



wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 02:39 am GMT

PDB ID : 6ZVI
EMDB ID : EMD-11457
Title : Mbf1-ribosome complex
Authors : Best, K.M.; Denk, T.; Cheng, J.; Thoms, M.; Berninghausen, O.; Beckmann, R.
Deposited on : 2020-07-24
Resolution : 3.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

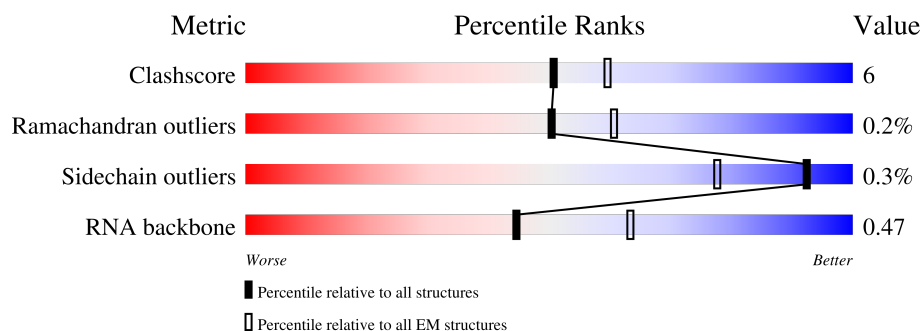
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.



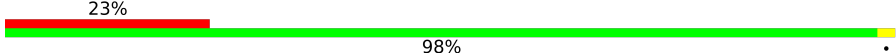
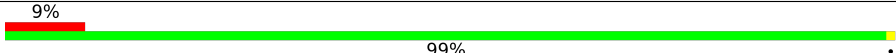
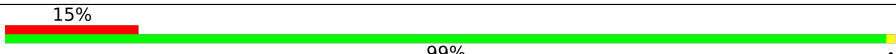
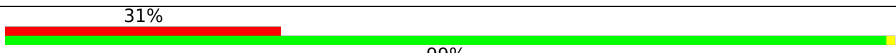
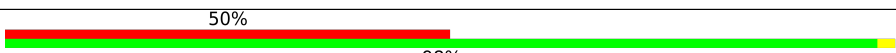
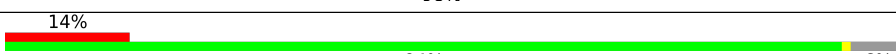
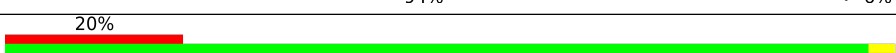
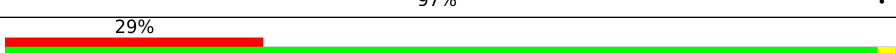
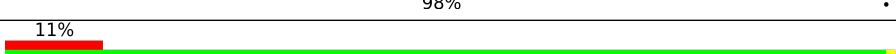
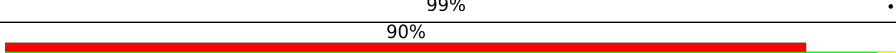
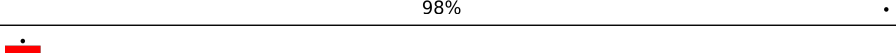
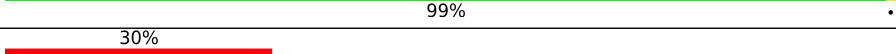
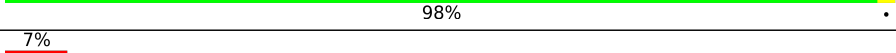
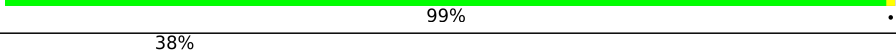
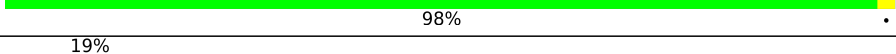


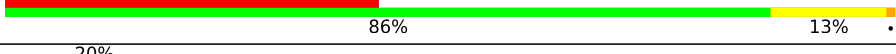
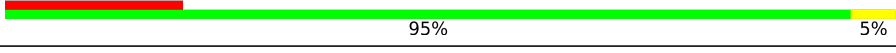
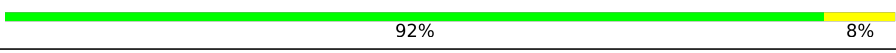





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. 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	d	76	<div> <div>70%</div> <div>57%</div> <div>37%</div> <div>7%</div> </div>
2	e	77	<div> <div>75%</div> <div>47%</div> <div>51%</div> <div>.</div> </div>
3	f	35	<div> <div>69%</div> <div>37%</div> <div>54%</div> <div>9%</div> </div>
4	h	1758	<div> <div>14%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
5	i	206	<div> <div>17%</div> <div>98%</div> <div>.</div> </div>
6	j	216	<div> <div>27%</div> <div>100%</div> </div>
7	k	217	<div> <div>6%</div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
8	l	223	
9	m	260	
10	n	206	
11	o	218	
12	p	185	
13	q	199	
14	r	185	
15	s	92	
16	t	146	
17	u	124	
18	v	150	
19	x	119	
20	y	141	
21	z	125	
22	A	145	
23	B	143	
24	C	101	
25	D	87	
26	E	129	
27	H	144	
28	I	134	
29	J	69	
30	L	81	
31	N	63	
32	P	46	

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Mol	Chain	Length	Quality of chain
33	Q	73	<div> <div>85%</div> <div>71%</div> <div>29%</div> </div>
34	R	313	<div> <div>68%</div> <div>86%</div> <div>14%</div> </div>
35	T	111	<div> <div>86%</div> <div>88%</div> <div>12%</div> </div>
36	O	53	<div> <div>87%</div> <div>13%</div> </div>
37	w	128	<div> <div>9%</div> <div>100%</div> </div>
38	K	97	<div> <div>7%</div> <div>84%</div> <div>15%</div> </div>

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 80088 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 A/P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	d	76	Total	C	N	O	P	0	0
			1620	723	290	532	75		

- Molecule 2 is a RNA chain called P/E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	e	77	Total	C	N	O	P	0	0
			1644	732	297	538	77		

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	f	35	Total	C	N	O	P	0	0
			724	325	102	262	35		

- Molecule 4 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	h	1758	Total	C	N	O	P	0	0
			37455	16745	6624	12328	1758		

- Molecule 5 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	i	206	Total	C	N	O	S	0	0
			1583	1017	281	283	2		

- Molecule 6 is a protein called RPS1A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	j	216	Total	C	N	O	S	0	0
			1722	1091	312	315	4		

- Molecule 7 is a protein called RPS2 isoform 1.

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

- Molecule 8 is a protein called RPS3 isoform 1.

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

- Molecule 9 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 10 is a protein called Rps5p.

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

- Molecule 11 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	o	218	Total	C	N	O	S	0	0
			1755	1102	337	313	3		

- Molecule 12 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	p	185	Total	C	N	O	0	0
			1486	954	266	266		

- Molecule 13 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 14 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 15 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	s	92	Total	C	N	O	S	0	0
			741	478	121	140	2		

- Molecule 16 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	t	146	Total	C	N	O	S	0	0
			1168	747	221	197	3		

- Molecule 17 is a protein called RPS12 isoform 1.

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

- Molecule 18 is a protein called 40S ribosomal protein S13.

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

- Molecule 19 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	x	119	Total	C	N	O	S	0	0
			939	595	176	161	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	z	125	Total	C	N	O	S	0	0
			1001	625	188	186	2		

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

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

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

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

- Molecule 24 is a protein called RPS20 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C	101	Total	C	N	O	S	0	0
			805	512	145	147	1		

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

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

- Molecule 26 is a protein called RPS22A isoform 1.

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

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

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

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

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

- Molecule 29 is a protein called RPS25A isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	J	69	Total	C	N	O	0	0
			558	357	103	98		

- Molecule 30 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 31 is a protein called RPS28A isoform 1.

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

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	P	46	Total	C	N	O	0	0
			370	236	75	59		

- Molecule 33 is a protein called RPS31 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Q	73	Total	C	N	O	S	0	0
			556	352	105	95	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	97	ALA	LYS	conflict	UNP A0A6A5PU37

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	R	313	Total	C	N	O	S	0	0
			2403	1521	411	463	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	161	ALA	LYS	conflict	UNP P38011

- Molecule 35 is a protein called MBF1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	T	111	Total	C	N	O	S	0	0
			870	528	174	167	1		

- Molecule 36 is a protein called RPS29A isoform 1.

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

- Molecule 37 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	w	128	Total	C	N	O	S	0	0
			949	582	188	176	3		

- Molecule 38 is a protein called RPS26B isoform 1.

