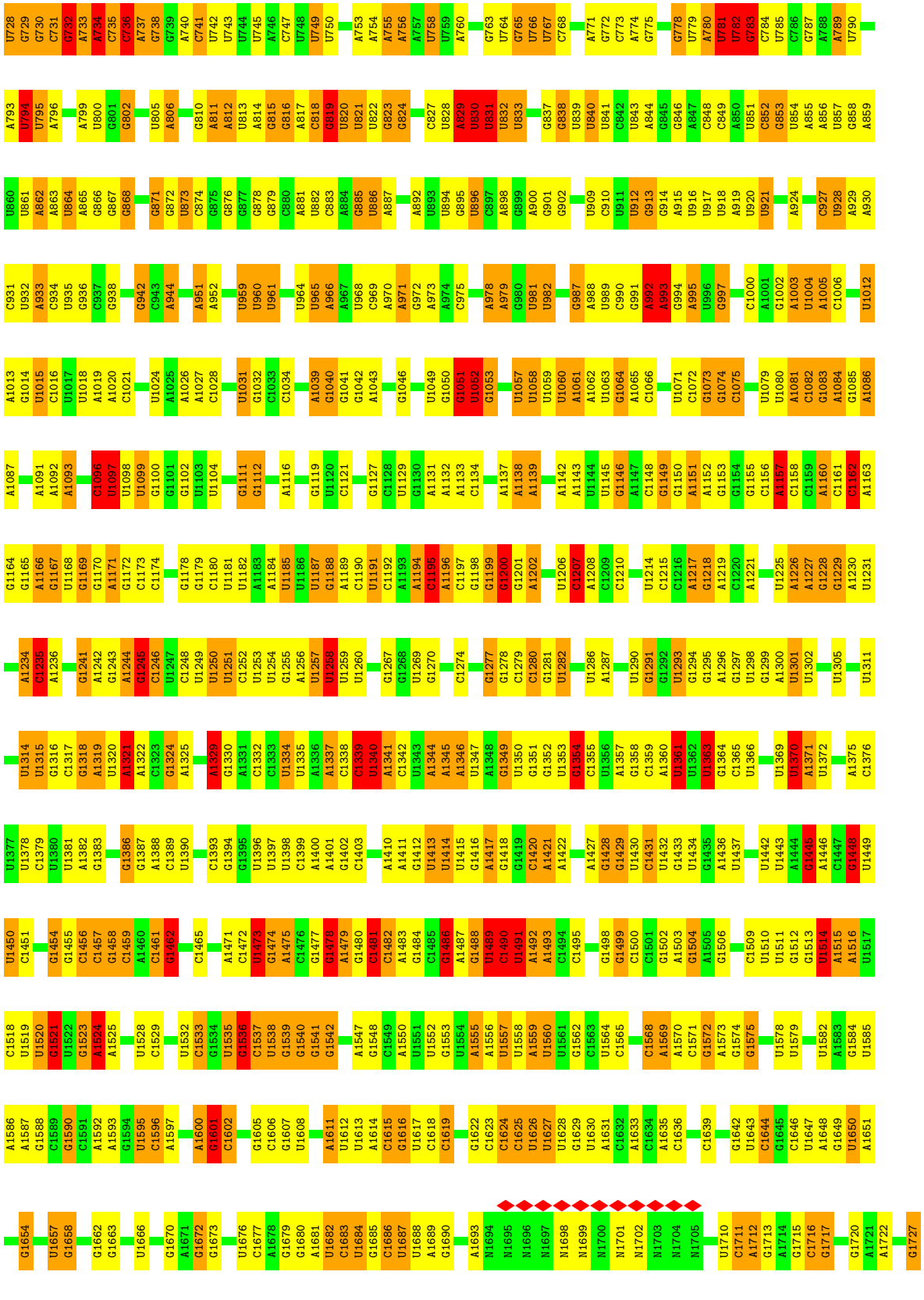


• Molecule 11: 18S RRNA

Chain A:

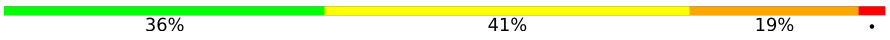


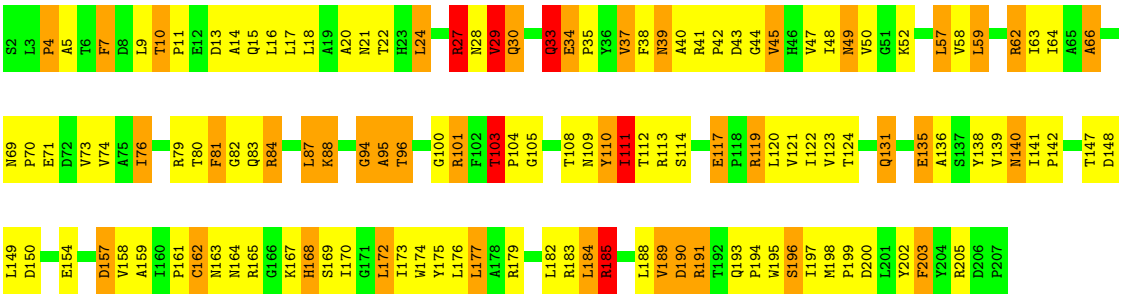




- Molecule 12: US2

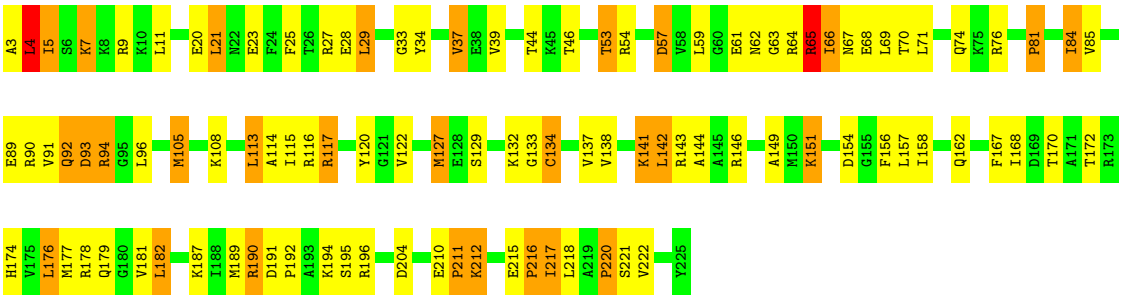
Chain B:





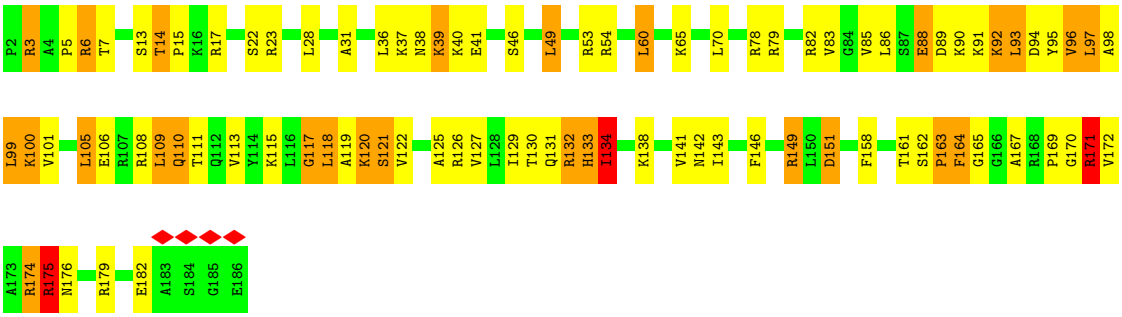
- Molecule 13: US3

Chain C:



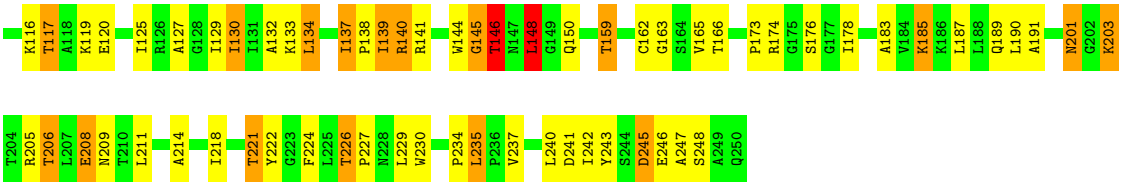
- Molecule 14: US4

Chain D:



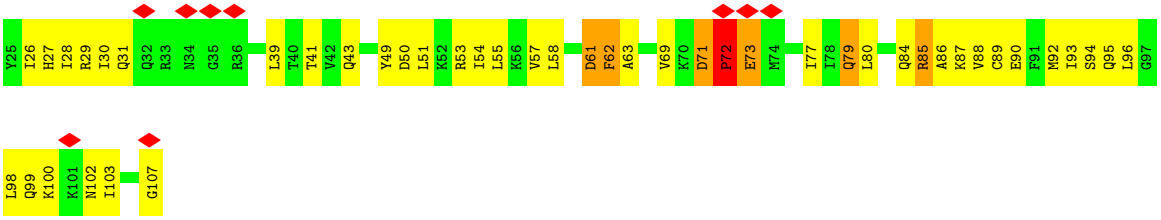
- Molecule 15: US5

Chain E:



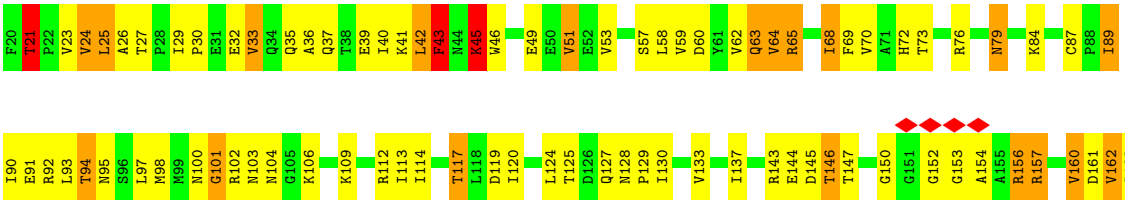
• Molecule 16: EIF1

Chain F:



