



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 02:09 PM EST

PDB ID : 3J81
EMDB ID : EMD-2763
Title : CryoEM structure of a partial yeast 48S preinitiation complex
Authors : Hussain, T.; Llacer, J.L.; Fernandez, I.S.; Savva, C.G.; Ramakrishnan, V.
Deposited on : 2014-08-29
Resolution : 4.00 Å(reported)
Based on initial models : 3V11, 3U5C, 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 ⓘ 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

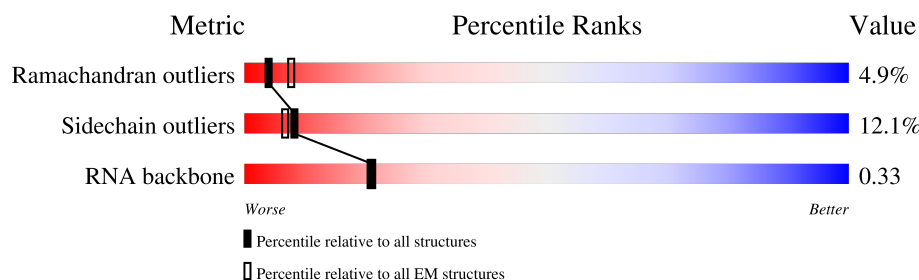
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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








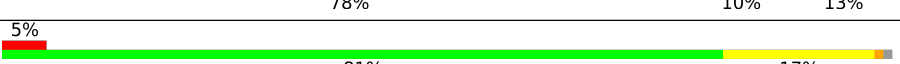
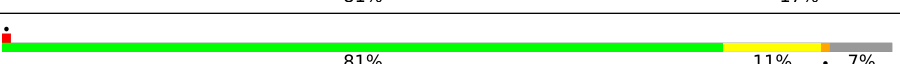
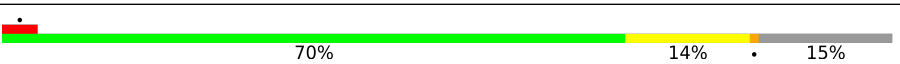


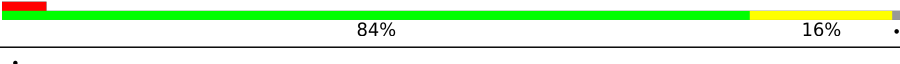
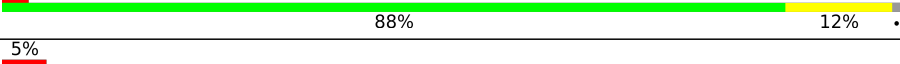

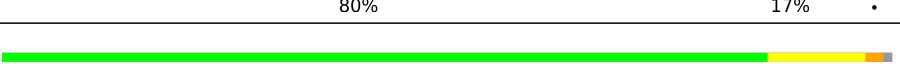
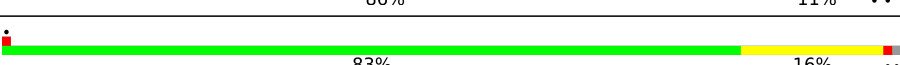










Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1799	
2	A	254	
3	B	255	
4	C	259	
5	D	237	
6	E	261	
7	F	227	
8	G	236	

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Mol	Chain	Length	Quality of chain
9	H	190	
10	I	201	
11	J	188	
12	K	106	
13	L	156	
14	M	134	
15	N	151	
16	O	137	
17	P	140	
18	Q	143	
19	R	136	
20	S	146	
21	T	144	
22	U	117	
23	V	87	
24	W	130	
25	X	145	
26	Y	135	
27	Z	108	
28	a	119	
29	b	82	
30	c	67	
31	f	150	
32	g	326	
33	d	56	

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Mol	Chain	Length	Quality of chain
34	e	63	
35	h	25	
36	1	75	
37	3	25	
38	i	153	
39	j	300	
40	m	108	
41	k	527	
42	l	285	

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 83760 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1780	Total	C	N	O	P	0	0
			37797	16892	6658	12467	1780		

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	207	Total	C	N	O	S	0	0
			1625	1040	286	297	2		

- Molecule 3 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	215	Total	C	N	O	S	0	0
			1727	1092	314	318	3		

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 5 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 6 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 7 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 8 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 9 is a protein called eS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	H	184	Total	C	N	O	0	0
			1483	950	270	263		

- Molecule 10 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	188	Total	C	N	O	S	0	0
			1493	926	301	265	1		

- Molecule 11 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 12 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 13 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 14 is a protein called eS12.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	117	Total	C	N	O	0	0
			885	553	161	171		

- Molecule 15 is a protein called uS15.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	N	150	Total	C	N	O	S	0
			1187	756	223	206	2	0

- Molecule 16 is a protein called uS11.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	O	127	Total	C	N	O	S	0
			942	578	188	173	3	0

- Molecule 17 is a protein called uS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	P	119	Total	C	N	O	S	0
			943	604	171	163	5	0

- Molecule 18 is a protein called uS9.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Q	141	Total	C	N	O		0
			1105	709	204	192		0

- Molecule 19 is a protein called eS17.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	R	120	Total	C	N	O	S	0
			959	598	178	180	3	0

- Molecule 20 is a protein called uS13.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	S	145	Total	C	N	O	S	0
			1193	741	240	210	2	0

- Molecule 21 is a protein called eS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 22 is a protein called uS10.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	U	106	Total	C	N	O	S	0
			845	540	152	152	1	0

- Molecule 23 is a protein called eS21.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	V	87	Total	C	N	O	S	0
			687	424	126	135	2	0

- Molecule 24 is a protein called uS8.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	W	129	Total	C	N	O	S	0
			1021	651	187	180	3	0

- Molecule 25 is a protein called uS12.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	144	Total	C	N	O	S	0
			1119	708	218	191	2	0

- Molecule 26 is a protein called eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Y	134	Total	C	N	O	0	0
			1061	665	207	189		

- Molecule 27 is a protein called eS25.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Z	70	Total	C	N	O	S	0
			558	355	104	98	1	0

- Molecule 28 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	97	Total	C	N	O	S	0	0
			770	475	163	127	5		

- Molecule 29 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	81	Total	C	N	O	S	0	0
			609	379	112	113	5		

- Molecule 30 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	62	Total	C	N	O	S	0	0
			487	301	97	88	1		

- Molecule 31 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	69	Total	C	N	O	S	0	0
			546	351	101	90	4		

- Molecule 32 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 33 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	53	Total	C	N	O	S	0	0
			446	280	89	76	1		

- Molecule 34 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	54	Total	C	N	O	S	0	0
			433	271	88	73	1		

- Molecule 35 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 36 is a RNA chain called Met-tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1	74	Total	C	N	O	P	0	0
			1584	706	291	513	74		

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	22	Total	C	N	O	P	0	0
			447	201	62	162	22		

- Molecule 38 is a protein called eIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	111	Total	C	N	O	S	0	0
			884	542	170	167	5		

- Molecule 39 is a protein called eIF2 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	252	Total	C	N	O	S	0	0
			2025	1294	336	386	9		

- Molecule 40 is a protein called eIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	m	90	Total	C	N	O	S	0	0
			716	452	132	128	4		

- Molecule 41 is a protein called eIF2 gamma.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	k	365	Total	C	N	O	0	0
			1798	1068	365	365		

- Molecule 42 is a protein called eIF2 beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	1	17	Total	C	N	O	0	0
			84	50	17	17		

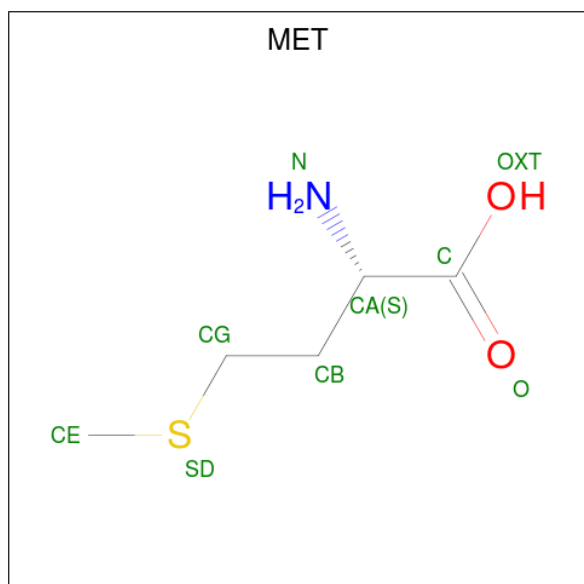
- Molecule 43 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
43	2	80	Total	Mg	0
			80	80	
43	G	1	Total	Mg	0
			1	1	

- Molecule 44 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
44	a	1	Total	Zn	0
			1	1	
44	b	1	Total	Zn	0
			1	1	
44	f	1	Total	Zn	0
			1	1	