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

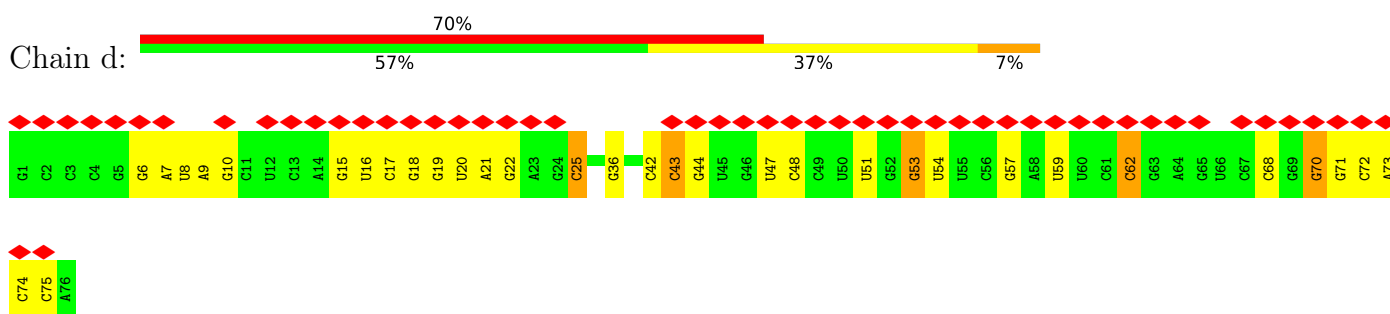
- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
39	L	1	Total	Zn	0
			1	1	
39	O	1	Total	Zn	0
			1	1	

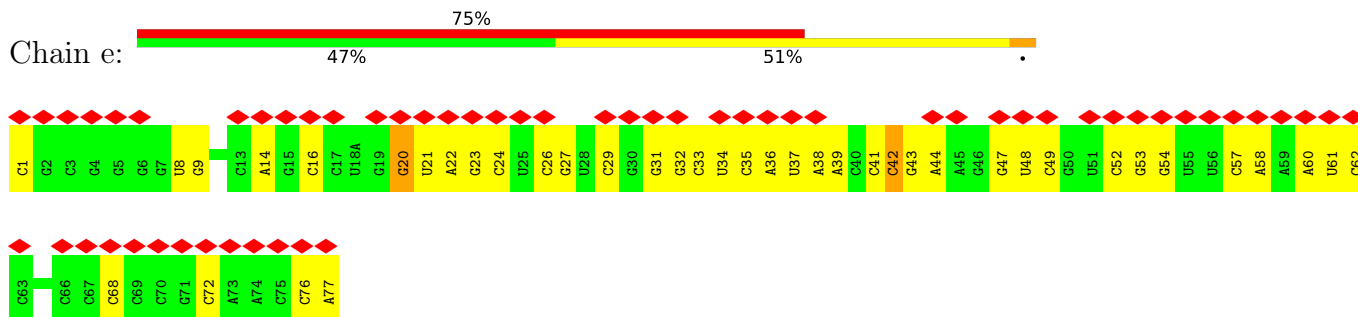
3 Residue-property plots [i](#)

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

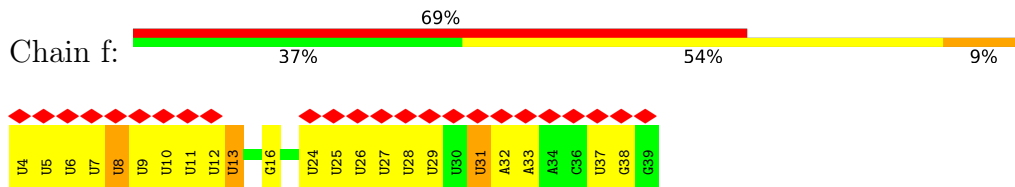
• Molecule 1: A/P-site tRNA



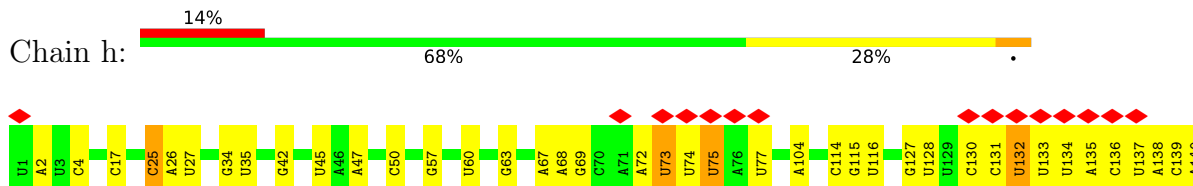
• Molecule 2: P/E-site tRNA

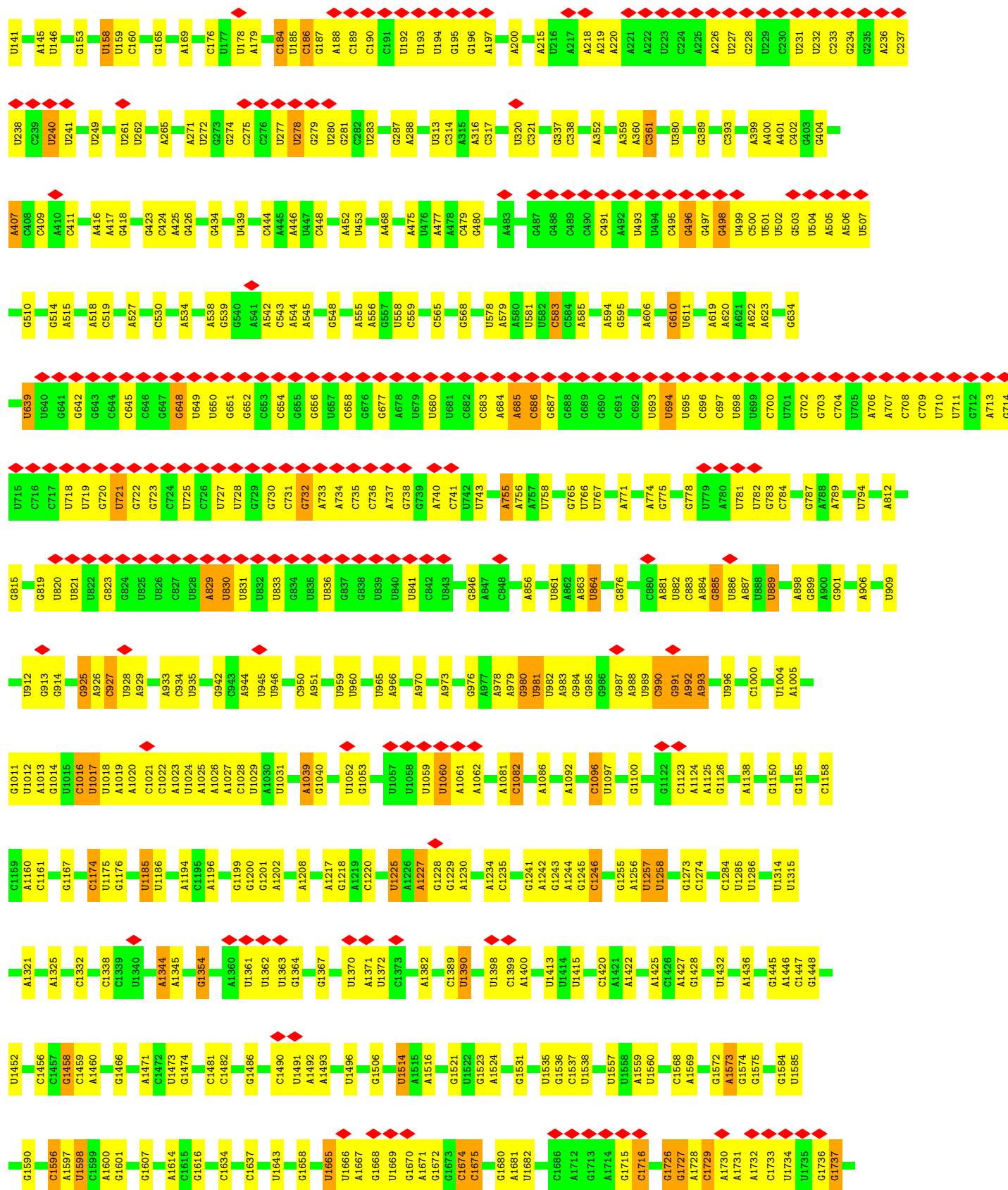


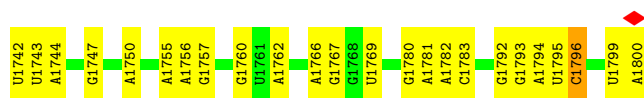
• Molecule 3: mRNA



• Molecule 4: 18S rRNA

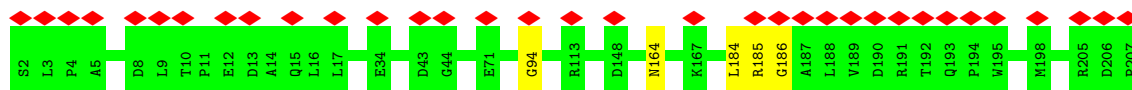






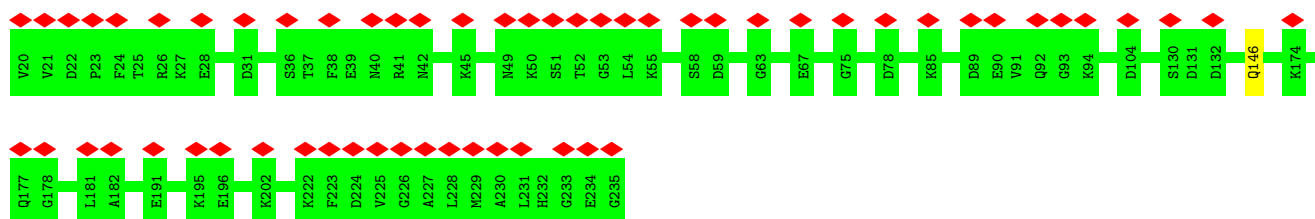
- Molecule 5: 40S ribosomal protein S0-A