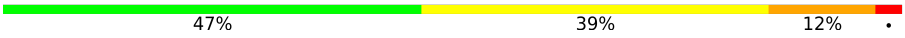
• Molecule 17: US7

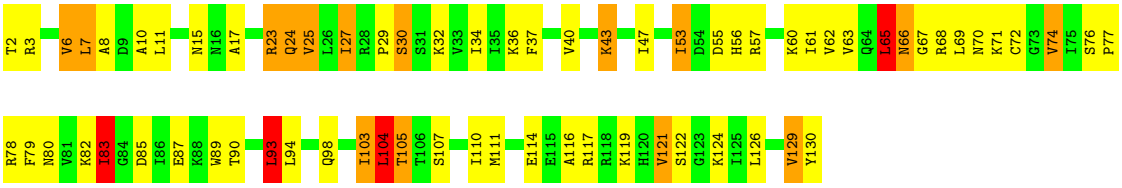
Chain G:



• Molecule 18: US8

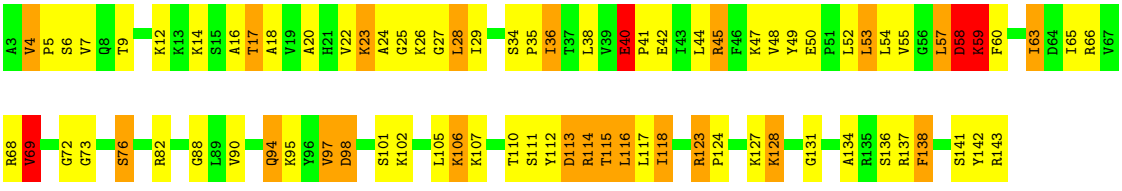
Chain H:





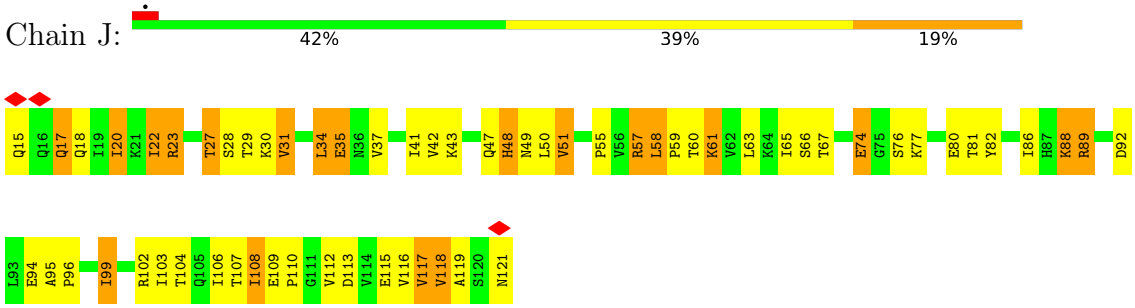
• Molecule 19: US9

Chain I:



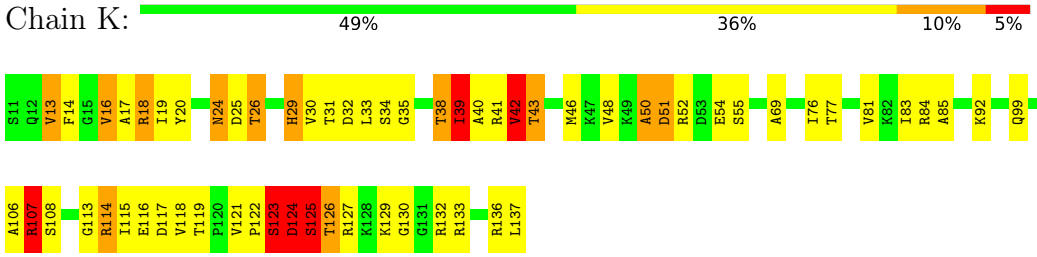
- Molecule 20: US10

Chain J:



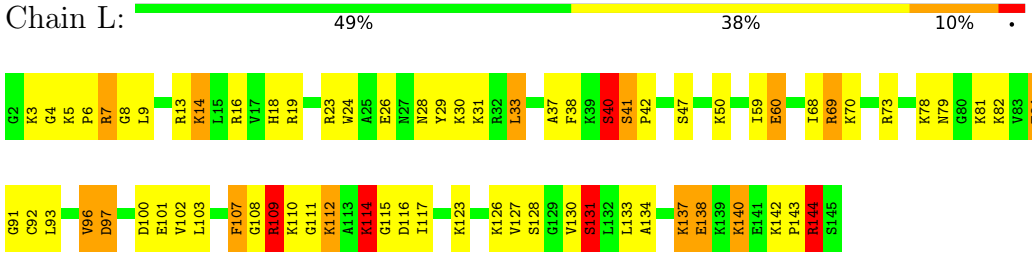
- Molecule 21: US11

Chain K:



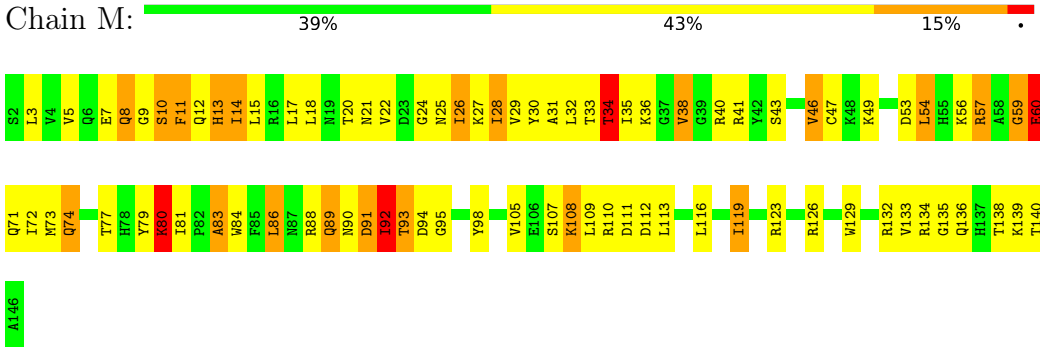
- Molecule 22: US12

Chain L:



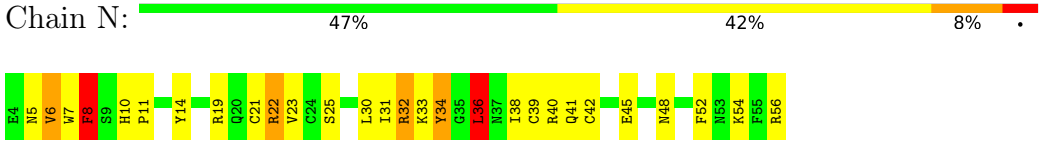
- Molecule 23: US13

Chain M:



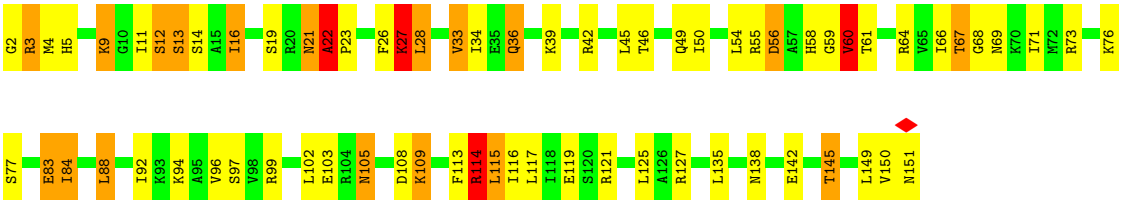
- Molecule 24: US14

Chain N:



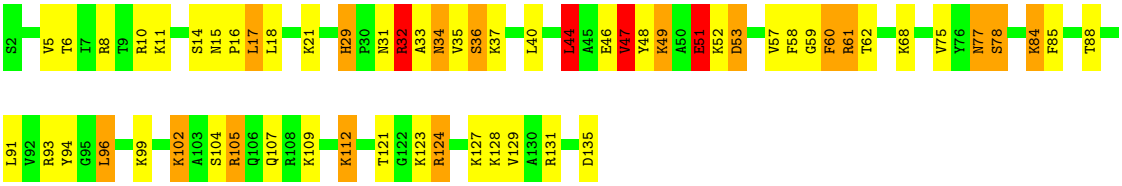
• Molecule 25: US15

Chain O:



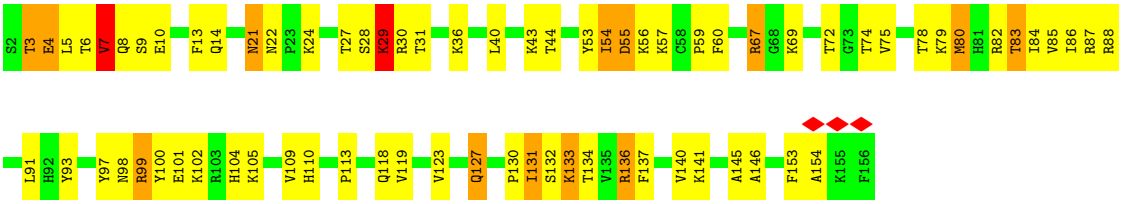
• Molecule 26: ES24

Chain P:



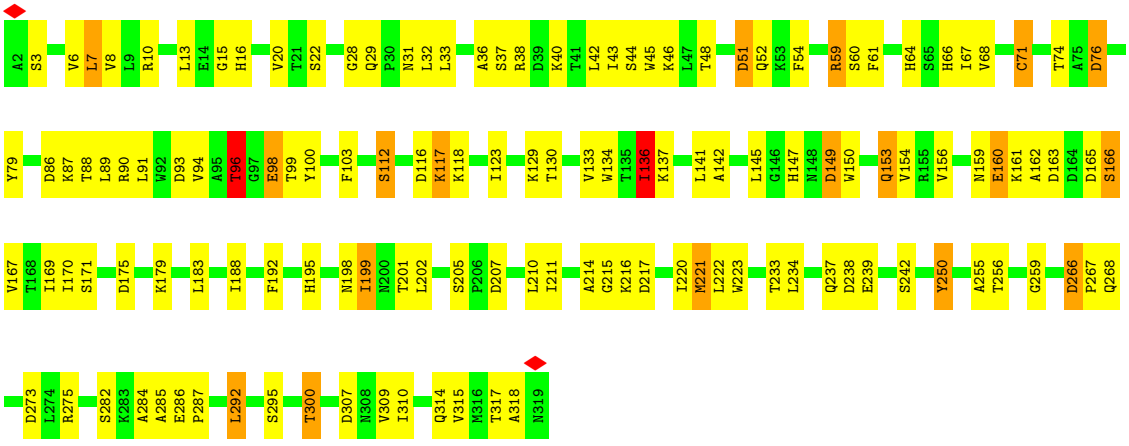
• Molecule 27: US17

Chain Q:

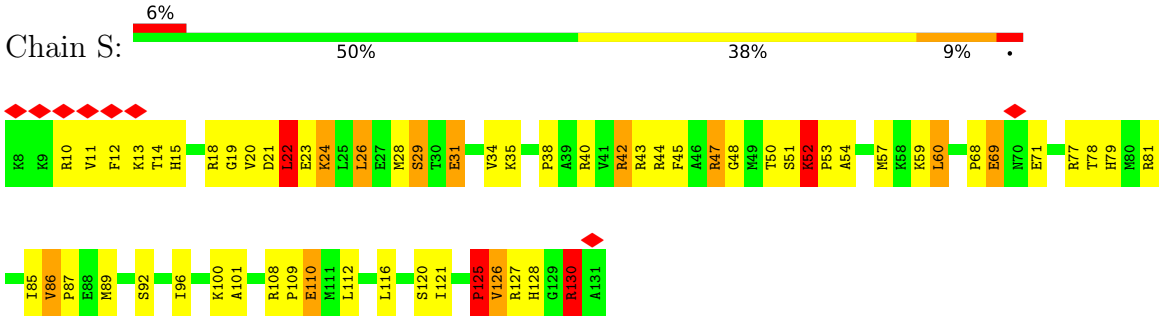


• Molecule 28: RACK1

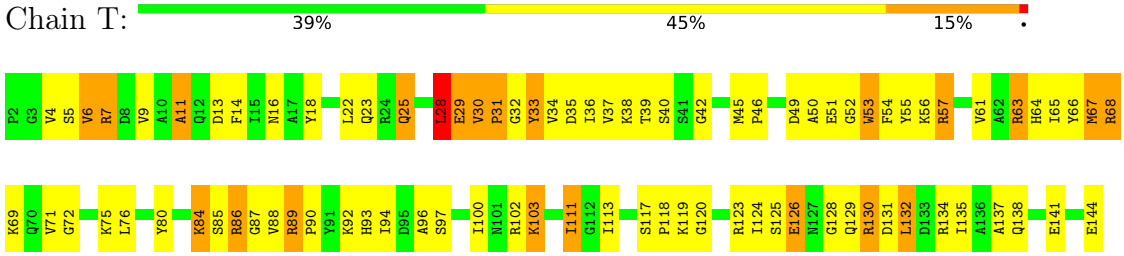
Chain R:



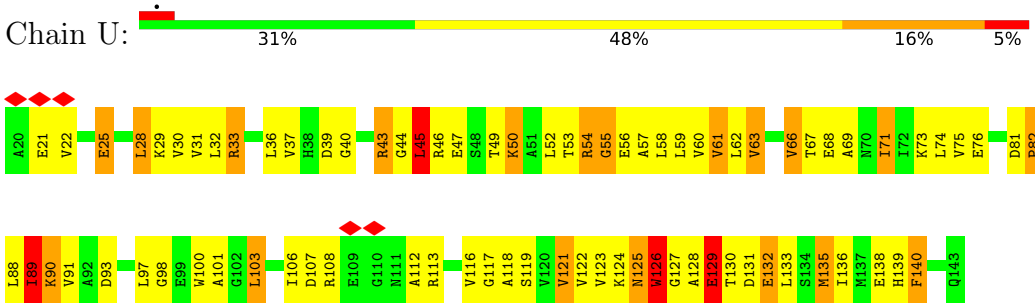
• Molecule 29: US19



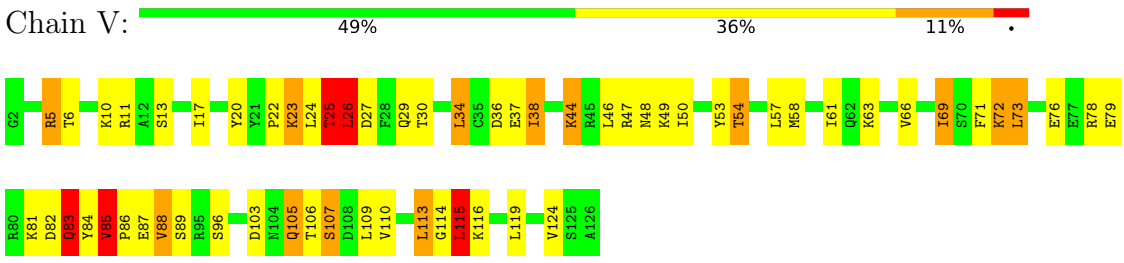
• Molecule 30: ES19



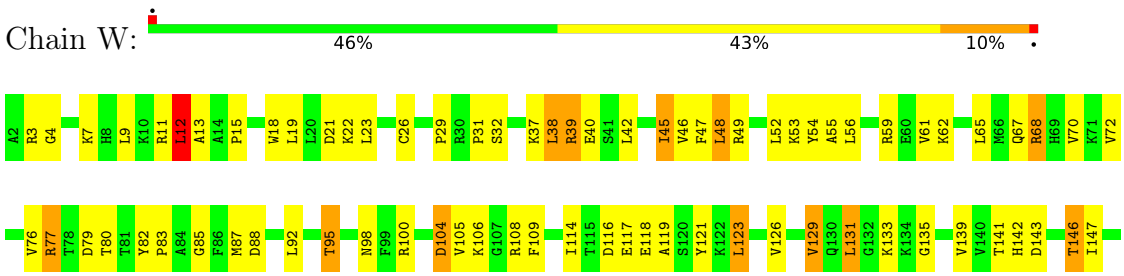
• Molecule 31: ES12

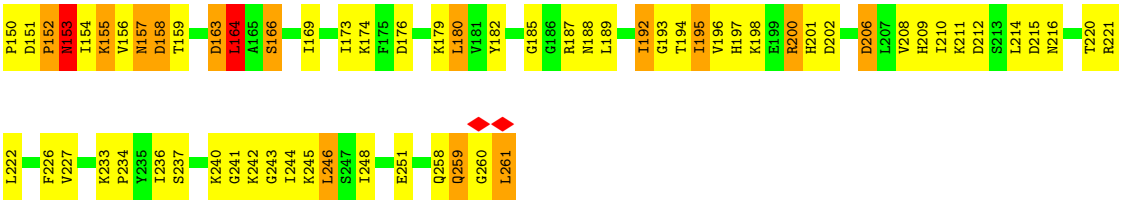


• Molecule 32: ES17



• Molecule 33: ES4



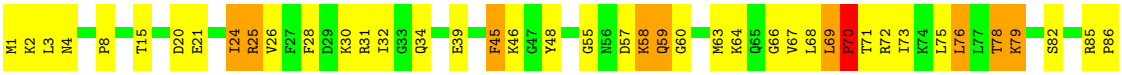


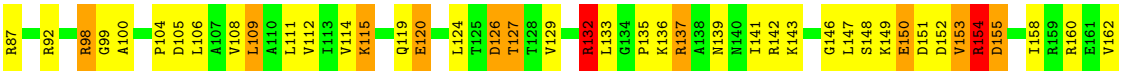
• Molecule 34: ES30

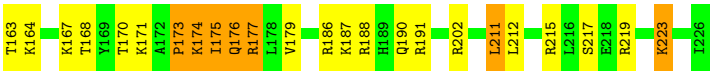
Chain X:

• Molecule 35: ES6

Chain Y:

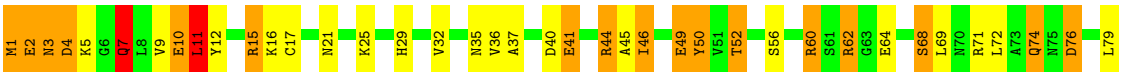


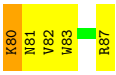




• Molecule 36: ES21

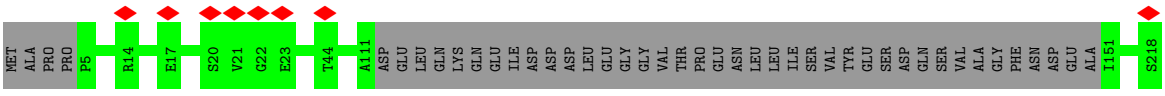
Chain Z:

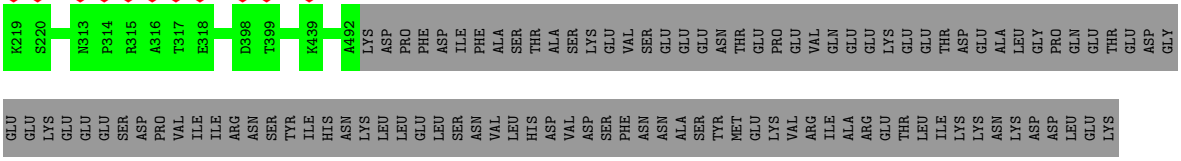




• Molecule 37: EIF3A

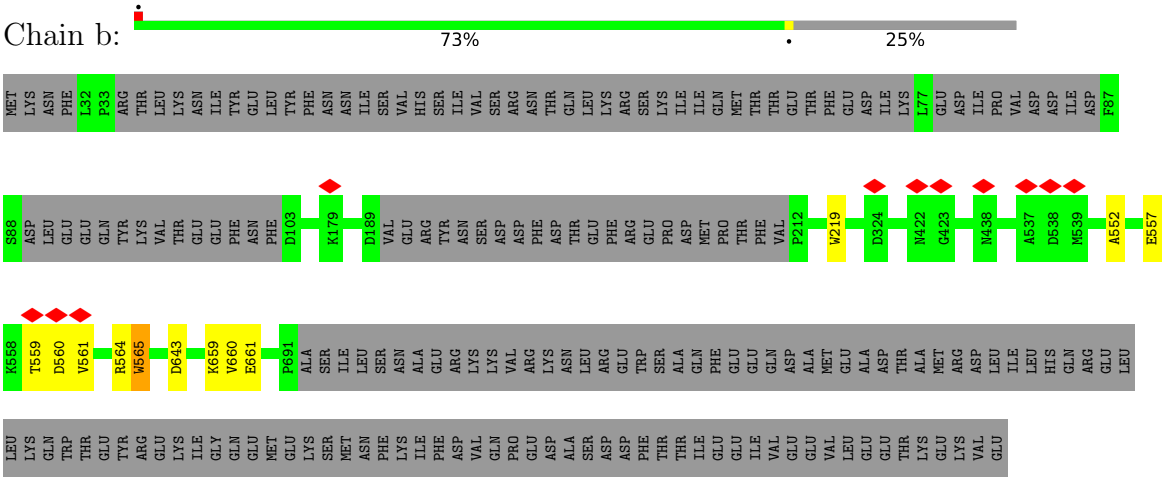
Chain a:





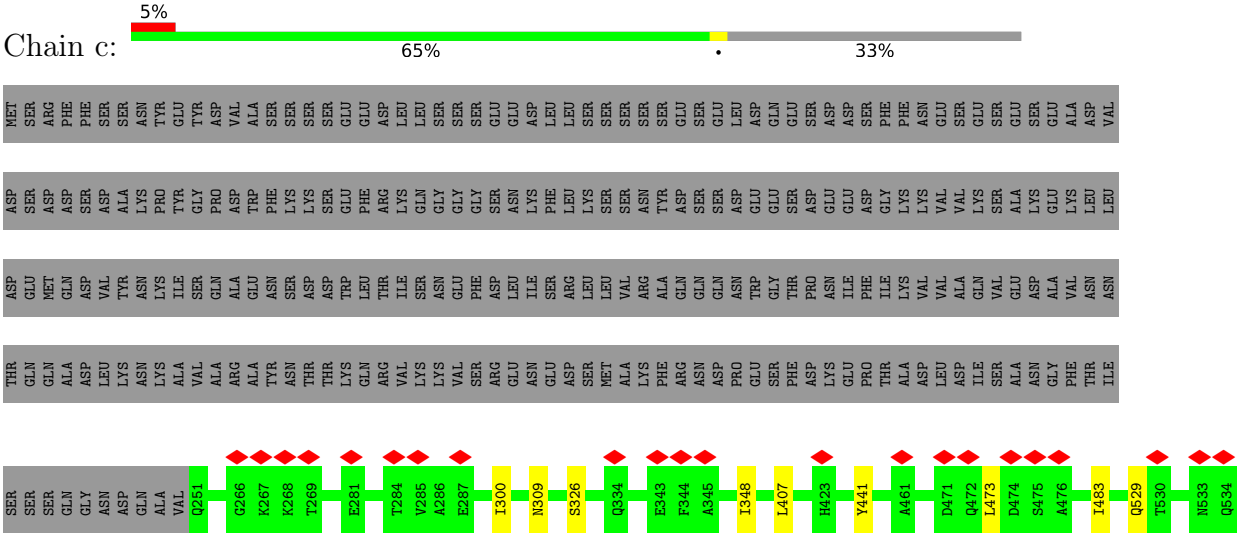
• Molecule 38: EIF3B

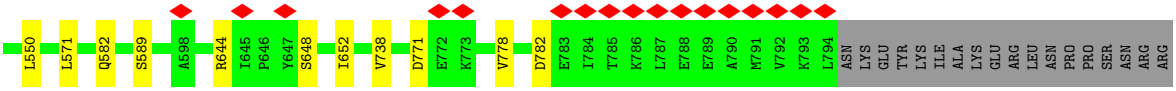
Chain b:



• Molecule 39: EIF3C

Chain c:




L550
L571
Q582
S589
A598
R644
I645
P646
Y647
S648
I652
V738
D771
E772
K773
V778
D782
E783
I784
T785
K786
L787
E788
E789
A790
M791
V792
K793
L794
ASN
LYS
GLU
TYR
LYS
ILE
ALA
LYS
GLU
ARG
LEU
ASN
PRO
PRO
SER
ASN
ARG
ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27354	Depositor
Resolution determination method	Not provided	
CTF correction method	BY IMAGE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	100719	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.115	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	355.84, 355.84, 355.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.64	0/815	1.14	3/1087 (0.3%)
2	1	0.44	0/499	0.72	0/670
3	2	0.68	0/1514	0.88	2/2021 (0.1%)
4	3	0.52	0/1506	0.77	0/2028
5	4	0.45	0/1735	0.81	0/2335
6	5	0.54	0/782	0.77	0/1047
7	6	0.53	0/620	0.82	1/838 (0.1%)
8	7	0.56	0/789	0.83	3/1067 (0.3%)
9	8	0.50	0/571	0.86	1/768 (0.1%)
10	9	0.53	0/404	0.99	1/542 (0.2%)
11	A	0.96	38/42127 (0.1%)	1.50	830/65638 (1.3%)
12	B	0.54	0/1617	0.80	0/2215
13	C	0.59	0/1759	0.74	0/2368
14	D	0.60	0/1519	0.82	1/2035 (0.0%)
15	E	0.60	0/1665	0.78	0/2263
16	F	0.64	0/678	1.18	6/903 (0.7%)
17	G	0.49	0/1629	0.72	0/2202
18	H	0.66	0/1038	0.86	3/1395 (0.2%)
19	I	0.57	0/1125	0.85	3/1510 (0.2%)
20	J	0.55	0/865	0.76	0/1169
21	K	0.49	0/901	0.82	1/1217 (0.1%)
22	L	0.72	0/1139	0.91	2/1518 (0.1%)
23	M	0.59	0/1211	0.80	0/1628
24	N	0.71	0/452	0.94	1/600 (0.2%)
25	O	0.61	0/1215	0.83	3/1638 (0.2%)
26	P	0.56	0/1087	0.77	1/1449 (0.1%)
27	Q	0.70	0/1239	0.81	0/1673
28	R	0.49	0/2490	0.70	0/3389
29	S	0.60	0/998	0.86	2/1341 (0.1%)
30	T	0.57	0/1130	0.81	0/1517
31	U	0.49	0/898	0.76	0/1220
32	V	0.54	0/935	0.81	0/1254

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	W	0.58	0/2109	0.86	1/2839 (0.0%)
34	X	0.50	0/483	0.72	0/643
35	Y	0.55	0/1823	0.75	0/2439
36	Z	0.53	0/693	0.75	0/935
37	a	0.32	0/3729	0.51	0/5041
38	b	0.42	1/3999 (0.0%)	0.57	2/5440 (0.0%)
39	c	0.33	0/4525	0.53	0/6120
All	All	0.75	39/94313 (0.0%)	1.18	867/136002 (0.6%)

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	0	0	1
4	3	0	1
5	4	0	1
7	6	0	1
9	8	0	3
10	9	0	2
16	F	0	1
21	K	0	1
27	Q	0	1
32	V	0	2
39	c	0	1
All	All	0	15

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1626	U	O3'-P	48.27	2.19	1.61
11	A	553	G	C6-N1	8.08	1.45	1.39
11	A	377	G	N9-C4	-7.20	1.32	1.38
11	A	1456	C	N3-C4	-7.04	1.29	1.33
11	A	1455	G	C6-O6	6.88	1.30	1.24

The worst 5 of 867 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1626	U	O3'-P-O5'	27.80	156.82	104.00
11	A	1626	U	OP1-P-O3'	-21.44	58.04	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1626	U	P-O3'-C3'	-19.41	96.41	119.70
11	A	553	G	N1-C6-O6	18.48	130.99	119.90
11	A	1200	G	N1-C6-O6	17.91	130.65	119.90

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	23	LYS	Peptide
4	3	131	PHE	Peptide
5	4	131	ASP	Peptide
7	6	42	ASN	Peptide
9	8	54	VAL	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	805	0	790	147	0
2	1	497	0	535	36	0
3	2	1489	0	1525	59	0
4	3	1481	0	1572	80	0
5	4	1709	0	1784	125	0
6	5	769	0	814	51	0
7	6	610	0	630	24	0
8	7	772	0	727	42	0
9	8	563	0	603	45	0
10	9	516	0	517	42	0
11	A	37835	0	19056	1169	0
12	B	1577	0	1566	221	0
13	C	1734	0	1817	80	0
14	D	1494	0	1573	81	0
15	E	1635	0	1715	88	0
16	F	671	0	707	80	0
17	G	1609	0	1675	70	0
18	H	1021	0	1060	54	0
19	I	1105	0	1166	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	J	855	0	917	41	0
21	K	891	0	883	63	0
22	L	1121	0	1196	61	0
23	M	1192	0	1222	63	0
24	N	442	0	428	24	0
25	O	1192	0	1255	45	0
26	P	1073	0	1132	41	0
27	Q	1213	0	1257	50	0
28	R	2437	0	2386	77	0
29	S	977	0	1002	41	0
30	T	1112	0	1124	69	0
31	U	890	0	887	43	0
32	V	926	0	930	76	0
33	W	2068	0	2154	71	0
34	X	475	0	523	86	0
35	Y	1799	0	1879	88	0
36	Z	684	0	672	39	0
37	a	3656	0	3708	0	0
38	b	3978	0	3768	0	0
39	c	4442	0	4474	0	0
40	5	1	0	0	0	0
40	6	1	0	0	0	0
40	9	1	0	0	0	0
40	N	1	0	0	0	0
All	All	89319	0	71629	2908	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 20.