- Molecule 45 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



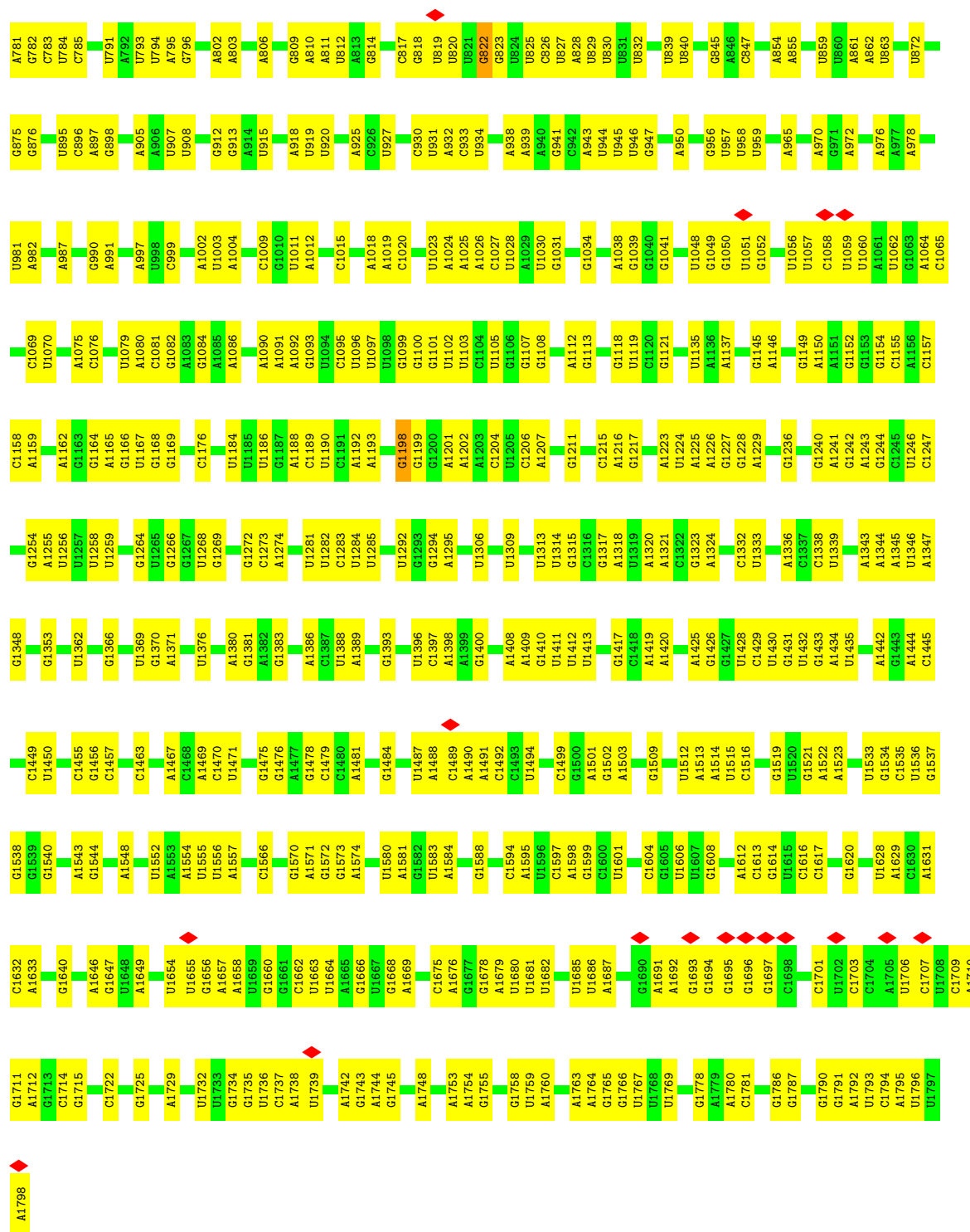
Mol	Chain	Residues	Atoms					AltConf
45	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

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.

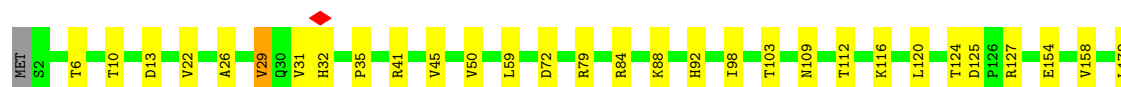
• Molecule 1: 18S rRNA



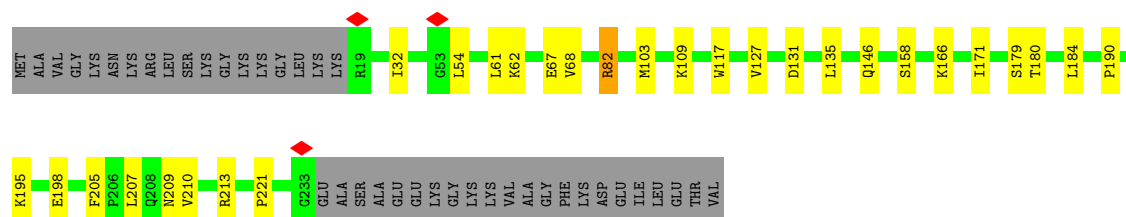


• Molecule 2: uS2

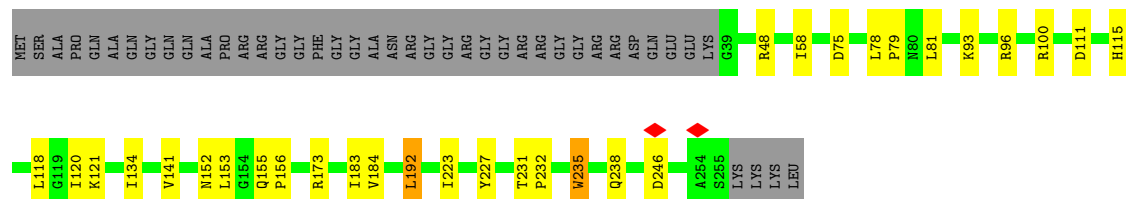
Chain A: 66% 14% 19%



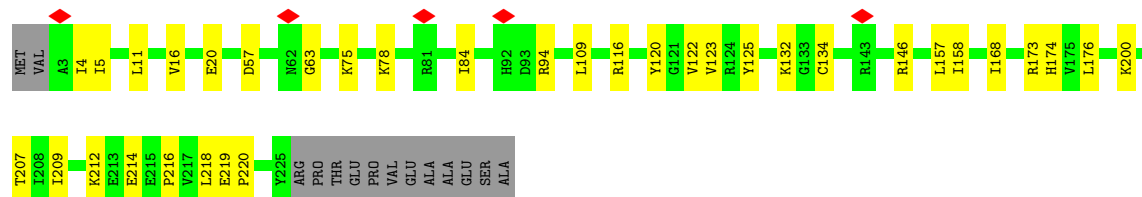
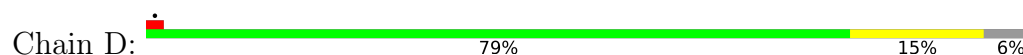
- Molecule 3: eS1



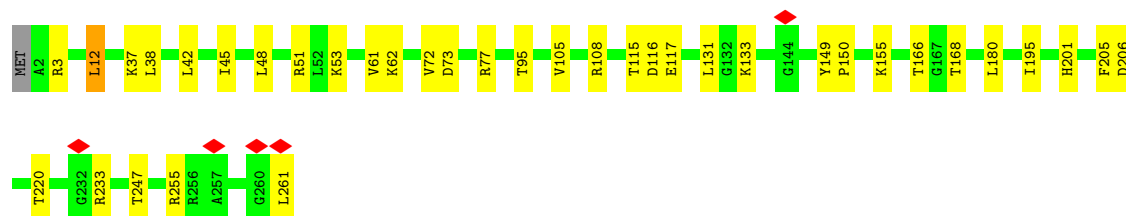
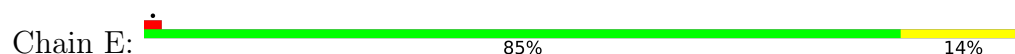
- Molecule 4: uS5




- Molecule 5: uS3

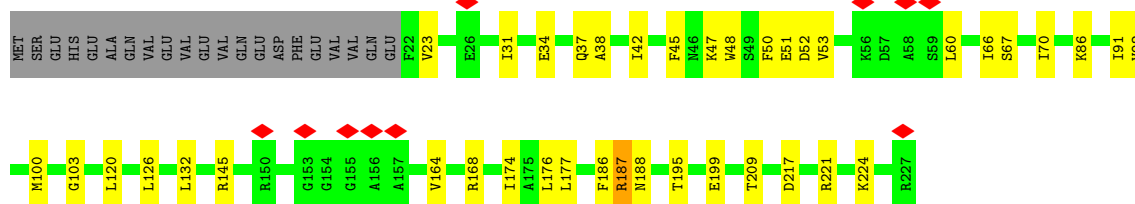


- Molecule 6: eS4




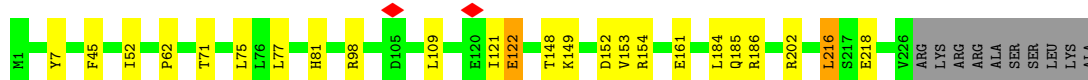
- Molecule 7: uS7

Chain F:  73% 17% 9%




- Molecule 8: eS6

Chain G:  86% 9% . .




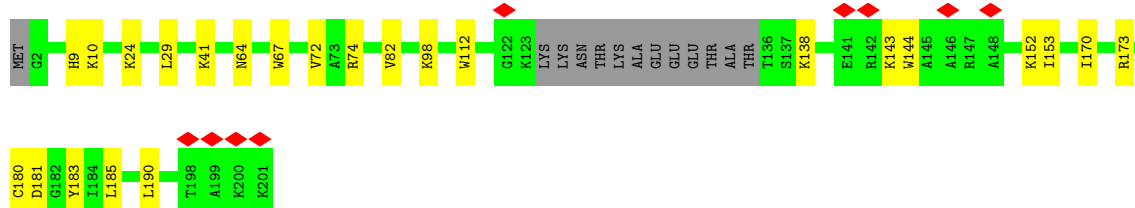
- Molecule 9: eS7

Chain H:  84% 13% .




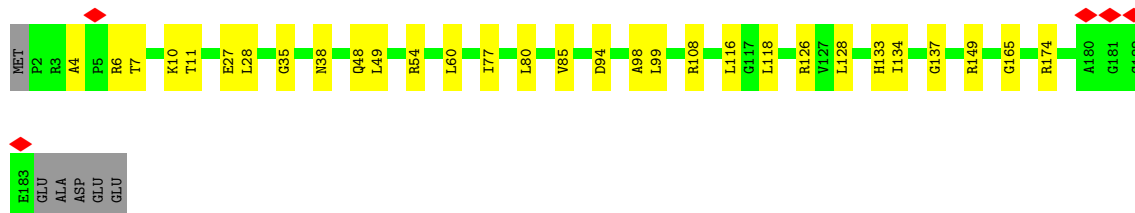
- Molecule 10: eS8

Chain I:  82% 12% 6%



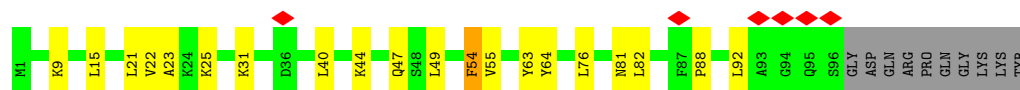
- Molecule 11: uS4

Chain J:  81% 16% .