Chain i: 17% 98%



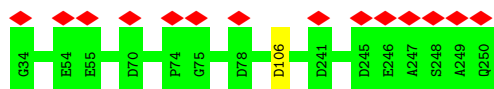
- Molecule 6: RPS1A isoform 1

Chain j: 27% 100%



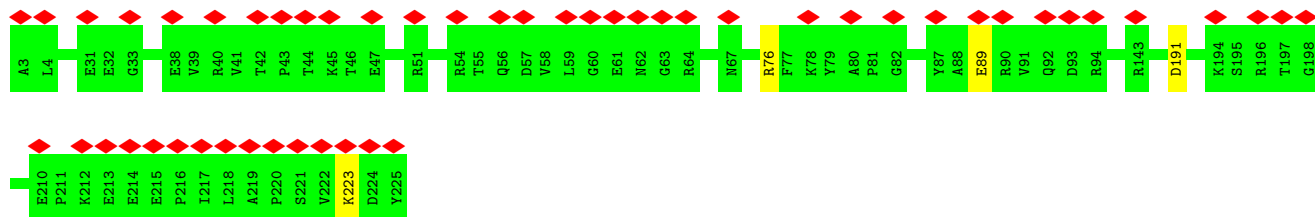
- Molecule 7: RPS2 isoform 1

Chain k: 6% 100%



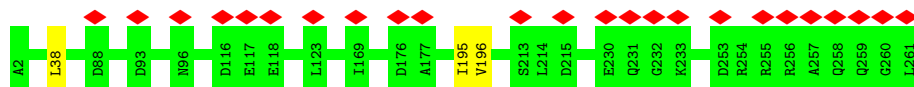
- Molecule 8: RPS3 isoform 1

Chain l: 23% 98%

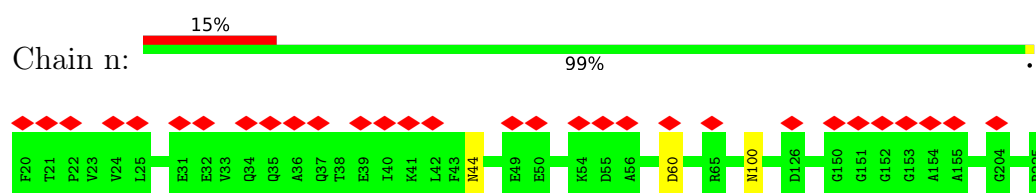


- Molecule 9: 40S ribosomal protein S4-A

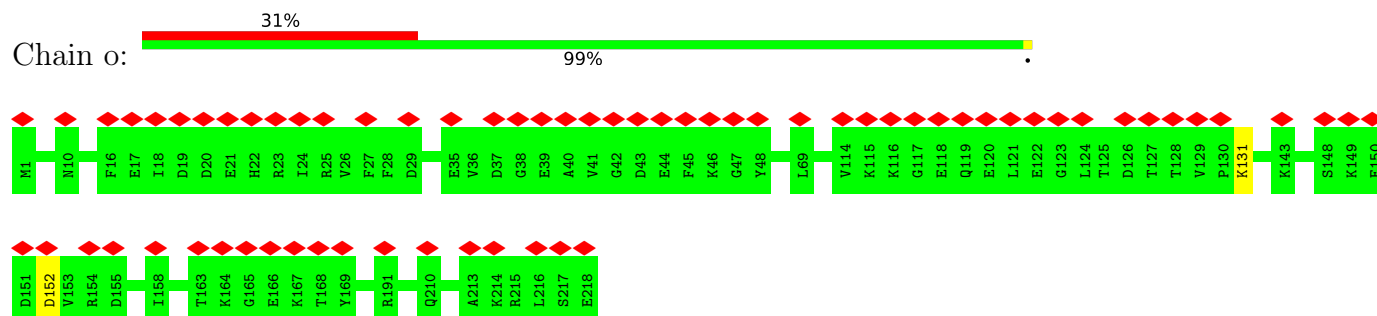
Chain m: 9% 99%



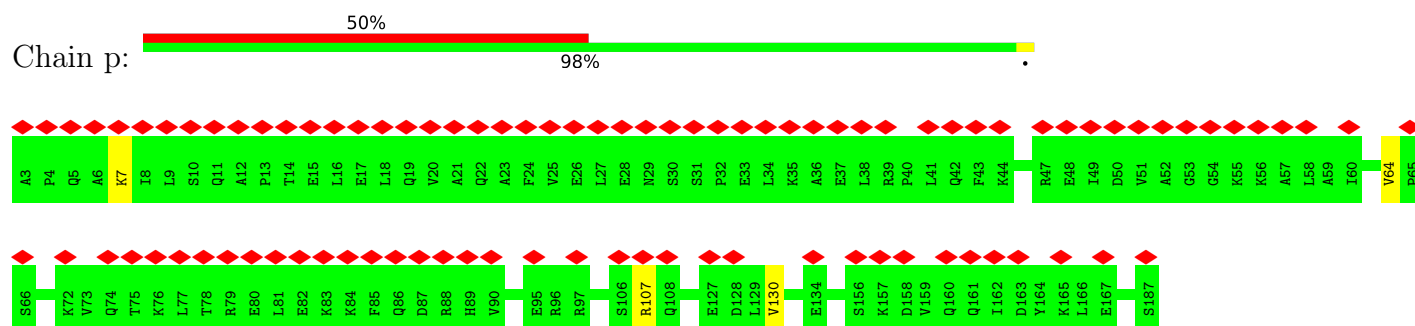
- Molecule 10: Rps5p



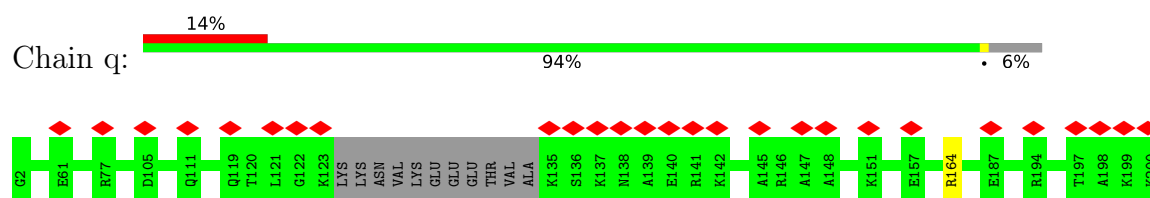
• Molecule 11: 40S ribosomal protein S6-A



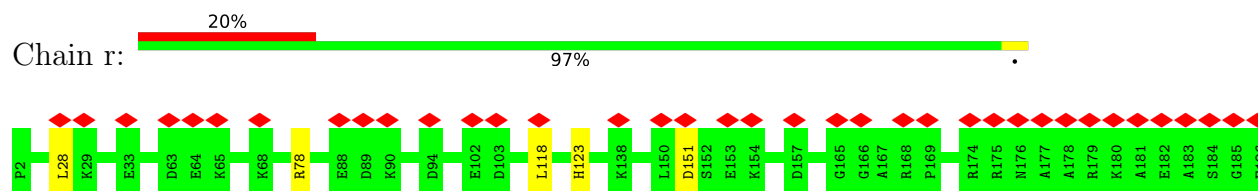
• Molecule 12: 40S ribosomal protein S7-A



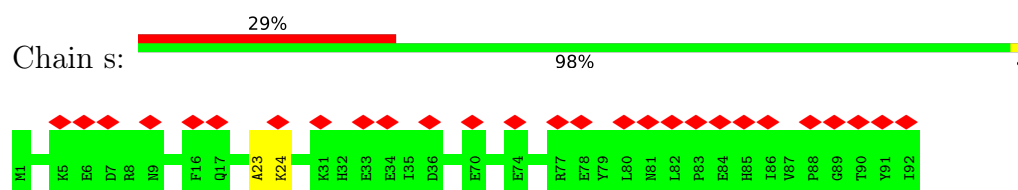
• Molecule 13: 40S ribosomal protein S8-A



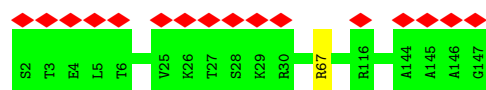
• Molecule 14: 40S ribosomal protein S9-A



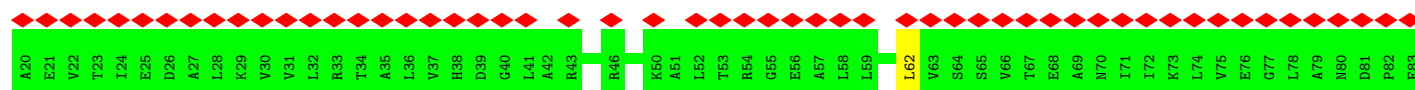
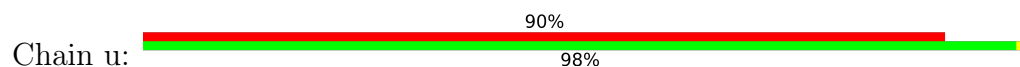
• Molecule 15: 40S ribosomal protein S10-A



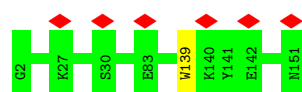
- Molecule 16: 40S ribosomal protein S11-A



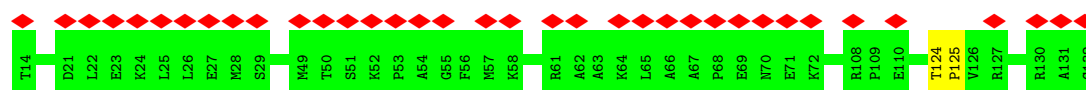
- Molecule 17: RPS12 isoform 1



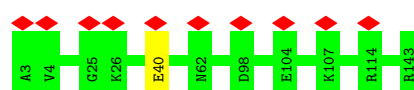
- Molecule 18: 40S ribosomal protein S13



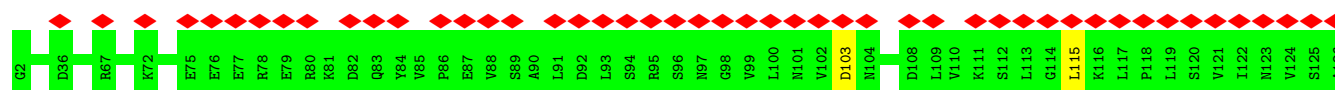
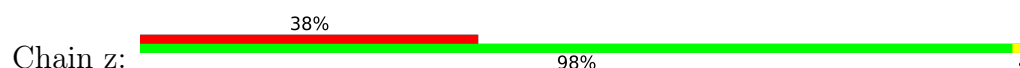
- Molecule 19: RPS15 isoform 1