The worst 5 of 2908 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)
11:A:1151:A:C2'	11:A:1152:A:H5'	1.10	1.57
11:A:1151:A:C6	11:A:1152:A:C8	1.93	1.57
11:A:1293:U:H1'	12:B:111:ILE:CB	1.21	1.57
11:A:1293:U:H1'	12:B:111:ILE:CG1	1.27	1.56
1:0:46:ARG:CD	34:X:3:LYS:HE3	1.39	1.53

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	0	98/100 (98%)	89 (91%)	6 (6%)	3 (3%)	4 27
2	1	61/63 (97%)	47 (77%)	9 (15%)	5 (8%)	1 12
3	2	184/188 (98%)	155 (84%)	14 (8%)	15 (8%)	1 12
4	3	182/184 (99%)	128 (70%)	27 (15%)	27 (15%)	0 3
5	4	212/214 (99%)	132 (62%)	42 (20%)	38 (18%)	0 2
6	5	95/97 (98%)	58 (61%)	20 (21%)	17 (18%)	0 2
7	6	79/81 (98%)	62 (78%)	13 (16%)	4 (5%)	2 19
8	7	94/96 (98%)	66 (70%)	18 (19%)	10 (11%)	0 8
9	8	68/70 (97%)	46 (68%)	11 (16%)	11 (16%)	0 3
10	9	50/71 (70%)	30 (60%)	9 (18%)	11 (22%)	0 1
12	B	204/206 (99%)	143 (70%)	35 (17%)	26 (13%)	0 5
13	C	221/223 (99%)	180 (81%)	28 (13%)	13 (6%)	1 17
14	D	183/185 (99%)	153 (84%)	18 (10%)	12 (7%)	1 15
15	E	215/217 (99%)	187 (87%)	16 (7%)	12 (6%)	2 18
16	F	81/83 (98%)	75 (93%)	5 (6%)	1 (1%)	13 50
17	G	204/206 (99%)	154 (76%)	31 (15%)	19 (9%)	0 10
18	H	127/129 (98%)	114 (90%)	10 (8%)	3 (2%)	6 33
19	I	139/141 (99%)	114 (82%)	14 (10%)	11 (8%)	1 13
20	J	105/107 (98%)	87 (83%)	13 (12%)	5 (5%)	2 21
21	K	125/127 (98%)	94 (75%)	16 (13%)	15 (12%)	0 6
22	L	142/144 (99%)	111 (78%)	13 (9%)	18 (13%)	0 5
23	M	143/145 (99%)	110 (77%)	19 (13%)	14 (10%)	0 9
24	N	51/53 (96%)	42 (82%)	7 (14%)	2 (4%)	3 23
25	O	148/150 (99%)	125 (84%)	15 (10%)	8 (5%)	2 19
26	P	132/134 (98%)	106 (80%)	13 (10%)	13 (10%)	0 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
27	Q	153/155 (99%)	125 (82%)	19 (12%)	9 (6%)	1 17
28	R	316/318 (99%)	273 (86%)	30 (10%)	13 (4%)	3 23
29	S	122/124 (98%)	92 (75%)	15 (12%)	15 (12%)	0 5
30	T	141/143 (99%)	111 (79%)	18 (13%)	12 (8%)	1 11
31	U	122/124 (98%)	66 (54%)	23 (19%)	33 (27%)	0 0
32	V	116/120 (97%)	87 (75%)	17 (15%)	12 (10%)	0 8
33	W	258/260 (99%)	202 (78%)	36 (14%)	20 (8%)	1 13
34	X	58/60 (97%)	49 (84%)	7 (12%)	2 (3%)	3 26
35	Y	224/226 (99%)	190 (85%)	22 (10%)	12 (5%)	2 19
36	Z	85/87 (98%)	64 (75%)	11 (13%)	10 (12%)	0 6
37	a	445/964 (46%)	438 (98%)	7 (2%)	0	100 100
38	b	478/763 (63%)	452 (95%)	24 (5%)	2 (0%)	34 72
39	c	542/812 (67%)	507 (94%)	35 (6%)	0	100 100
All	All	6403/7570 (85%)	5264 (82%)	686 (11%)	453 (7%)	2 14

5 of 453 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	24	ARG
2	1	36	THR
2	1	51	ASN
3	2	13	ALA
3	2	22	ARG

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	0	86/86 (100%)	84 (98%)	2 (2%)	50 70
2	1	56/56 (100%)	38 (68%)	18 (32%)	0 2
3	2	150/150 (100%)	118 (79%)	32 (21%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	3	165/165 (100%)	124 (75%)	41 (25%)	0 3
5	4	191/191 (100%)	137 (72%)	54 (28%)	0 2
6	5	83/83 (100%)	65 (78%)	18 (22%)	1 6
7	6	70/70 (100%)	62 (89%)	8 (11%)	5 21
8	7	77/89 (86%)	58 (75%)	19 (25%)	0 3
9	8	61/61 (100%)	43 (70%)	18 (30%)	0 2
10	9	43/43 (100%)	32 (74%)	11 (26%)	0 3
12	B	164/173 (95%)	122 (74%)	42 (26%)	0 3
13	C	182/182 (100%)	137 (75%)	45 (25%)	0 3
14	D	158/158 (100%)	117 (74%)	41 (26%)	0 3
15	E	176/176 (100%)	130 (74%)	46 (26%)	0 3
16	F	74/74 (100%)	73 (99%)	1 (1%)	67 80
17	G	173/173 (100%)	137 (79%)	36 (21%)	1 7
18	H	110/110 (100%)	84 (76%)	26 (24%)	1 4
19	I	117/117 (100%)	84 (72%)	33 (28%)	0 2
20	J	100/100 (100%)	71 (71%)	29 (29%)	0 2
21	K	81/96 (84%)	57 (70%)	24 (30%)	0 2
22	L	119/119 (100%)	96 (81%)	23 (19%)	1 8
23	M	128/128 (100%)	87 (68%)	41 (32%)	0 2
24	N	47/47 (100%)	38 (81%)	9 (19%)	1 8
25	O	127/127 (100%)	91 (72%)	36 (28%)	0 2
26	P	112/112 (100%)	84 (75%)	28 (25%)	0 3
27	Q	129/136 (95%)	105 (81%)	24 (19%)	1 9
28	R	259/261 (99%)	222 (86%)	37 (14%)	3 16
29	S	101/104 (97%)	82 (81%)	19 (19%)	1 9
30	T	115/115 (100%)	84 (73%)	31 (27%)	0 3
31	U	88/100 (88%)	55 (62%)	33 (38%)	0 0
32	V	94/109 (86%)	70 (74%)	24 (26%)	0 3
33	W	221/221 (100%)	166 (75%)	55 (25%)	0 3
34	X	51/51 (100%)	43 (84%)	8 (16%)	2 14
35	Y	188/193 (97%)	149 (79%)	39 (21%)	1 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	Z	74/74 (100%)	56 (76%)	18 (24%)	0 4
37	a	404/846 (48%)	404 (100%)	0	100 100
38	b	430/693 (62%)	421 (98%)	9 (2%)	53 72
39	c	506/749 (68%)	487 (96%)	19 (4%)	33 57
All	All	5510/6538 (84%)	4513 (82%)	997 (18%)	4 10

5 of 997 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	I	28	LEU
33	W	192	ILE
23	M	14	ILE
33	W	153	ASN
35	Y	179	VAL

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

Mol	Chain	Res	Type
23	M	19	ASN
32	V	105	GLN
23	M	89	GLN
27	Q	110	HIS
35	Y	22	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1763/1781 (98%)	544 (30%)	86 (4%)

5 of 544 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	2	A
11	A	4	C
11	A	8	U
11	A	16	G
11	A	20	G

5 of 86 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	913	G
11	A	1339	C
11	A	1058	U
11	A	1196	A
11	A	1481	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)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
11	A	3
3	2	1

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Mol	Chain	Number of breaks
32	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	123:LYS	C	135:LYS	N	19.74
1	A	658:C	O3'	676:G	P	17.56
1	V	89:SER	C	95:ARG	N	3.95
1	A	1151:A	O3'	1152:A	P	3.15
1	A	1626:U	O3'	1627:U	P	2.19

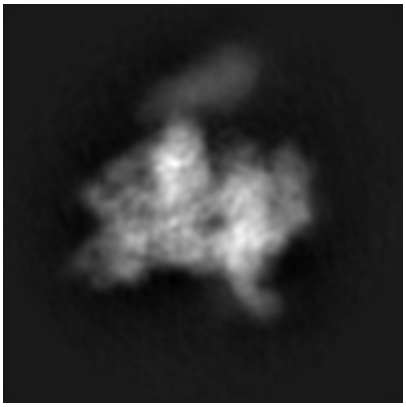
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2845. These allow visual inspection of the internal detail of the map and identification of artifacts.