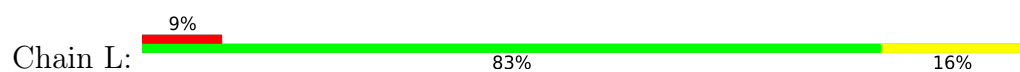


- Molecule 12: eS10

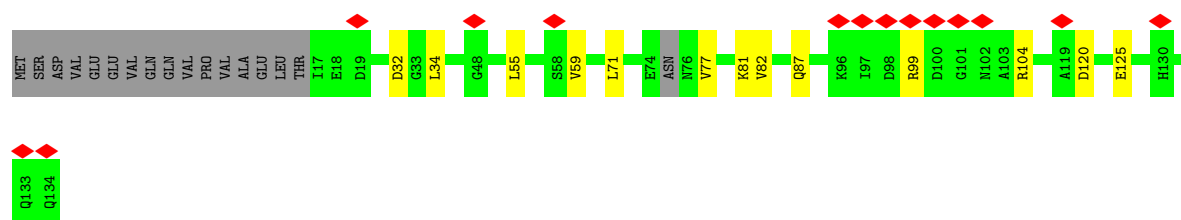
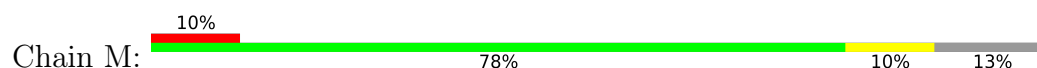
Chain K:  72% 18% . 9%



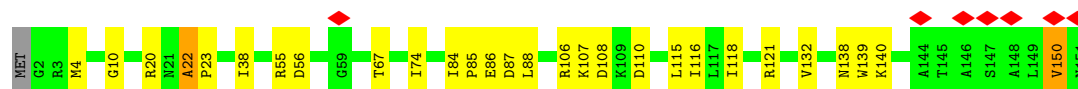
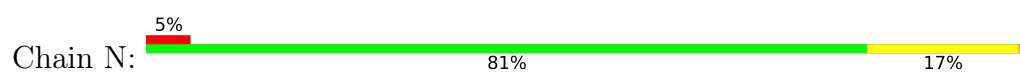
• Molecule 13: uS17



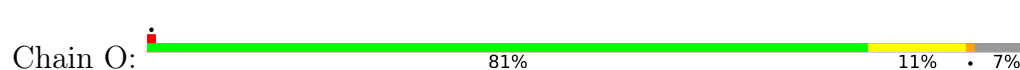
• Molecule 14: eS12



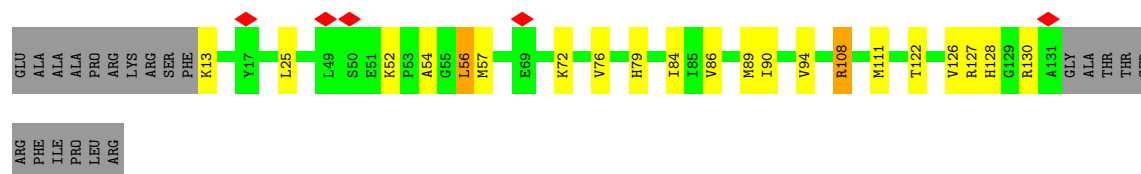
• Molecule 15: uS15



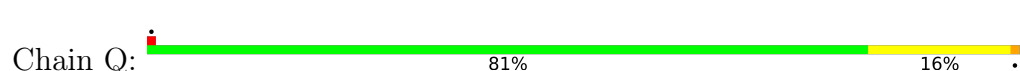
• Molecule 16: uS11

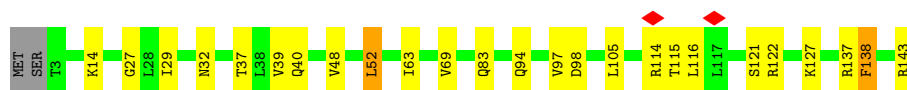


• Molecule 17: uS19

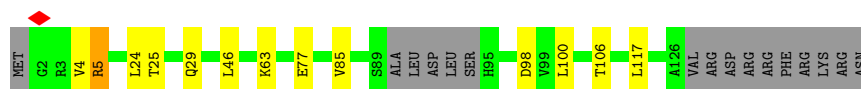
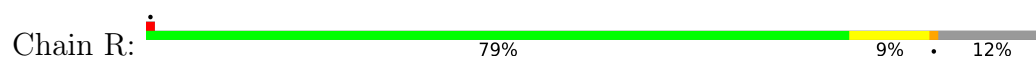


• Molecule 18: uS9

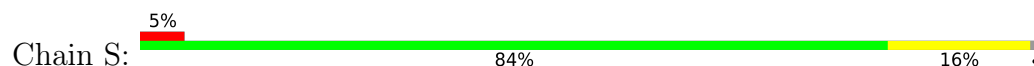




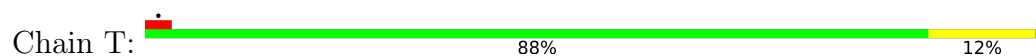
• Molecule 19: eS17



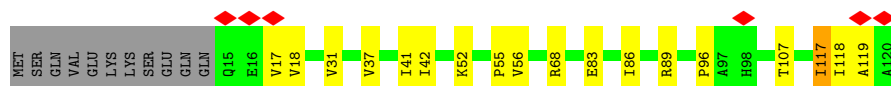
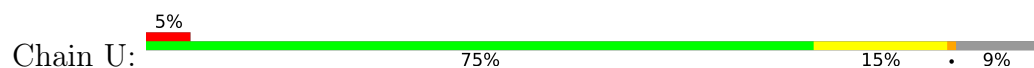
• Molecule 20: uS13



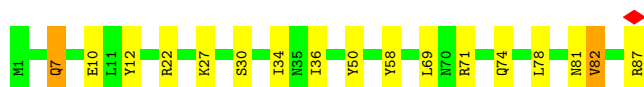
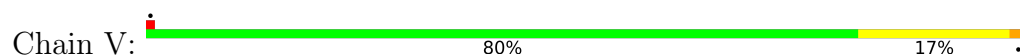
• Molecule 21: eS19



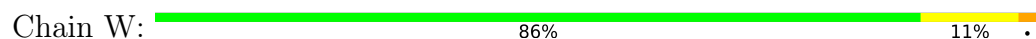
• Molecule 22: uS10



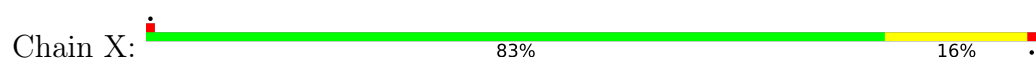
• Molecule 23: eS21



• Molecule 24: uS8

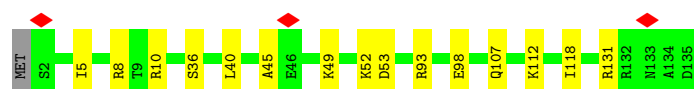
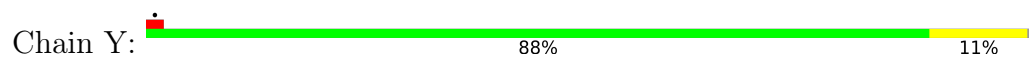


• Molecule 25: uS12

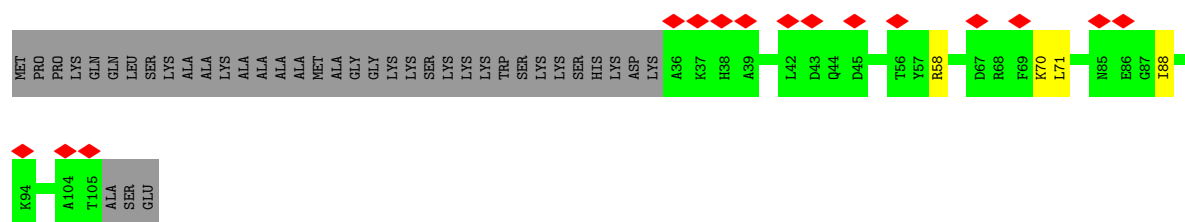




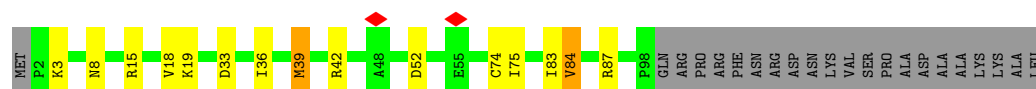
• Molecule 26: eS24



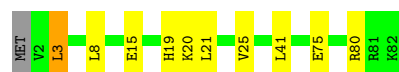
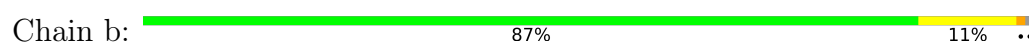
• Molecule 27: eS25



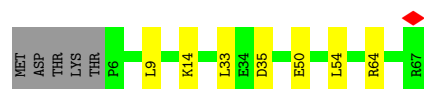
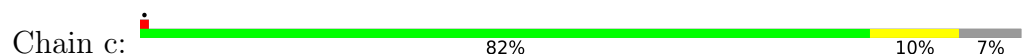
• Molecule 28: eS26