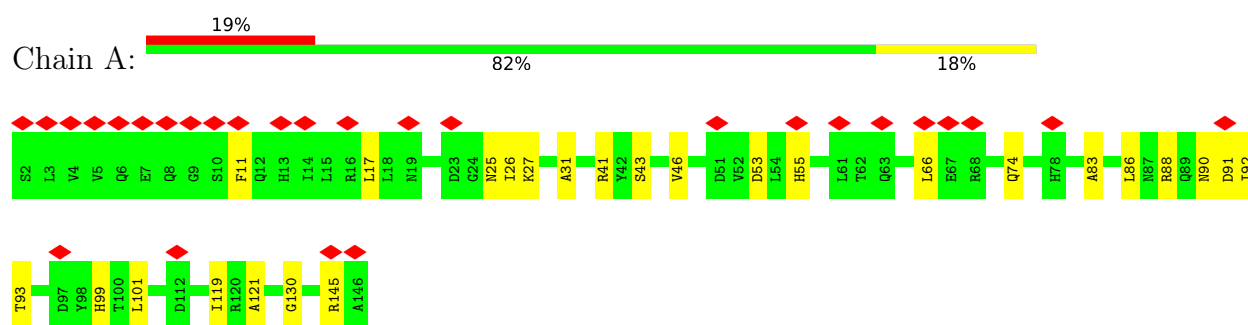
- Molecule 20: 40S ribosomal protein S16-A



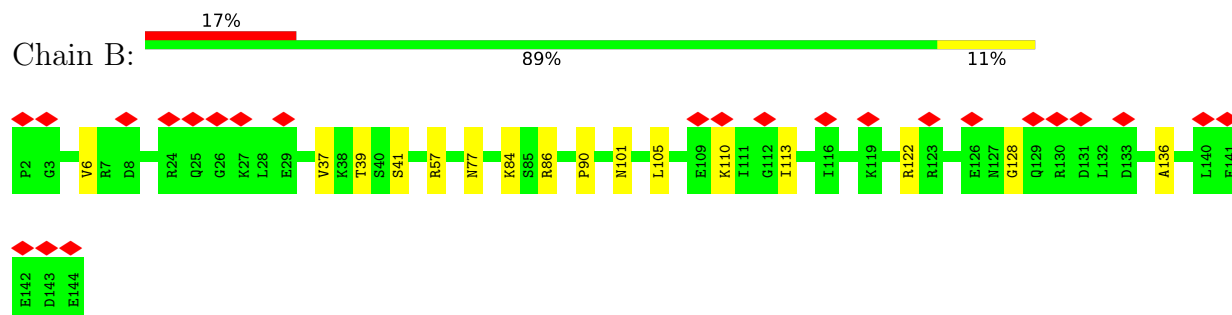
- Molecule 21: 40S ribosomal protein S17-A



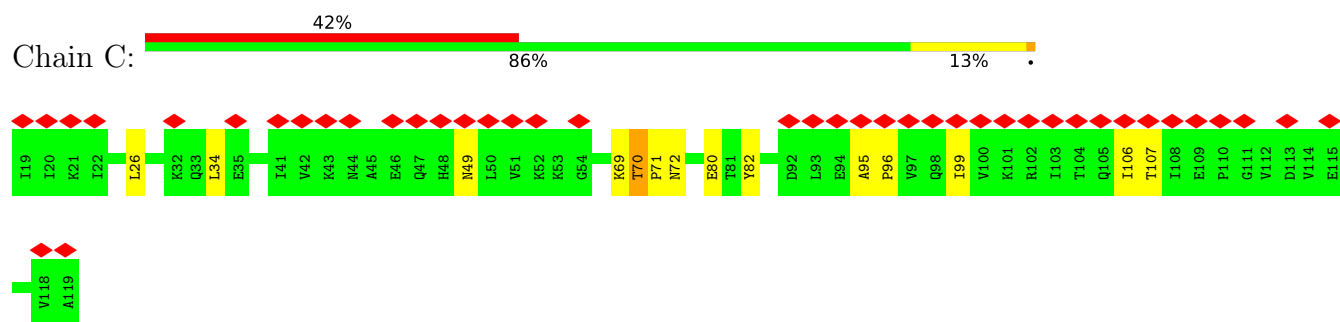
- Molecule 22: 40S ribosomal protein S18-A



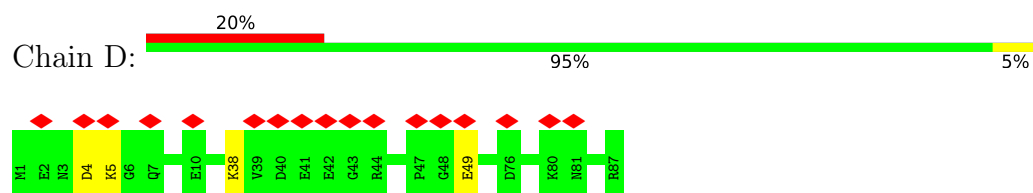
- Molecule 23: 40S ribosomal protein S19-A



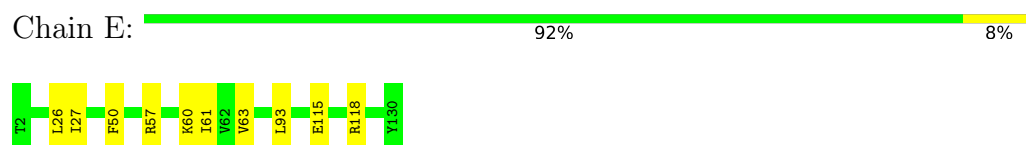
- Molecule 24: RPS20 isoform 1



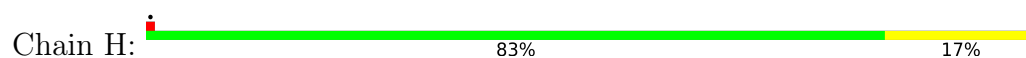
- Molecule 25: 40S ribosomal protein S21-A



- Molecule 26: RPS22A isoform 1

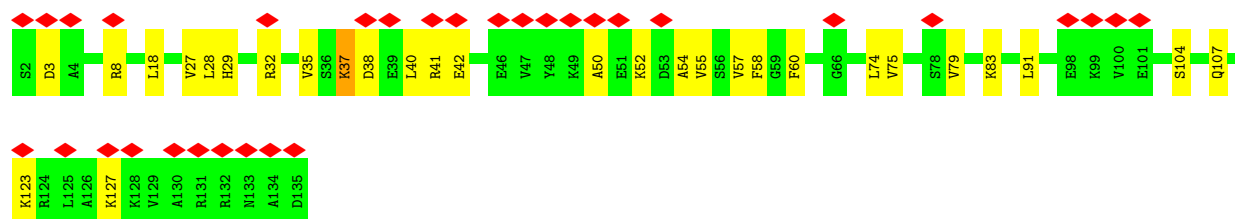
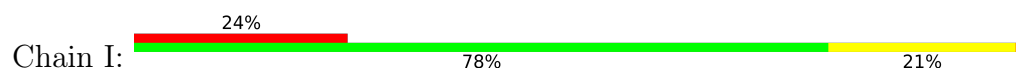


- Molecule 27: 40S ribosomal protein S23-A

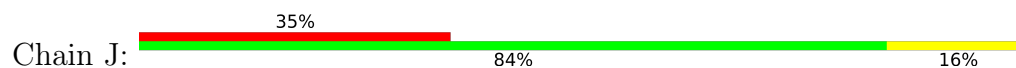




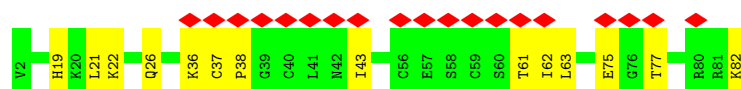
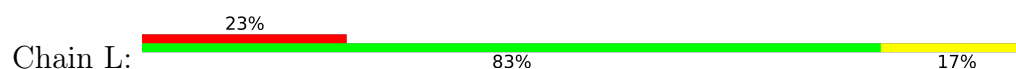
- Molecule 28: 40S ribosomal protein S24-A



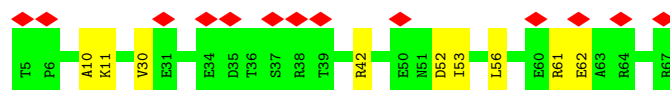
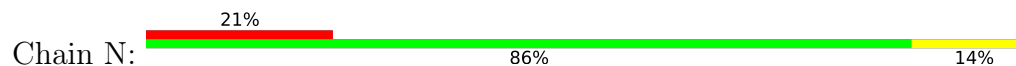
- Molecule 29: RPS25A isoform 1



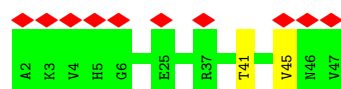
- Molecule 30: 40S ribosomal protein S27-A