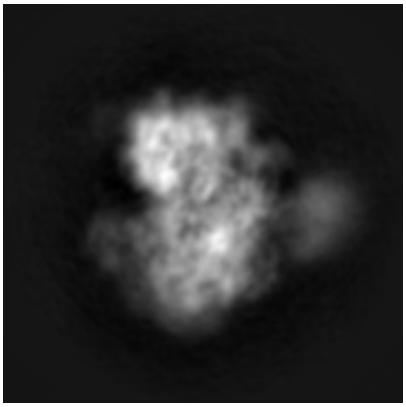
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

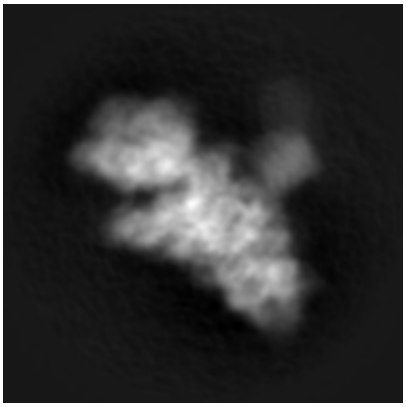
6.1.1 Primary map



X



Y

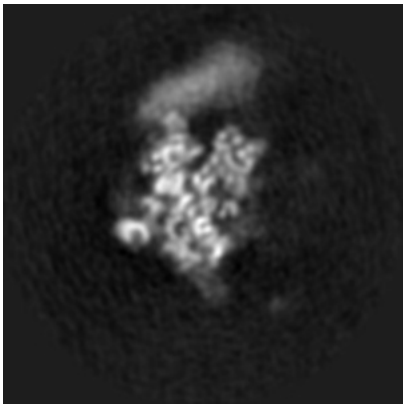


Z

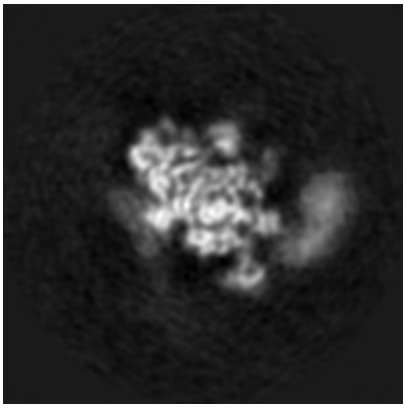
The images above show the map projected in three orthogonal directions.

6.2 Central slices

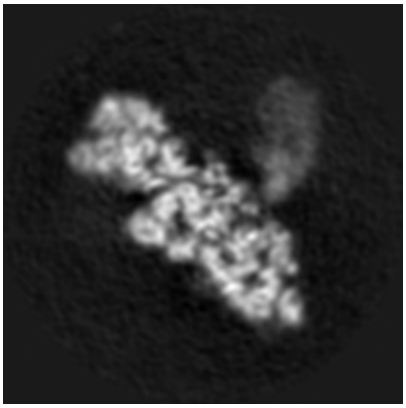
6.2.1 Primary map



X Index: 128



Y Index: 128

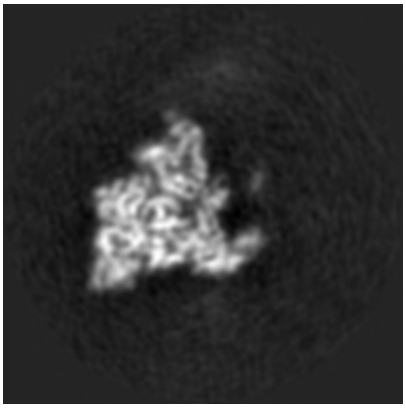


Z Index: 128

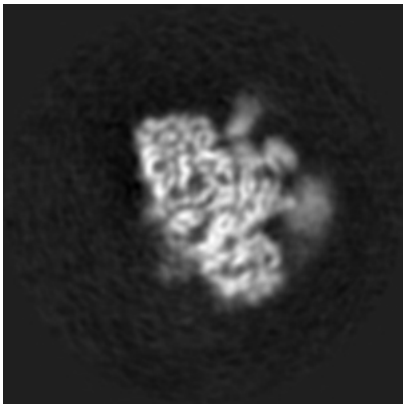
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

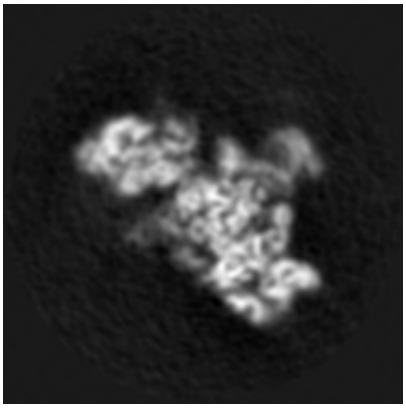
6.3.1 Primary map



X Index: 150



Y Index: 108

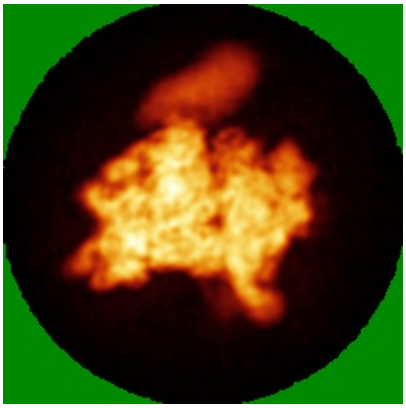


Z Index: 103

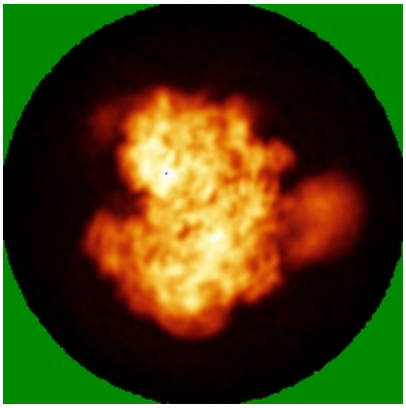
The images above show the largest variance slices of the map in three orthogonal directions.

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

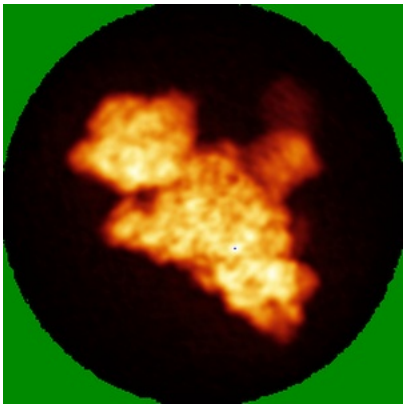
6.4.1 Primary map



X



Y

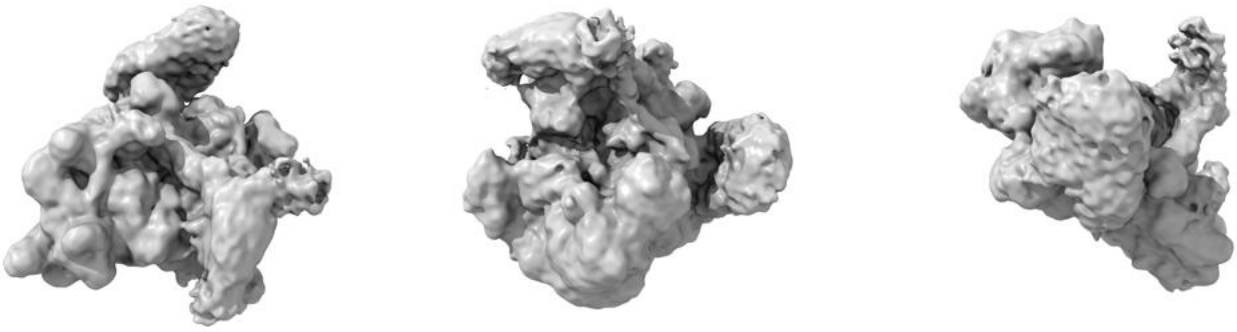


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

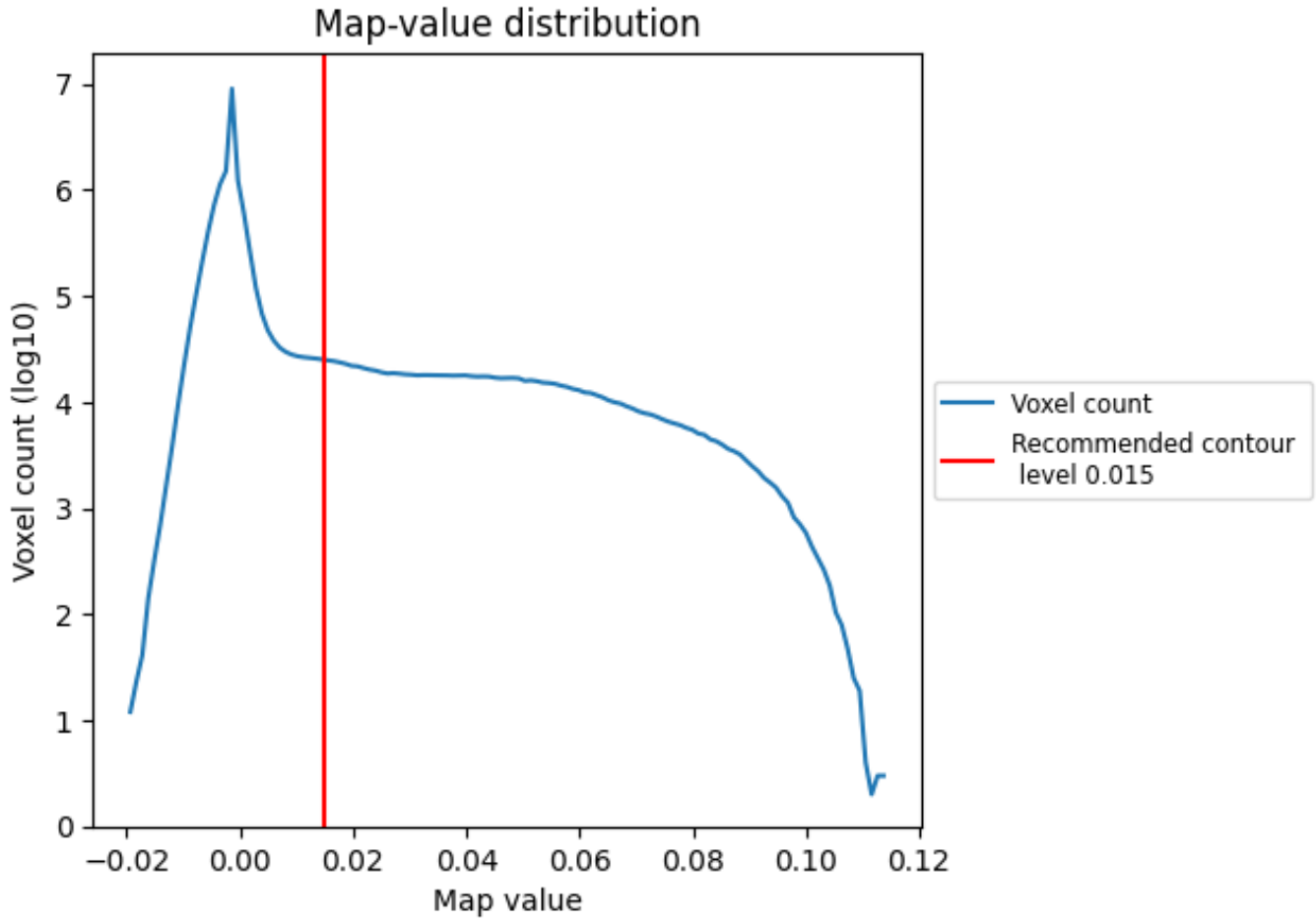
6.6 Mask visualisation (i)