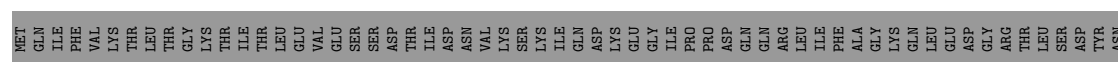
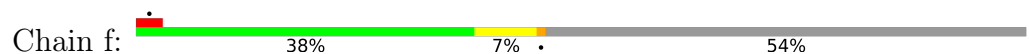
• Molecule 29: eS27



• Molecule 30: eS28



• Molecule 31: eS31





- Molecule 32: RACK1

Chain g: 88% 9%



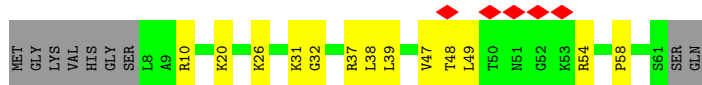
- Molecule 33: uS14

Chain d: 79% 16% 5%



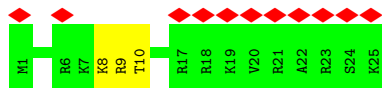
- Molecule 34: eS30

Chain e: 8% 65% 21% 14%



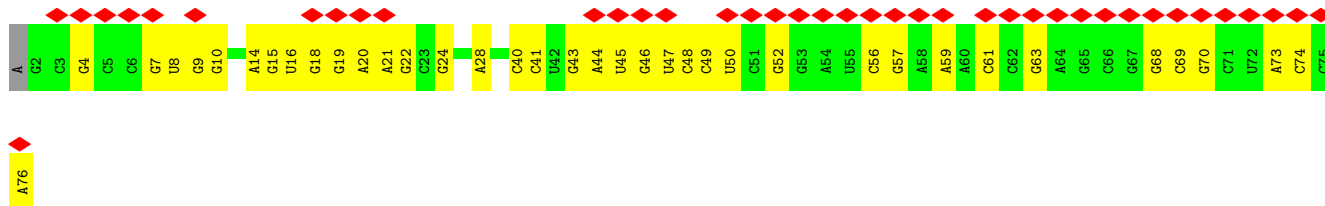
- Molecule 35: eL41

Chain h: 44% 88% 12%

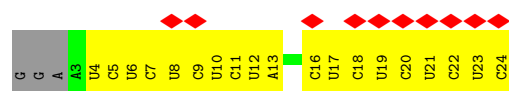


- Molecule 36: Met-tRNAi

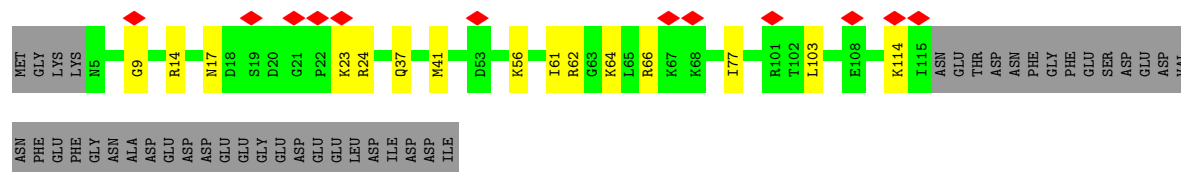
Chain 1: 53% 49% 49%



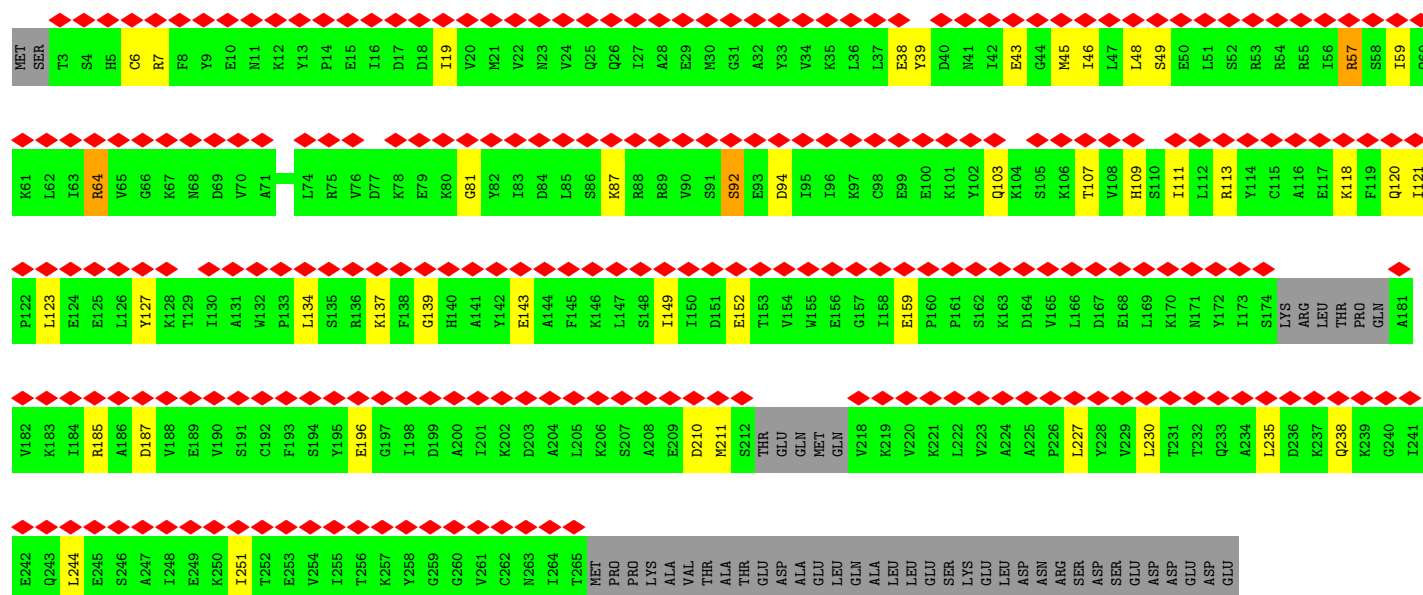
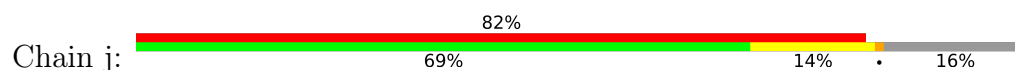
- Molecule 37: mRNA



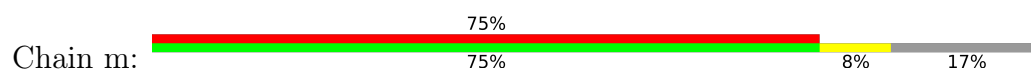
• Molecule 38: eIF1A



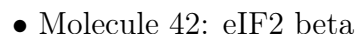
• Molecule 39: eIF2 alpha



• Molecule 40: eIF1



• Molecule 41: eIF2 gamma



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29698	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.467	Depositor
Minimum map value	-0.164	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.065	Depositor
Map size (\AA)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.34, 1.34, 1.34	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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.25	0/42269	0.67	6/65862 (0.0%)
2	A	0.42	0/1665	0.73	1/2276 (0.0%)
3	B	0.40	0/1752	0.67	1/2360 (0.0%)
4	C	0.39	0/1659	0.68	1/2252 (0.0%)
5	D	0.41	0/1769	0.69	0/2378
6	E	0.39	0/2122	0.66	2/2861 (0.1%)
7	F	0.41	0/1628	0.75	1/2198 (0.0%)
8	G	0.39	0/1835	0.66	2/2451 (0.1%)
9	H	0.40	0/1507	0.69	0/2028
10	I	0.40	0/1519	0.66	1/2033 (0.0%)
11	J	0.41	0/1495	0.73	0/2001
12	K	0.47	0/831	0.72	0/1123
13	L	0.40	0/1276	0.64	0/1718
14	M	0.41	0/891	0.69	0/1201
15	N	0.42	0/1210	0.75	1/1628 (0.1%)
16	O	0.38	0/953	0.67	0/1279
17	P	0.41	0/962	0.69	1/1294 (0.1%)
18	Q	0.42	0/1125	0.70	1/1510 (0.1%)
19	R	0.41	0/969	0.70	0/1299
20	S	0.40	0/1212	0.73	0/1629
21	T	0.39	0/1129	0.68	0/1520
22	U	0.39	0/857	0.66	0/1158
23	V	0.39	0/696	0.69	0/938
24	W	0.39	0/1039	0.69	0/1399
25	X	0.41	0/1137	0.71	0/1516
26	Y	0.38	0/1075	0.64	0/1433
27	Z	0.41	0/567	0.65	0/762
28	a	0.38	0/782	0.71	0/1047
29	b	0.38	0/619	0.66	0/837
30	c	0.36	0/489	0.67	0/655
31	f	0.43	0/559	0.70	1/747 (0.1%)
32	g	0.40	0/2521	0.61	0/3431

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.44	0/457	0.65	0/607
34	e	0.42	0/440	0.69	0/586
35	h	0.35	0/234	0.79	0/300
36	1	0.25	0/1771	0.65	0/2760
37	3	0.28	0/493	0.71	0/761
38	i	0.38	0/894	0.67	0/1188
39	j	0.41	0/2053	0.66	0/2762
40	m	0.39	0/724	0.65	0/968
41	k	0.47	1/1791 (0.1%)	0.74	1/2480 (0.0%)
42	l	0.42	0/83	0.69	0/114
All	All	0.34	1/89059 (0.0%)	0.67	20/129350 (0.0%)

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
10	I	0	1
15	N	0	1
25	X	0	1
41	k	0	2
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	k	497	GLU	N-CA	5.42	1.57	1.46