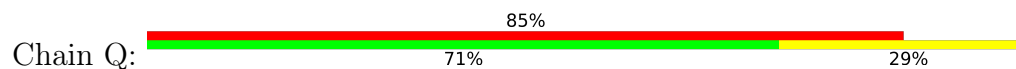
- Molecule 31: RPS28A isoform 1



- Molecule 32: 40S ribosomal protein S30-A

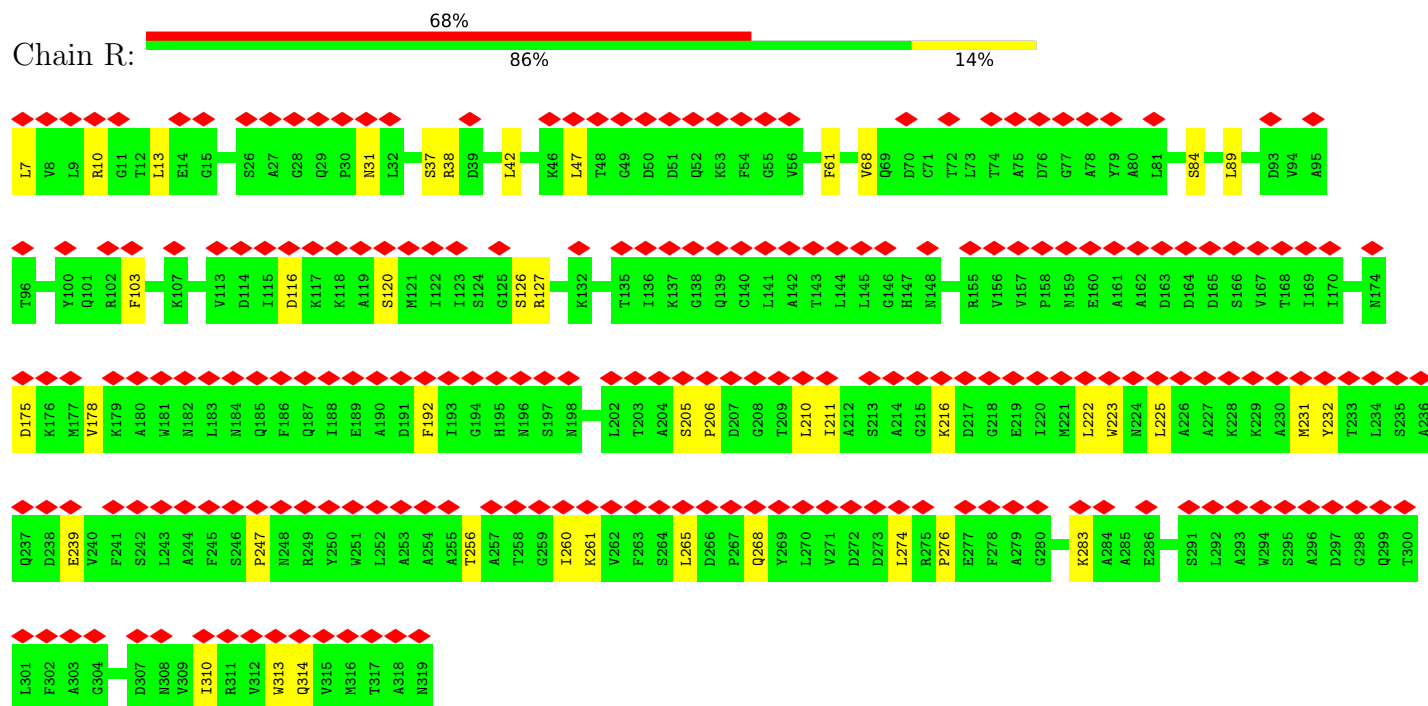


- Molecule 33: RPS31 isoform 1

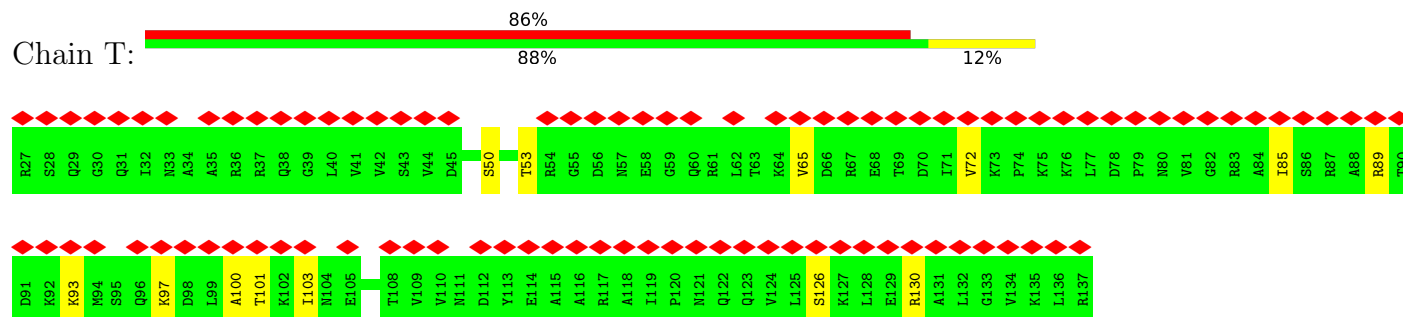




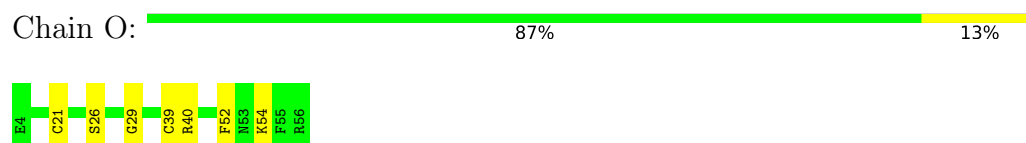
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



• Molecule 35: MBF1 isoform 1



• Molecule 36: RPS29A isoform 1

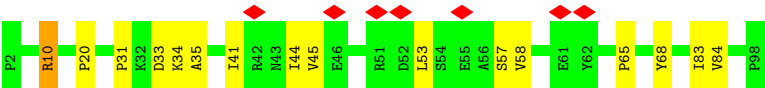
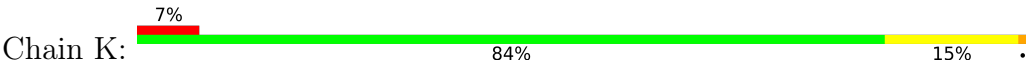


• Molecule 37: 40S ribosomal protein S14-B





• Molecule 38: RPS26B isoform 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57350	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.298	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	423.6, 423.6, 423.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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	d	0.42	0/1810	1.06	7/2821 (0.2%)
2	e	0.54	1/1836 (0.1%)	1.33	23/2859 (0.8%)
3	f	0.65	1/802 (0.1%)	1.08	9/1238 (0.7%)
4	h	0.78	2/41890 (0.0%)	1.08	264/65269 (0.4%)
5	i	0.38	0/1623	0.62	0/2222
6	j	0.36	0/1748	0.58	0/2352
7	k	0.41	0/1665	0.59	0/2263
8	l	0.38	0/1759	0.61	1/2368 (0.0%)
9	m	0.40	0/2109	0.59	1/2839 (0.0%)
10	n	0.36	0/1629	0.62	1/2202 (0.0%)
11	o	0.33	0/1779	0.57	1/2379 (0.0%)
12	p	0.33	0/1511	0.59	0/2036
13	q	0.39	0/1514	0.54	0/2021
14	r	0.38	0/1519	0.61	3/2035 (0.1%)
15	s	0.40	0/757	0.63	0/1022
16	t	0.47	0/1194	0.56	0/1610
17	u	0.30	0/898	0.74	1/1220 (0.1%)
18	v	0.41	0/1215	0.54	0/1638
19	x	0.36	0/959	0.54	0/1288
20	y	0.43	0/1125	0.61	0/1510
21	z	0.34	0/1011	0.63	2/1355 (0.1%)
22	A	0.34	0/1211	0.59	1/1628 (0.1%)
23	B	0.42	0/1130	0.57	0/1517
24	C	0.38	0/815	0.59	0/1102
25	D	0.42	0/693	0.62	0/935
26	E	0.47	0/1038	0.60	1/1395 (0.1%)
27	H	0.42	0/1139	0.58	0/1518
28	I	0.38	0/1087	0.59	0/1449
29	J	0.36	0/566	0.64	0/761
30	L	0.36	0/620	0.68	0/838
31	N	0.41	0/499	0.71	2/670 (0.3%)
32	P	0.41	0/376	0.56	0/499

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Q	0.36	0/567	0.83	1/764 (0.1%)
34	R	0.32	0/2456	0.58	0/3343
35	T	0.31	0/875	0.65	0/1170
36	O	0.48	0/452	0.54	0/600
37	w	0.41	0/960	0.64	0/1290
38	K	0.45	0/782	0.64	0/1047
All	All	0.61	4/85619 (0.0%)	0.92	318/125073 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	i	0	3
6	j	0	1
7	k	0	1
8	l	0	1
9	m	0	1
10	n	0	2
12	p	0	2
14	r	0	1
15	s	0	1
17	u	0	1
19	x	0	1
20	y	0	1
22	A	0	2
24	C	0	1
27	H	0	1
30	L	0	1
33	Q	0	2
35	T	0	1
38	K	0	1
All	All	0	25

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	1	C	OP3-P	-10.66	1.48	1.61
3	f	4	U	OP3-P	-10.49	1.48	1.61
4	h	993	A	N9-C4	5.62	1.41	1.37
4	h	976	G	C2-N3	-5.40	1.28	1.32

The worst 5 of 318 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	h	989	U	C5-C6-N1	11.79	128.60	122.70
4	h	1027	A	N1-C6-N6	-11.56	111.66	118.60
4	h	990	C	C5-C6-N1	11.39	126.70	121.00
4	h	989	U	C2-N1-C1'	11.34	131.30	117.70
2	e	33	C	N1-C2-O2	11.17	125.60	118.90

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	i	184	LEU	Peptide
5	i	186	GLY	Peptide
5	i	94	GLY	Peptide
6	j	146	GLN	Peptide
7	k	106	ASP	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	d	1620	0	822	0	0
2	e	1644	0	836	0	0
3	f	724	0	364	0	0
4	h	37455	0	18846	0	0
5	i	1583	0	1578	0	0
6	j	1722	0	1793	0	0
7	k	1635	0	1723	0	0
8	l	1734	0	1817	0	0
9	m	2068	0	2154	0	0
10	n	1609	0	1675	0	0
11	o	1755	0	1846	0	0
12	p	1486	0	1576	0	0
13	q	1489	0	1525	0	0
14	r	1494	0	1573	0	0
15	s	741	0	691	0	0
16	t	1168	0	1233	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	u	890	0	887	0	0
18	v	1192	0	1255	0	0
19	x	939	0	968	0	0
20	y	1105	0	1166	0	0
21	z	1001	0	1063	0	0
22	A	1192	0	1222	11	0
23	B	1112	0	1124	10	0
24	C	805	0	874	9	0
25	D	684	0	672	3	0
26	E	1021	0	1060	5	0
27	H	1121	0	1196	12	0
28	I	1073	0	1132	17	0
29	J	558	0	598	6	0
30	L	610	0	631	10	0
31	N	497	0	535	4	0
32	P	370	0	413	1	0
33	Q	556	0	552	10	0
34	R	2403	0	2353	28	0
35	T	870	0	917	6	0
36	O	442	0	431	6	0
37	w	949	0	985	0	0
38	K	769	0	818	9	0
39	L	1	0	0	0	0
39	O	1	0	0	0	0
All	All	80088	0	60904	143	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 6.