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

7 Map analysis

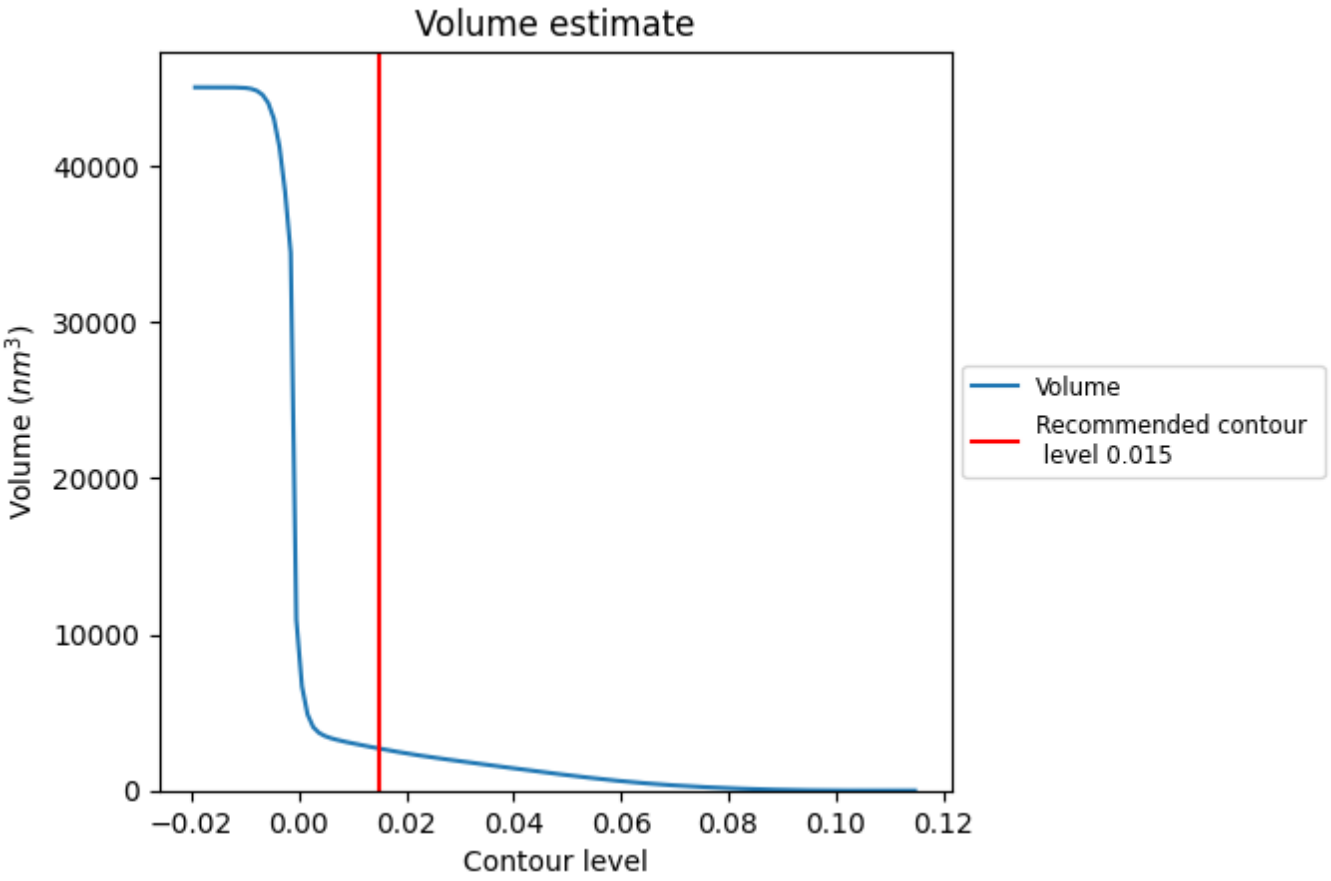
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

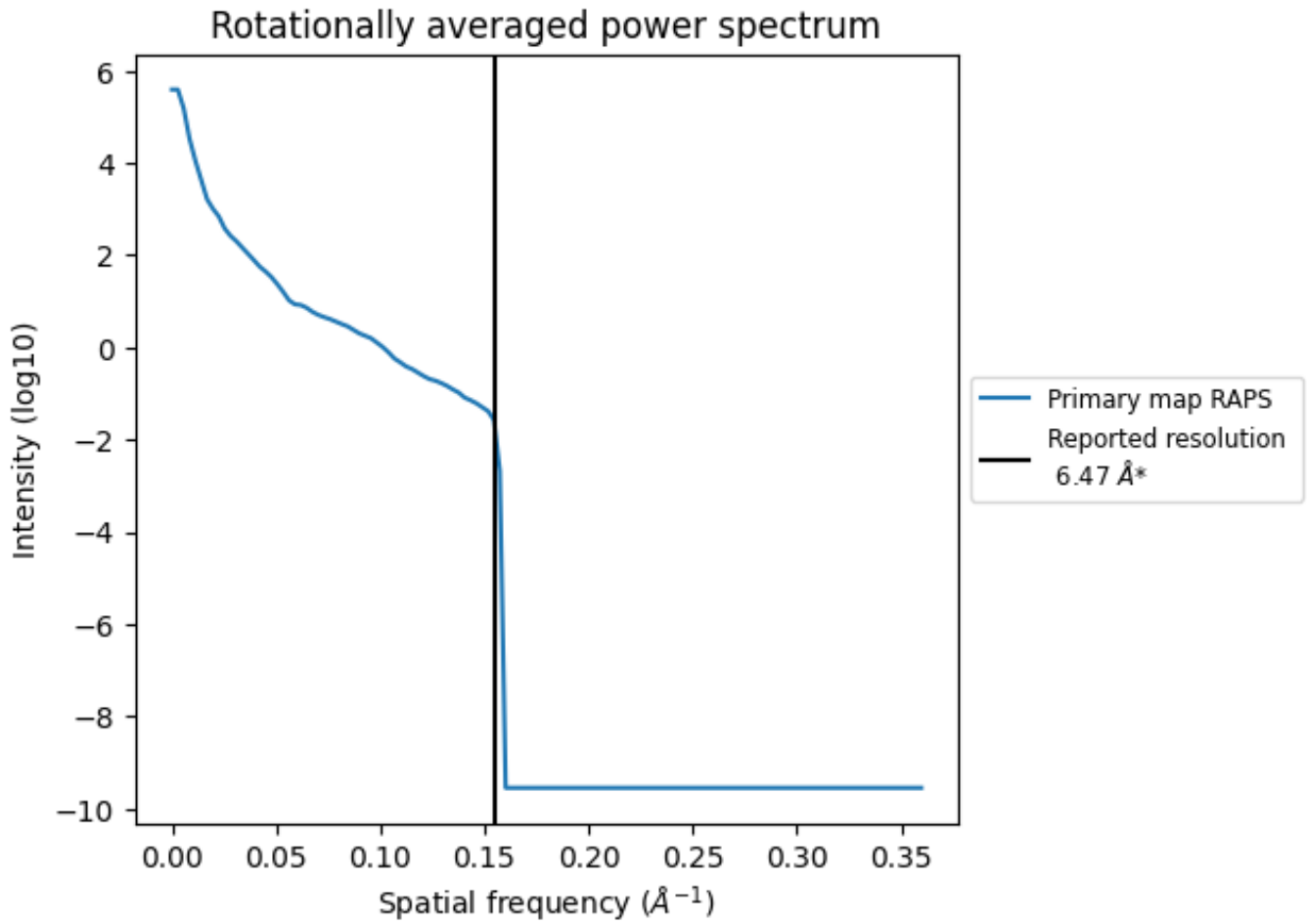
7.2 Volume estimate (i)



The volume at the recommended contour level is 2691 nm^3; this corresponds to an approximate mass of 2431 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 0.155 Å^{-1}

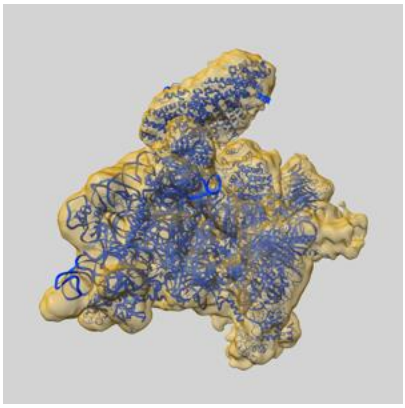
8 Fourier-Shell correlation (i)

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

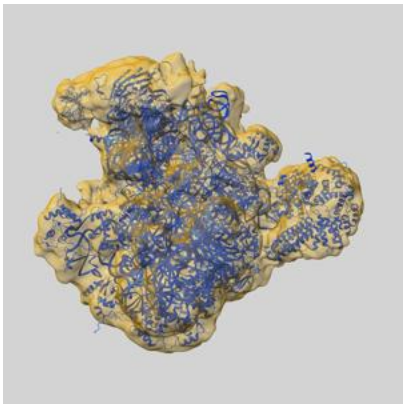
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2845 and PDB model 4UER. Per-residue inclusion information can be found in section 3 on page 11.