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	k	497	GLU	N-CA-C	8.38	133.61	111.00
1	2	685	A	C2'-C3'-O3'	7.22	125.38	109.50
17	P	56	LEU	CA-CB-CG	5.95	128.98	115.30
1	2	1198	G	C2'-C3'-O3'	5.93	123.19	113.70
4	C	192	LEU	CA-CB-CG	5.91	128.90	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	I	183	TYR	Peptide
15	N	22	ALA	Peptide
25	X	63	GLN	Peptide
41	k	179	CYS	Peptide
41	k	495	ILE	Mainchain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	205/254 (81%)	168 (82%)	26 (13%)	11 (5%)	2	21
3	B	213/255 (84%)	176 (83%)	23 (11%)	14 (7%)	1	17
4	C	215/259 (83%)	182 (85%)	23 (11%)	10 (5%)	2	23
5	D	221/237 (93%)	202 (91%)	13 (6%)	6 (3%)	5	34
6	E	258/261 (99%)	223 (86%)	25 (10%)	10 (4%)	3	26
7	F	204/227 (90%)	169 (83%)	24 (12%)	11 (5%)	2	21
8	G	224/236 (95%)	194 (87%)	24 (11%)	6 (3%)	5	34
9	H	182/190 (96%)	145 (80%)	23 (13%)	14 (8%)	1	14
10	I	184/201 (92%)	159 (86%)	21 (11%)	4 (2%)	6	37
11	J	180/188 (96%)	150 (83%)	21 (12%)	9 (5%)	2	22
12	K	94/106 (89%)	74 (79%)	12 (13%)	8 (8%)	1	12
13	L	153/156 (98%)	128 (84%)	16 (10%)	9 (6%)	1	19
14	M	113/134 (84%)	86 (76%)	21 (19%)	6 (5%)	2	21
15	N	148/151 (98%)	127 (86%)	11 (7%)	10 (7%)	1	17
16	O	125/137 (91%)	96 (77%)	24 (19%)	5 (4%)	3	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	P	117/140 (84%)	95 (81%)	15 (13%)	7 (6%)	1	19
18	Q	139/143 (97%)	115 (83%)	13 (9%)	11 (8%)	1	14
19	R	116/136 (85%)	101 (87%)	11 (10%)	4 (3%)	3	30
20	S	143/146 (98%)	119 (83%)	16 (11%)	8 (6%)	2	20
21	T	141/144 (98%)	129 (92%)	9 (6%)	3 (2%)	7	39
22	U	104/117 (89%)	88 (85%)	8 (8%)	8 (8%)	1	14
23	V	85/87 (98%)	69 (81%)	9 (11%)	7 (8%)	1	13
24	W	127/130 (98%)	107 (84%)	14 (11%)	6 (5%)	2	23
25	X	142/145 (98%)	111 (78%)	22 (16%)	9 (6%)	1	18
26	Y	132/135 (98%)	115 (87%)	13 (10%)	4 (3%)	4	32
27	Z	68/108 (63%)	58 (85%)	9 (13%)	1 (2%)	10	45
28	a	95/119 (80%)	71 (75%)	17 (18%)	7 (7%)	1	15
29	b	79/82 (96%)	65 (82%)	11 (14%)	3 (4%)	3	27
30	c	60/67 (90%)	55 (92%)	4 (7%)	1 (2%)	9	43
31	f	67/150 (45%)	47 (70%)	14 (21%)	6 (9%)	1	12
32	g	312/326 (96%)	270 (86%)	32 (10%)	10 (3%)	4	31
33	d	51/56 (91%)	39 (76%)	10 (20%)	2 (4%)	3	26
34	e	52/63 (82%)	40 (77%)	8 (15%)	4 (8%)	1	14
35	h	23/25 (92%)	23 (100%)	0	0	100	100
38	i	109/153 (71%)	90 (83%)	16 (15%)	3 (3%)	5	33
39	j	246/300 (82%)	213 (87%)	21 (8%)	12 (5%)	2	22
40	m	88/108 (82%)	80 (91%)	6 (7%)	2 (2%)	6	37
41	k	351/527 (67%)	270 (77%)	56 (16%)	25 (7%)	1	16
42	l	15/285 (5%)	11 (73%)	4 (27%)	0	100	100
All	All	5581/6684 (84%)	4660 (84%)	645 (12%)	276 (5%)	4	22

5 of 276 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	29	VAL
4	C	96	ARG
4	C	141	VAL
4	C	235	TRP
5	D	4	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	175/211 (83%)	145 (83%)	30 (17%)	2	13
3	B	196/228 (86%)	181 (92%)	15 (8%)	13	40
4	C	176/203 (87%)	154 (88%)	22 (12%)	4	22
5	D	185/196 (94%)	156 (84%)	29 (16%)	2	16
6	E	223/224 (100%)	197 (88%)	26 (12%)	5	24
7	F	174/194 (90%)	145 (83%)	29 (17%)	2	14
8	G	192/200 (96%)	174 (91%)	18 (9%)	8	31
9	H	164/170 (96%)	154 (94%)	10 (6%)	18	47
10	I	148/159 (93%)	130 (88%)	18 (12%)	5	23
11	J	153/158 (97%)	132 (86%)	21 (14%)	3	20
12	K	88/96 (92%)	75 (85%)	13 (15%)	3	17
13	L	136/137 (99%)	120 (88%)	16 (12%)	5	24
14	M	93/109 (85%)	86 (92%)	7 (8%)	13	41
15	N	127/128 (99%)	109 (86%)	18 (14%)	3	19
16	O	96/104 (92%)	84 (88%)	12 (12%)	4	22
17	P	101/117 (86%)	86 (85%)	15 (15%)	3	17
18	Q	117/119 (98%)	102 (87%)	15 (13%)	4	22
19	R	109/124 (88%)	99 (91%)	10 (9%)	9	32
20	S	128/129 (99%)	113 (88%)	15 (12%)	5	24
21	T	117/118 (99%)	103 (88%)	14 (12%)	5	23
22	U	96/107 (90%)	85 (88%)	11 (12%)	5	25
23	V	73/73 (100%)	61 (84%)	12 (16%)	2	14
24	W	110/111 (99%)	96 (87%)	14 (13%)	4	22
25	X	119/120 (99%)	103 (87%)	16 (13%)	4	21
26	Y	108/109 (99%)	97 (90%)	11 (10%)	7	28
27	Z	60/88 (68%)	57 (95%)	3 (5%)	24	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	a	82/100 (82%)	72 (88%)	10 (12%)	5	23
29	b	71/72 (99%)	63 (89%)	8 (11%)	6	25
30	c	54/59 (92%)	48 (89%)	6 (11%)	6	26
31	f	57/133 (43%)	50 (88%)	7 (12%)	4	23
32	g	265/272 (97%)	245 (92%)	20 (8%)	13	41
33	d	46/48 (96%)	39 (85%)	7 (15%)	3	16
34	e	47/55 (86%)	38 (81%)	9 (19%)	1	9
35	h	23/23 (100%)	20 (87%)	3 (13%)	4	22
38	i	93/130 (72%)	81 (87%)	12 (13%)	4	22
39	j	226/270 (84%)	190 (84%)	36 (16%)	2	16
40	m	77/96 (80%)	70 (91%)	7 (9%)	9	33
All	All	4505/4990 (90%)	3960 (88%)	545 (12%)	8	23

5 of 545 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	g	188	LEU
33	d	41	GLN
32	g	151	TRP
39	j	123	LEU
10	I	181	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
18	Q	100	GLN
24	W	12	ASN
39	j	238	GLN
33	d	20	GLN
18	Q	139	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1778/1799 (98%)	807 (45%)	139 (7%)
36	1	73/75 (97%)	34 (46%)	6 (8%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
37	3	21/25 (84%)	18 (85%)	6 (28%)
All	All	1872/1899 (98%)	859 (45%)	151 (8%)

5 of 859 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	5	U
1	2	8	U

5 of 151 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1514	A
36	1	47	U
1	2	1566	C
1	2	1711	G
37	3	22	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 85 ligands modelled in this entry, 84 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	MET	k	601	-	6,7,8	0.46	0	2,7,9	0.35	0

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
45	MET	k	601	-	-	1/5/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	k	601	MET	N-CA-CB-CG

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](#)

There are no chain breaks in this entry.

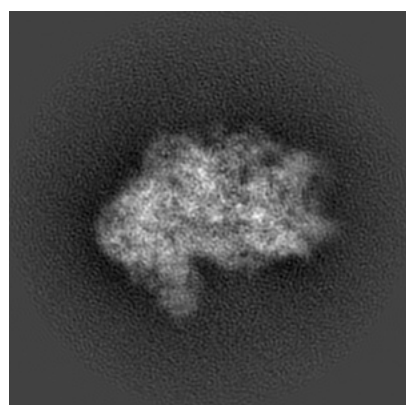
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2763. These allow visual inspection of the internal detail of the map and identification of artifacts.