The worst 5 of 143 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)
28:I:27:VAL:HG21	28:I:35:VAL:HG21	1.74	0.69
34:R:205:SER:HB3	34:R:210:LEU:HB2	1.75	0.68
34:R:13:LEU:HB2	34:R:310:ILE:HB	1.75	0.68
25:D:38:LYS:HD3	25:D:49:GLU:HG2	1.75	0.68
28:I:57:VAL:HB	28:I:60:PHE:HE2	1.59	0.67

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
5	i	204/206 (99%)	181 (89%)	22 (11%)	1 (0%)	29	68
6	j	214/216 (99%)	207 (97%)	7 (3%)	0	100	100
7	k	215/217 (99%)	211 (98%)	4 (2%)	0	100	100
8	l	221/223 (99%)	209 (95%)	12 (5%)	0	100	100
9	m	258/260 (99%)	249 (96%)	8 (3%)	1 (0%)	34	72
10	n	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
11	o	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
12	p	183/185 (99%)	173 (94%)	10 (6%)	0	100	100
13	q	184/199 (92%)	182 (99%)	2 (1%)	0	100	100
14	r	183/185 (99%)	173 (94%)	10 (6%)	0	100	100
15	s	90/92 (98%)	76 (84%)	13 (14%)	1 (1%)	14	50
16	t	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
17	u	122/124 (98%)	102 (84%)	19 (16%)	1 (1%)	19	57
18	v	148/150 (99%)	143 (97%)	4 (3%)	1 (1%)	22	60
19	x	117/119 (98%)	110 (94%)	6 (5%)	1 (1%)	17	55
20	y	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
21	z	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
22	A	143/145 (99%)	132 (92%)	11 (8%)	0	100	100
23	B	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
24	C	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	7	34
25	D	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
26	E	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
27	H	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
28	I	132/134 (98%)	125 (95%)	5 (4%)	2 (2%)	10	42
29	J	67/69 (97%)	64 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	L	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
31	N	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
32	P	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
33	Q	71/73 (97%)	58 (82%)	13 (18%)	0	100	100
34	R	311/313 (99%)	307 (99%)	4 (1%)	0	100	100
35	T	109/111 (98%)	96 (88%)	13 (12%)	0	100	100
36	O	51/53 (96%)	51 (100%)	0	0	100	100
37	w	126/128 (98%)	116 (92%)	10 (8%)	0	100	100
38	K	95/97 (98%)	87 (92%)	8 (8%)	0	100	100
All	All	4848/4929 (98%)	4588 (95%)	250 (5%)	10 (0%)	50	82

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	x	125	PRO
24	C	71	PRO
24	C	72	ASN
18	v	139	TRP
5	i	164	ASN

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	
5	i	165/173 (95%)	164 (99%)	1 (1%)	86	95
6	j	192/192 (100%)	192 (100%)	0	100	100
7	k	176/176 (100%)	176 (100%)	0	100	100
8	l	182/182 (100%)	180 (99%)	2 (1%)	73	90
9	m	221/221 (100%)	221 (100%)	0	100	100
10	n	173/173 (100%)	173 (100%)	0	100	100
11	o	187/187 (100%)	186 (100%)	1 (0%)	88	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	p	165/165 (100%)	163 (99%)	2 (1%)	71	90
13	q	150/160 (94%)	149 (99%)	1 (1%)	84	94
14	r	158/158 (100%)	157 (99%)	1 (1%)	86	95
15	s	73/85 (86%)	73 (100%)	0	100	100
16	t	129/129 (100%)	128 (99%)	1 (1%)	81	93
17	u	88/100 (88%)	88 (100%)	0	100	100
18	v	127/127 (100%)	127 (100%)	0	100	100
19	x	98/98 (100%)	98 (100%)	0	100	100
20	y	117/117 (100%)	117 (100%)	0	100	100
21	z	113/113 (100%)	113 (100%)	0	100	100
22	A	128/128 (100%)	126 (98%)	2 (2%)	62	86
23	B	115/115 (100%)	115 (100%)	0	100	100
24	C	94/94 (100%)	94 (100%)	0	100	100
25	D	74/74 (100%)	74 (100%)	0	100	100
26	E	110/110 (100%)	110 (100%)	0	100	100
27	H	119/119 (100%)	119 (100%)	0	100	100
28	I	112/112 (100%)	111 (99%)	1 (1%)	78	92
29	J	61/61 (100%)	61 (100%)	0	100	100
30	L	70/70 (100%)	70 (100%)	0	100	100
31	N	56/56 (100%)	56 (100%)	0	100	100
32	P	39/39 (100%)	39 (100%)	0	100	100
33	Q	56/63 (89%)	55 (98%)	1 (2%)	59	85
34	R	255/256 (100%)	255 (100%)	0	100	100
35	T	95/95 (100%)	95 (100%)	0	100	100
36	O	47/47 (100%)	47 (100%)	0	100	100
37	w	97/97 (100%)	97 (100%)	0	100	100
38	K	83/83 (100%)	83 (100%)	0	100	100
All	All	4125/4175 (99%)	4112 (100%)	13 (0%)	92	97

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	r	78	ARG

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Mol	Chain	Res	Type
16	t	67	ARG
33	Q	92	LYS
22	A	74	GLN
28	I	123	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
8	l	74	GLN
9	m	67	GLN
10	n	131	GLN
12	p	5	GLN
21	z	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	d	75/76 (98%)	32 (42%)	0
2	e	76/77 (98%)	33 (43%)	0
3	f	33/35 (94%)	21 (63%)	0
4	h	1754/1758 (99%)	506 (28%)	0
All	All	1938/1946 (99%)	592 (30%)	0

5 of 592 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	d	6	G
1	d	7	A
1	d	8	U
1	d	9	A
1	d	10	G

There are no RNA pucker outliers to report.

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

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 2 ligands modelled in this entry, 2 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
4	h	3
3	f	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	h	1686:C	O3'	1712:A	P	17.71
1	h	658:C	O3'	676:G	P	17.06
1	f	33:A	O3'	34:A	P	3.69
1	h	540:G	O3'	541:A	P	3.24

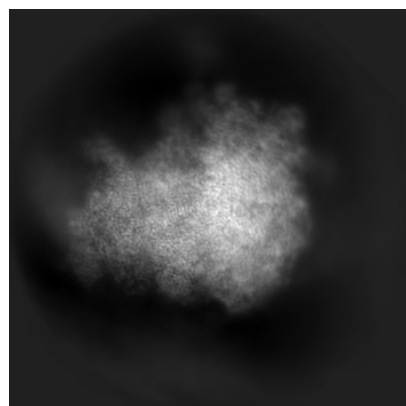
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11457. These allow visual inspection of the internal detail of the map and identification of artifacts.

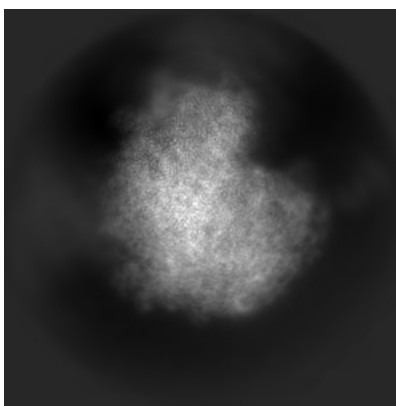
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