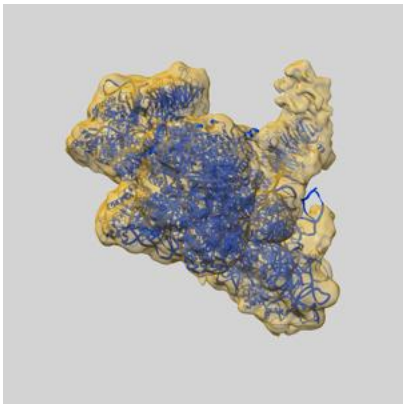
9.1 Map-model overlay



X



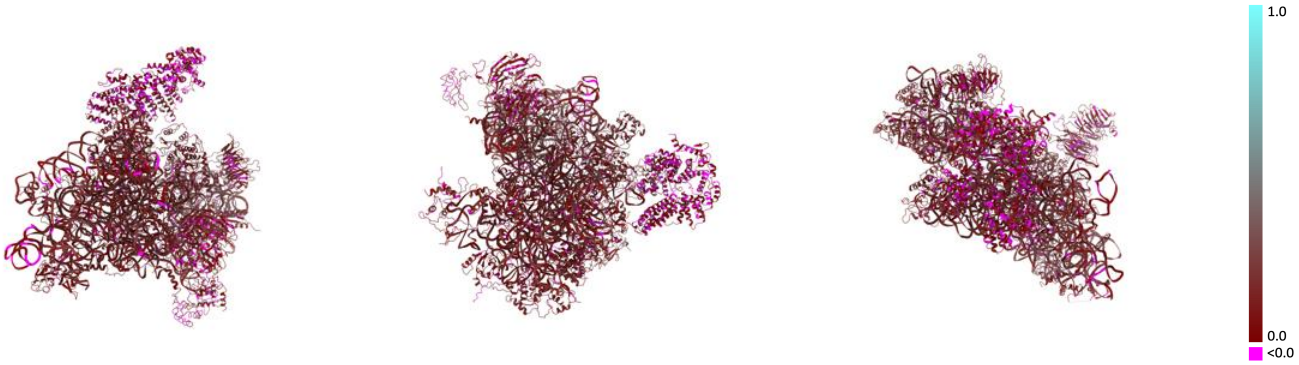
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

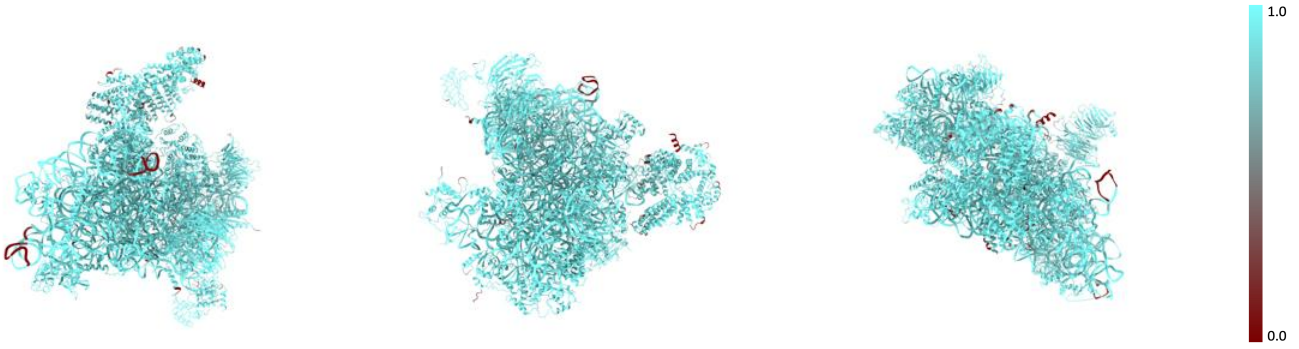
9.2 Q-score mapped to coordinate model



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.

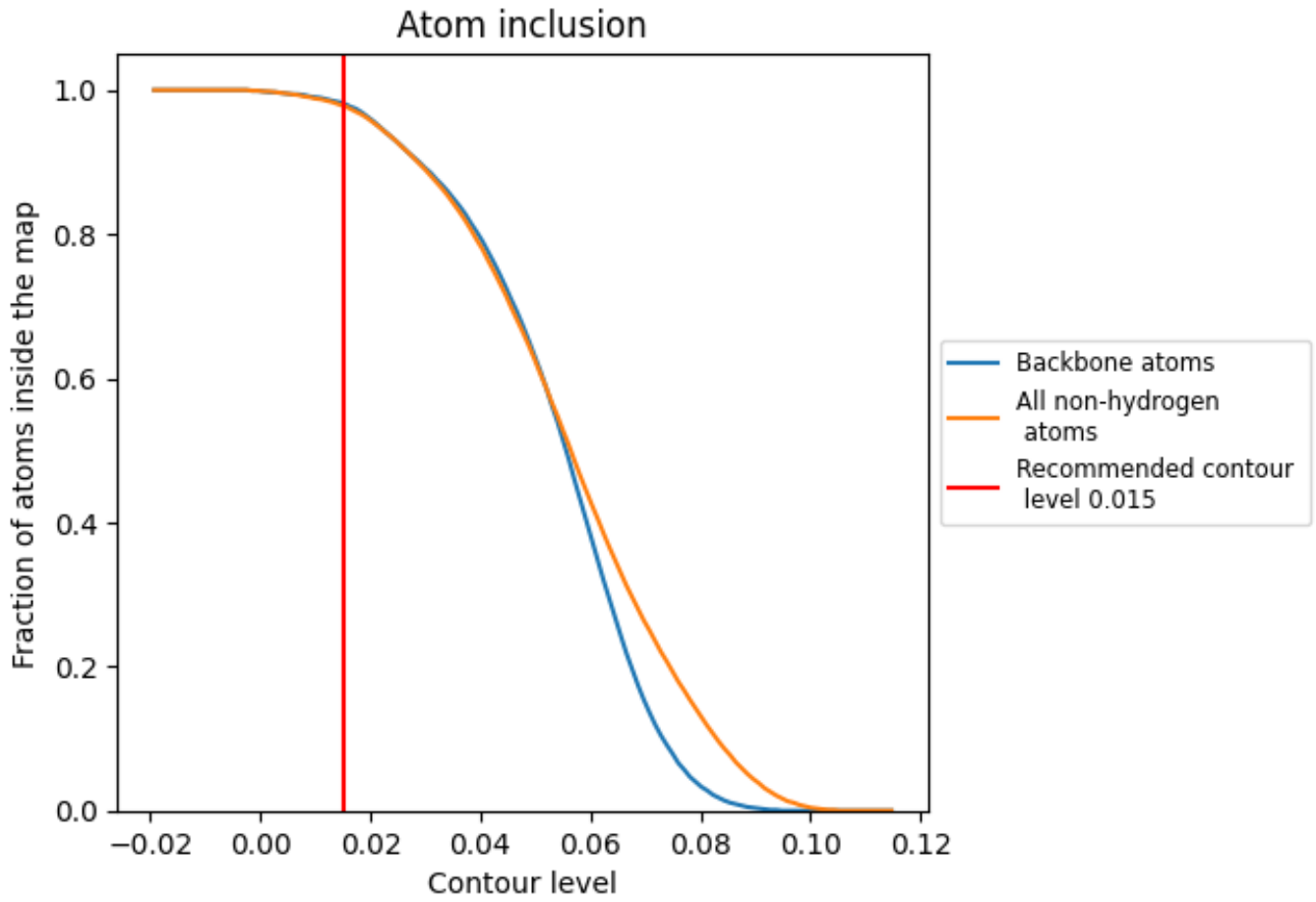
9.3 Atom inclusion mapped to coordinate model



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9780	0.1350
0	0.8020	0.0540
1	0.9620	0.1270
2	1.0000	0.1290
3	0.9840	0.1470
4	0.9960	0.1490
5	0.9890	0.1260
6	0.9920	0.1280
7	0.9960	0.1280
8	0.9840	0.1230
9	0.9700	0.0710
A	0.9860	0.1700
B	0.9960	0.1640
C	0.9870	0.1340
D	0.9710	0.1340
E	0.9940	0.1390
F	0.8670	0.0800
G	0.9910	0.1300
H	0.9980	0.1310
I	1.0000	0.1110
J	0.9680	0.1150
K	1.0000	0.1160
L	0.9950	0.1310
M	0.9960	0.0980
N	1.0000	0.0830
O	0.9890	0.1440
P	0.9950	0.1390
Q	0.9810	0.1280
R	0.9910	0.1140
S	0.9370	0.0960
T	1.0000	0.1060
U	0.9500	0.0950
V	0.9820	0.1350
W	0.9930	0.1350
X	0.9670	0.0830

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Chain	Atom inclusion	Q-score
Y	0.9940	0.1210
Z	0.9900	0.1390
a	0.9480	0.0430
b	0.9750	0.0910
c	0.9070	0.0430