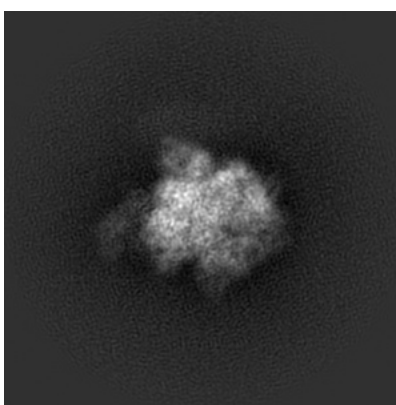
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

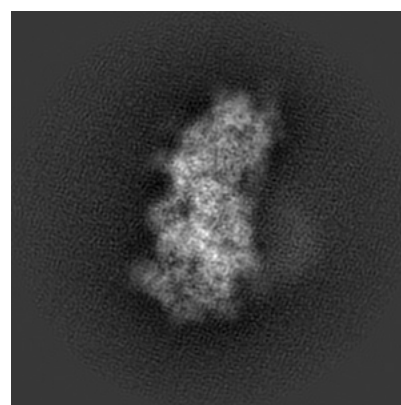
6.1.1 Primary map



X



Y

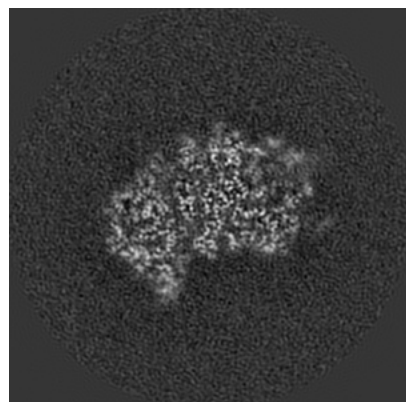


Z

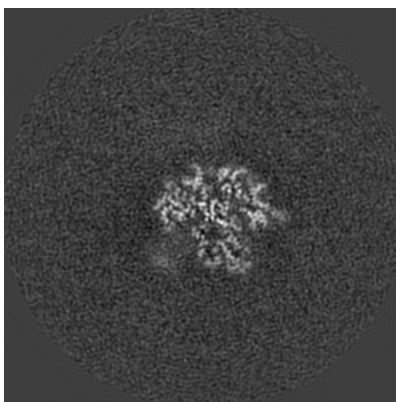
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

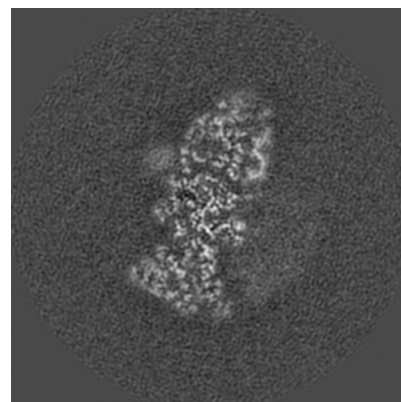
6.2.1 Primary map



X Index: 150



Y Index: 150

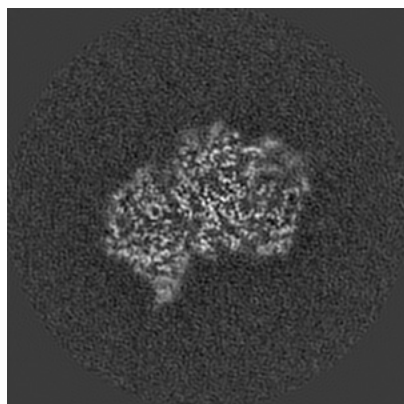


Z Index: 150

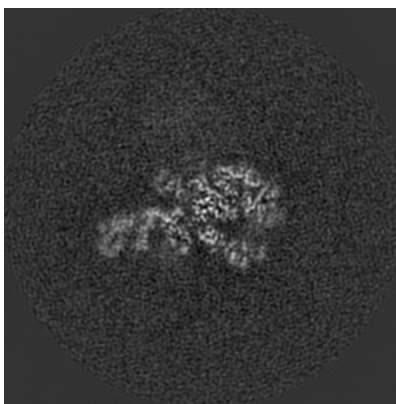
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

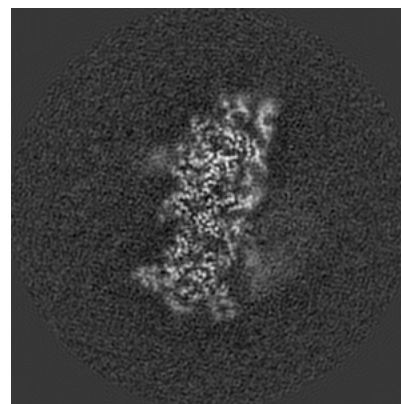
6.3.1 Primary map



X Index: 148



Y Index: 133



Z Index: 145

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

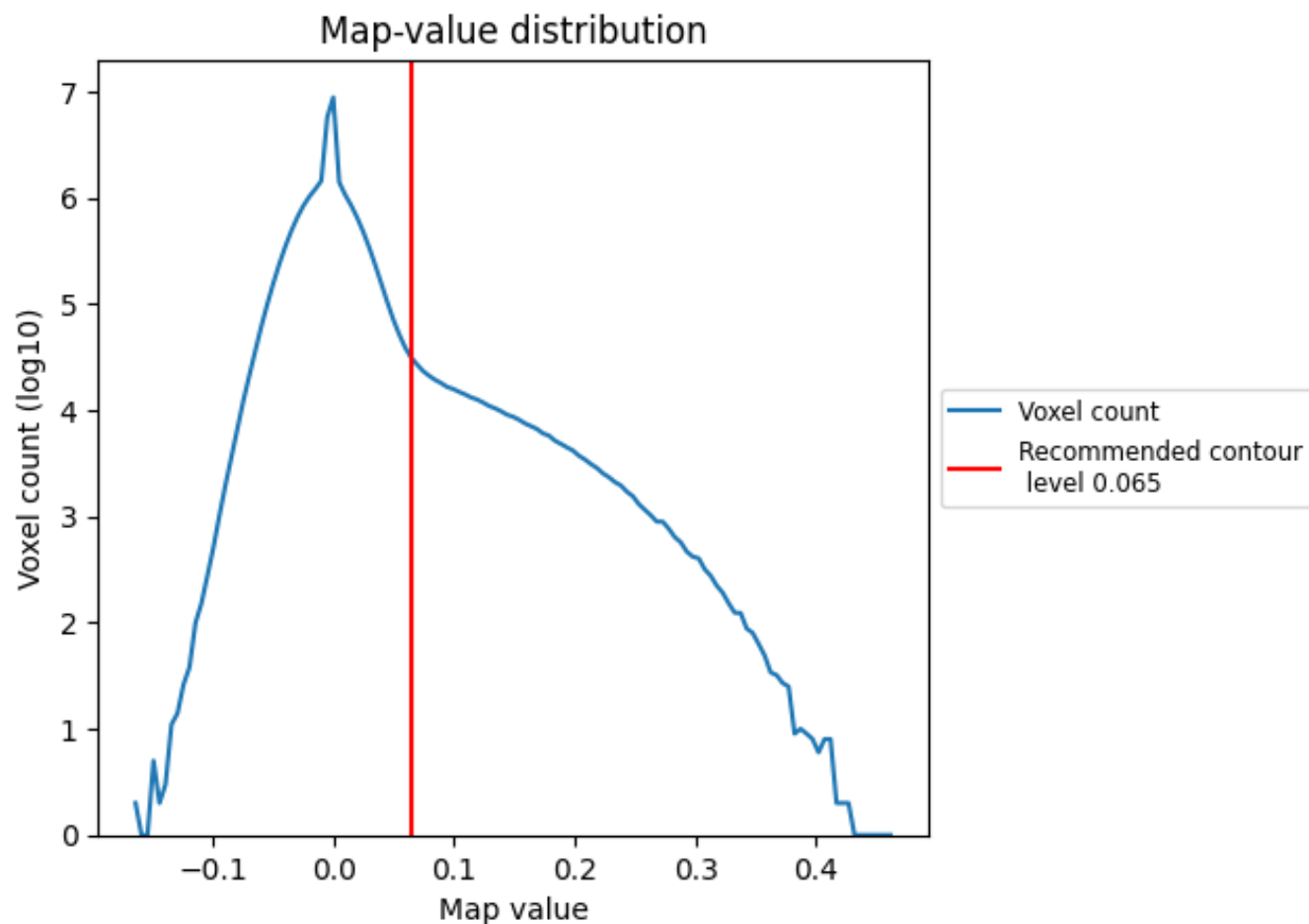
6.5 Mask visualisation

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

7 Map analysis [i](#)

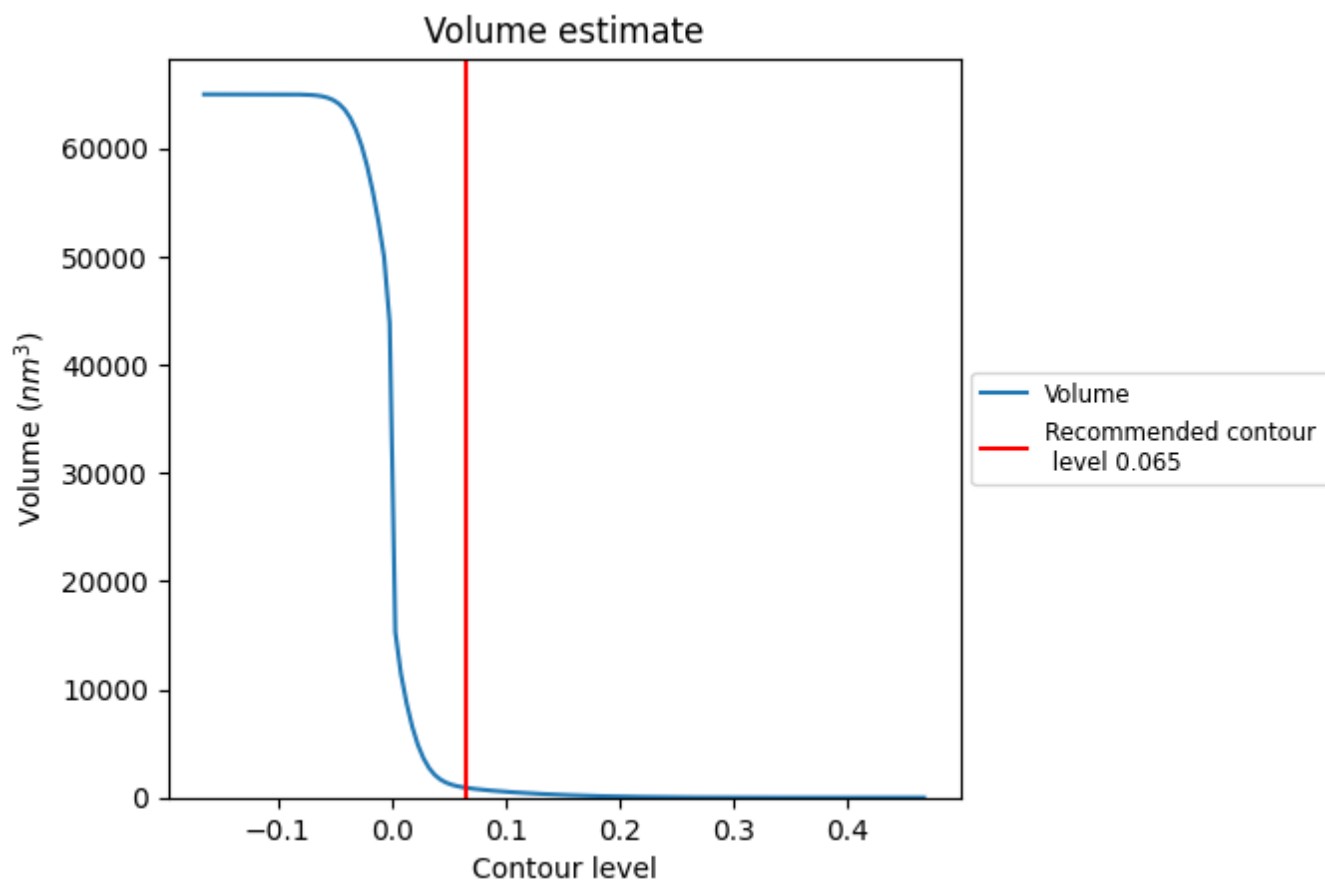
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