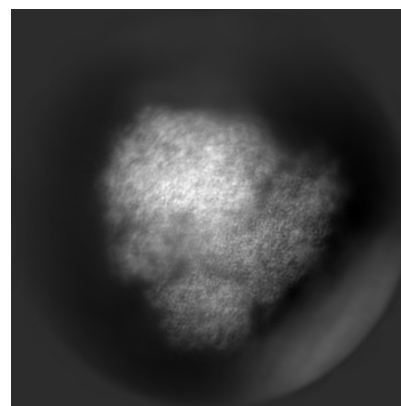
6.1.1 Primary map



X

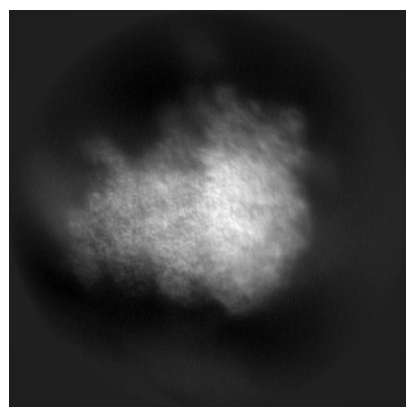


Y

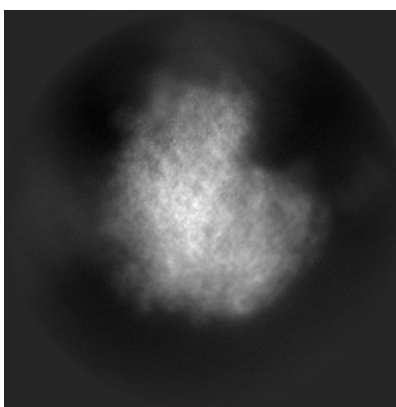


Z

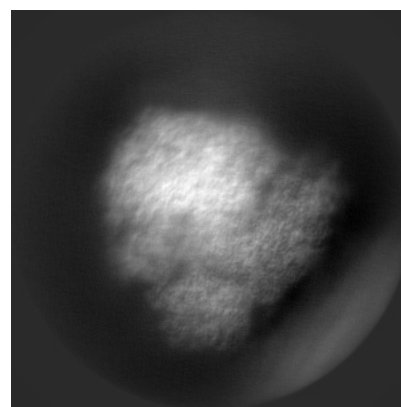
6.1.2 Raw map



X



Y

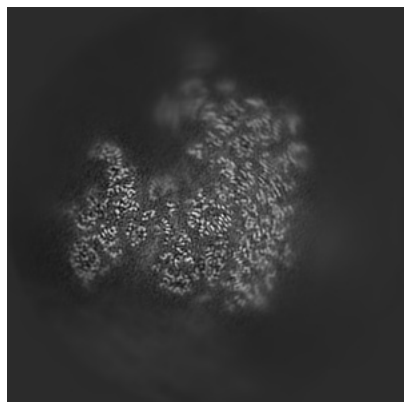


Z

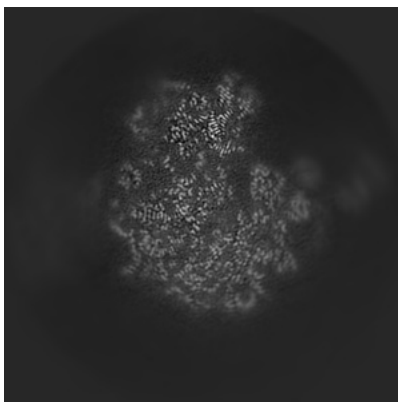
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

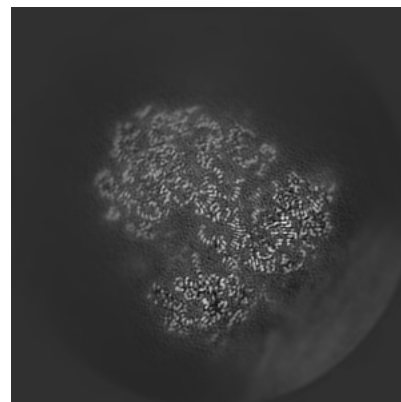
6.2.1 Primary map



X Index: 200

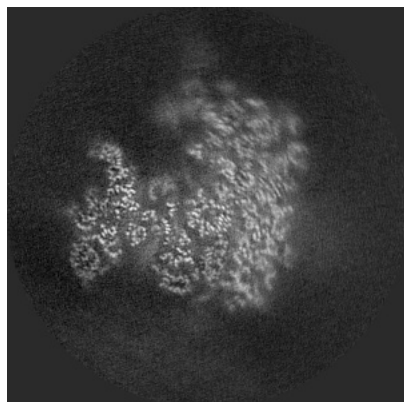


Y Index: 200

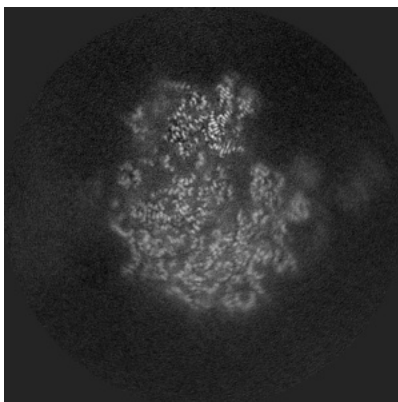


Z Index: 200

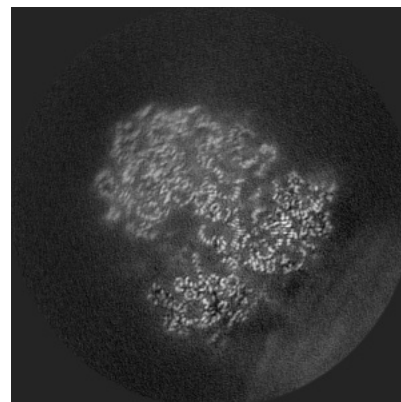
6.2.2 Raw map



X Index: 200



Y Index: 200

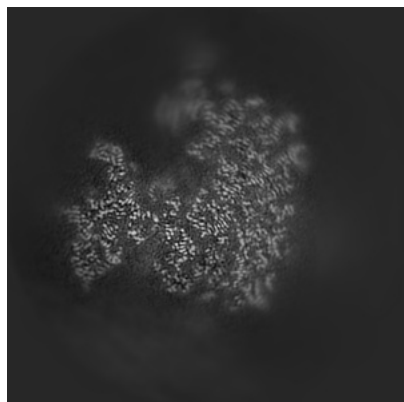


Z Index: 200

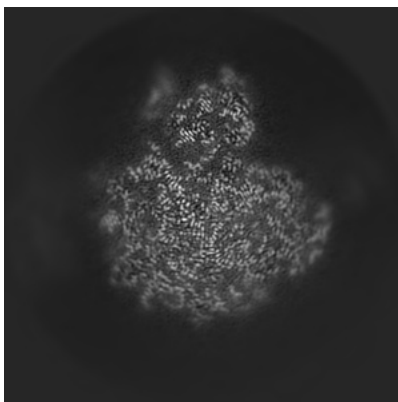
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

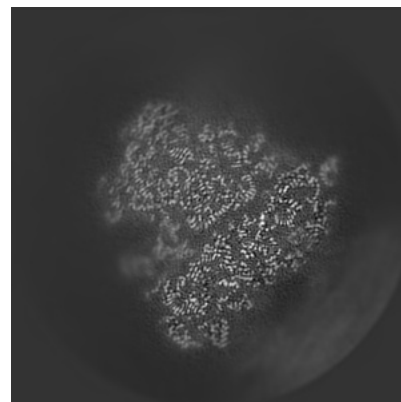
6.3.1 Primary map



X Index: 202

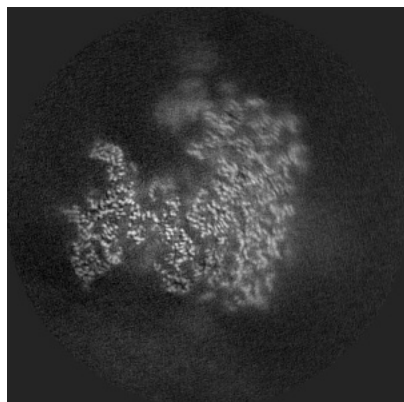


Y Index: 217

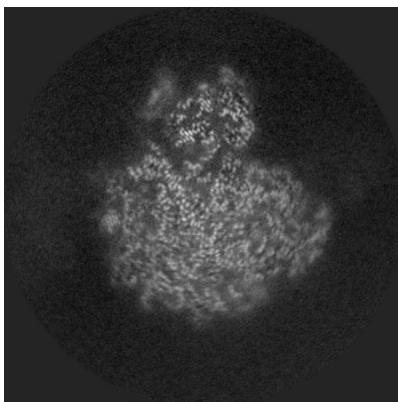


Z Index: 186

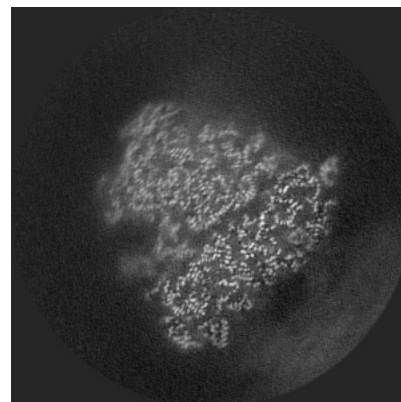
6.3.2 Raw map



X Index: 202



Y Index: 217



Z Index: 186

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

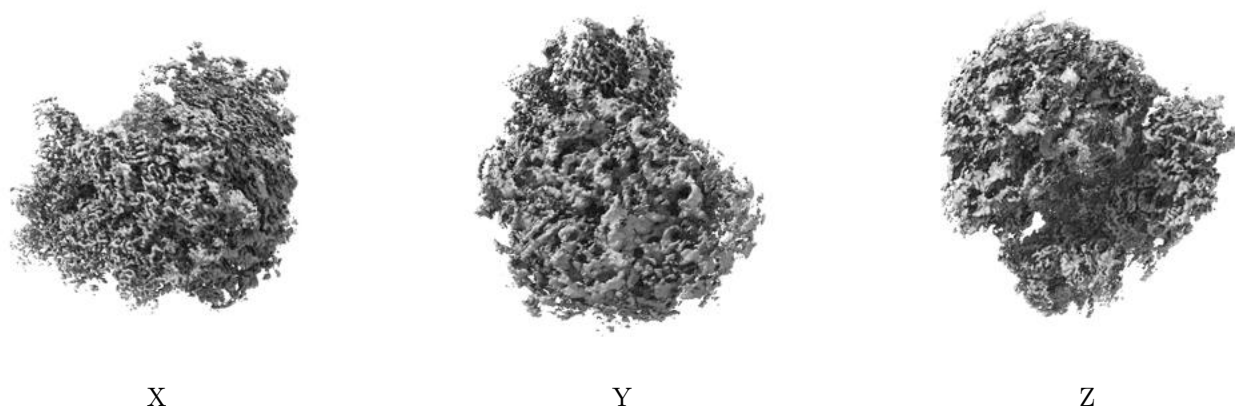
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