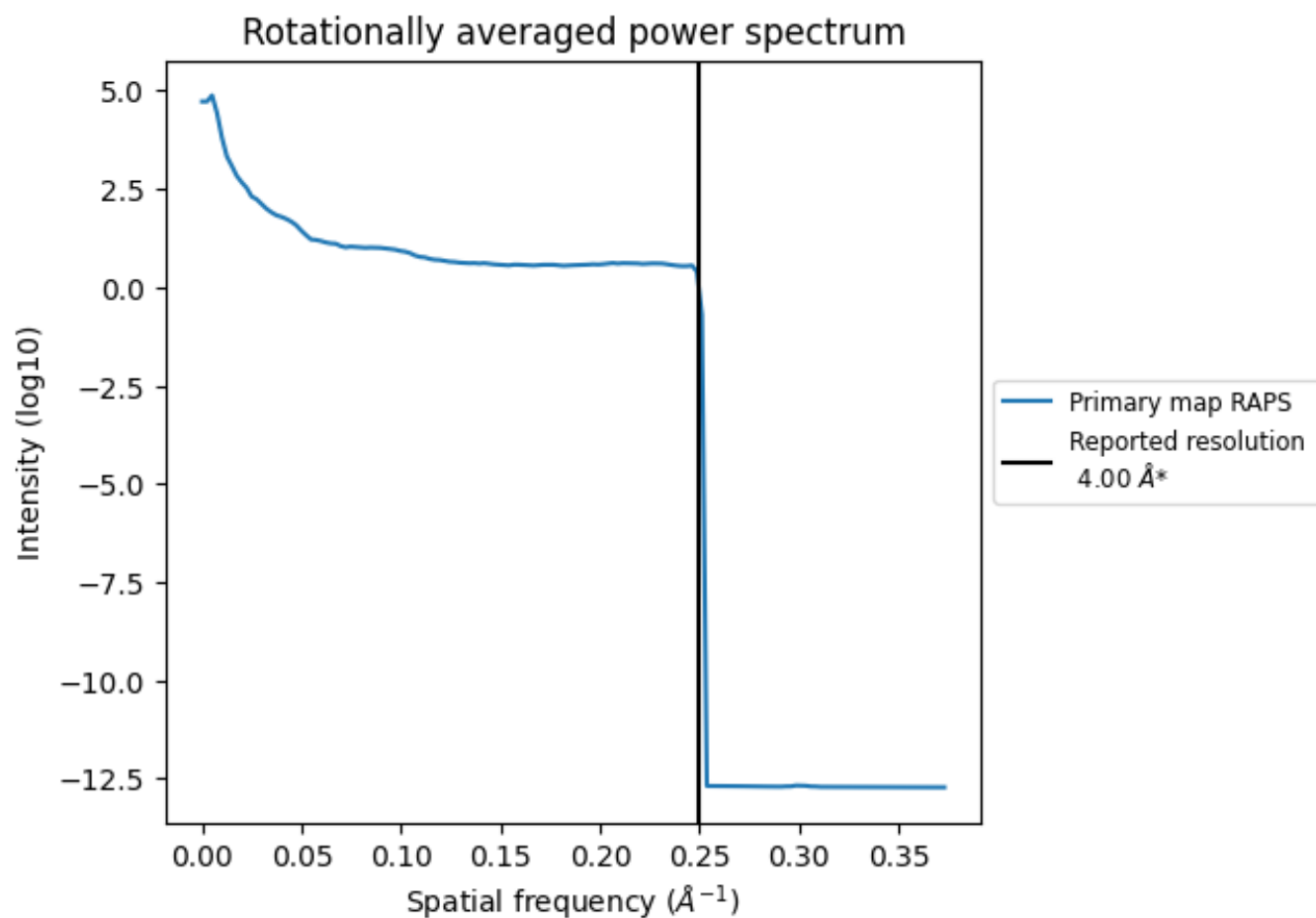
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 912 nm³; this corresponds to an approximate mass of 824 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 ⓘ

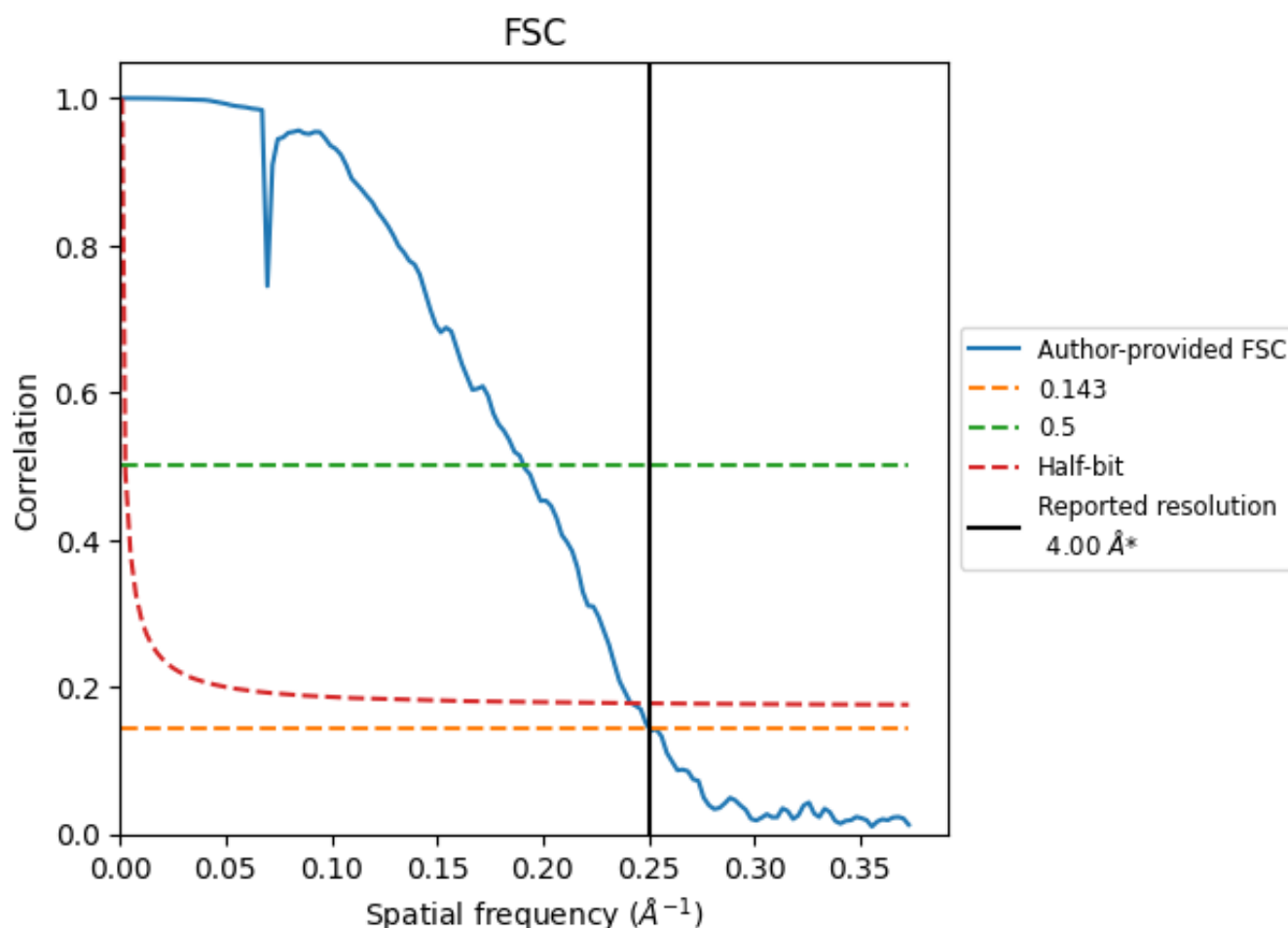


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 \AA^{-1}

8.2 Resolution estimates [i](#)

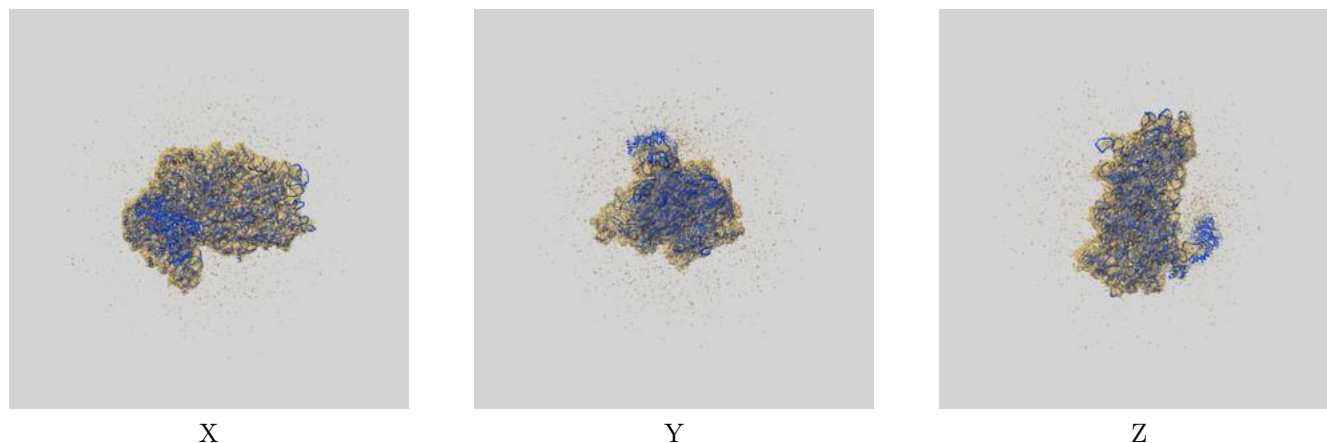
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.99	5.23	4.13
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

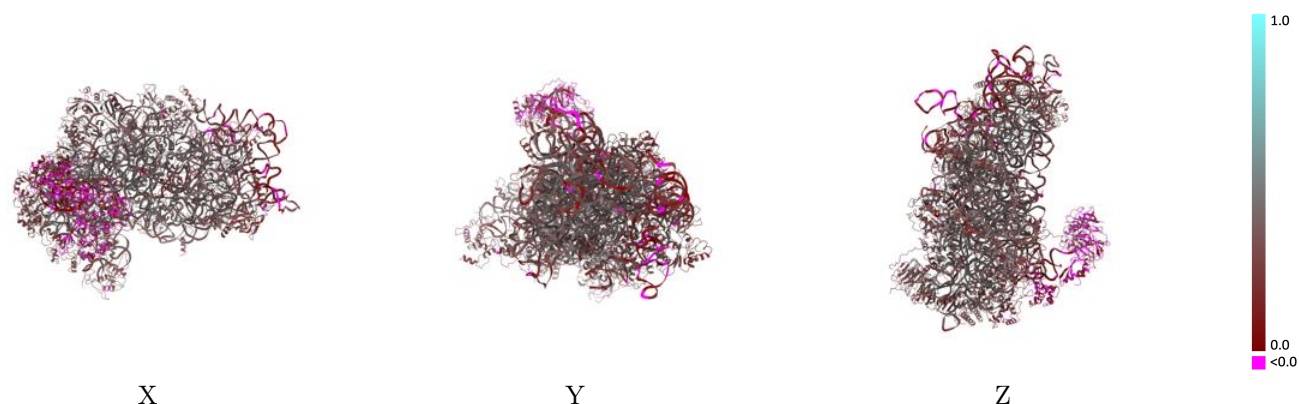
This section contains information regarding the fit between EMDB map EMD-2763 and PDB model 3J81. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



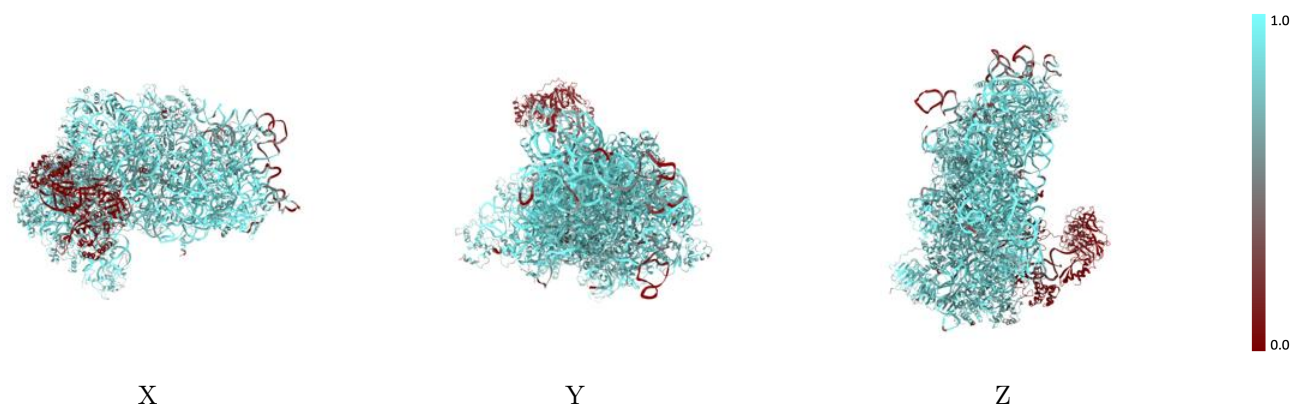
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



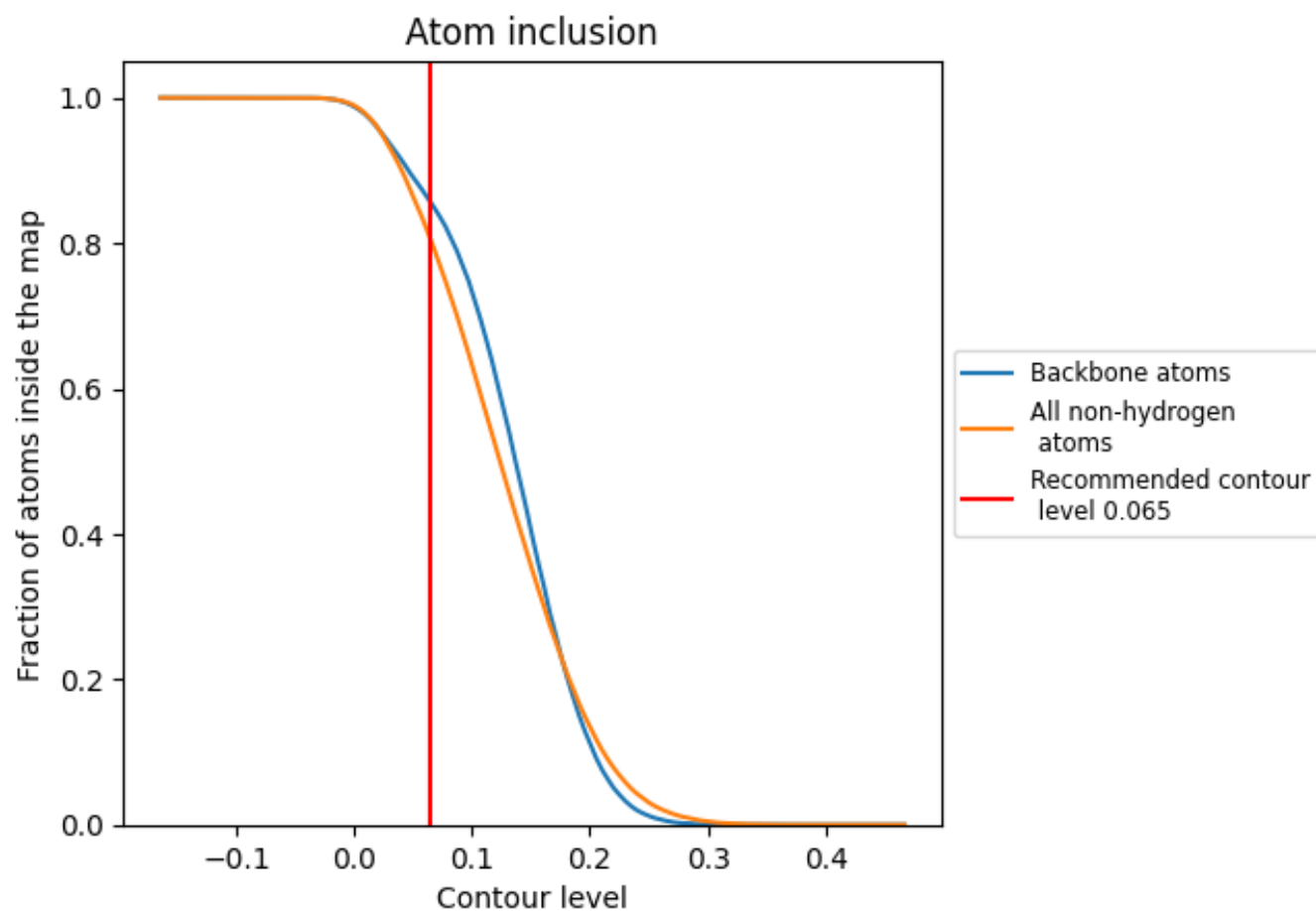
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.065).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8040	 0.3260
1	 0.4249	 0.1400
2	 0.9162	 0.3460
3	 0.4340	 0.2930
A	 0.8470	 0.3670
B	 0.8412	 0.3410
C	 0.8070	 0.3760
D	 0.7972	 0.3470
E	 0.8055	 0.3770
F	 0.7875	 0.3340
G	 0.8295	 0.3140
H	 0.7868	 0.3140
I	 0.8074	 0.3450
J	 0.8150	 0.3620
K	 0.8040	 0.3260
L	 0.7646	 0.3730
M	 0.7227	 0.2410
N	 0.8005	 0.3400
O	 0.8342	 0.3590
P	 0.8094	 0.3190
Q	 0.8019	 0.3540
R	 0.8128	 0.3400
S	 0.7658	 0.3040
T	 0.8231	 0.3260
U	 0.7771	 0.3530
V	 0.8306	 0.3750
W	 0.8120	 0.3880
X	 0.8480	 0.4070
Y	 0.8375	 0.3520
Z	 0.6077	 0.2240
a	 0.8331	 0.3810
b	 0.8140	 0.3500
c	 0.8094	 0.3950
d	 0.8431	 0.3840
e	 0.7852	 0.3640



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Chain	Atom inclusion	Q-score
f	 0.8007	 0.2860
g	 0.8271	 0.3350
h	 0.4717	 0.2570
i	 0.6914	 0.3310
j	 0.0685	 0.0950
k	 0.0144	 0.0250
l	 0.0000	 0.0230
m	 0.1364	 0.1940