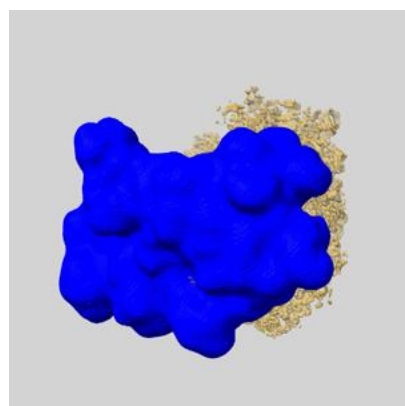
6.5 Mask visualisation [i](#)

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

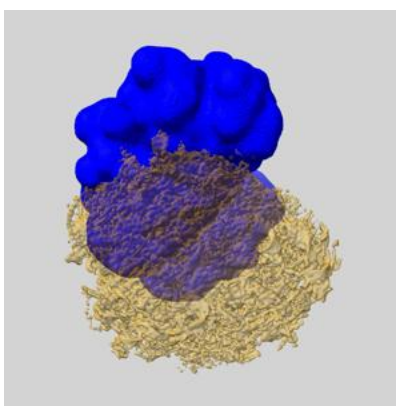
A mask typically either:

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

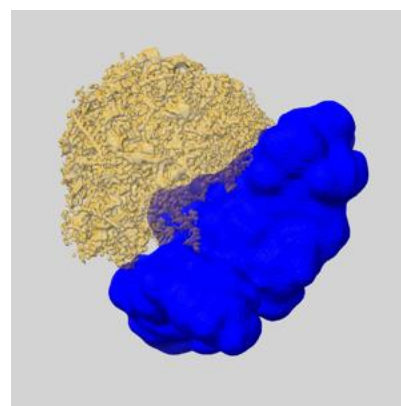
6.5.1 emd_11457_msk_1.map [i](#)



X



Y

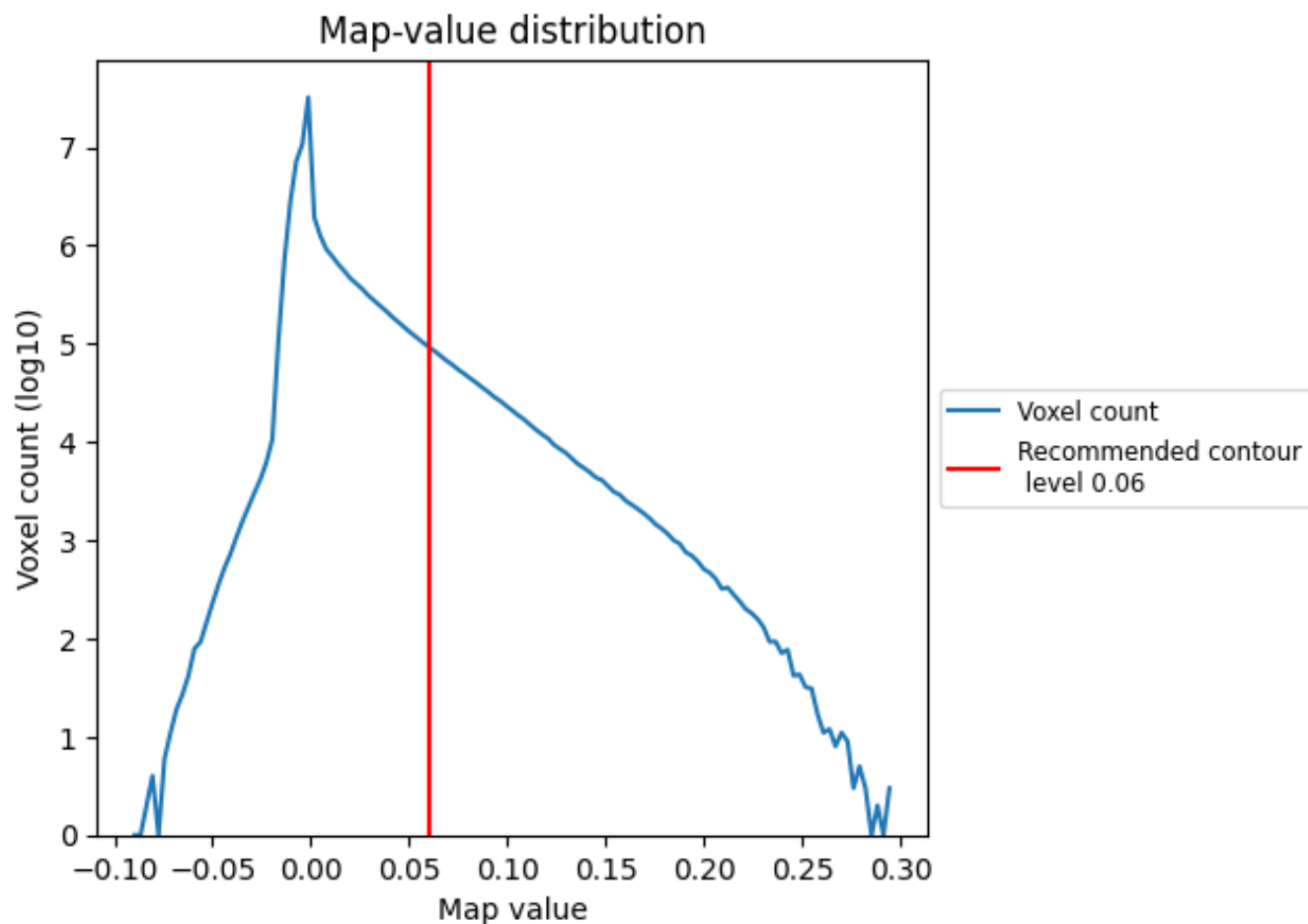


Z

7 Map analysis [i](#)

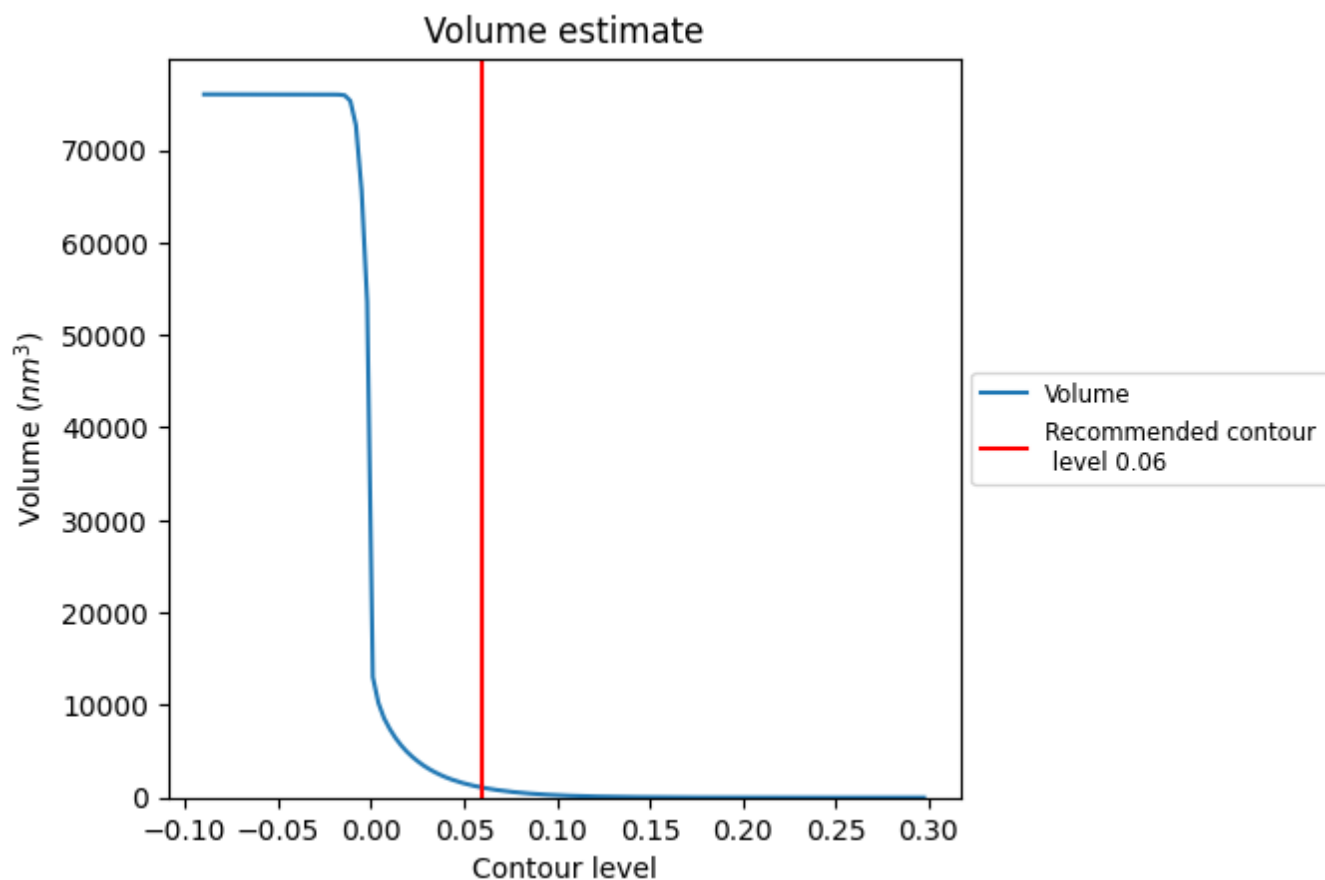
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

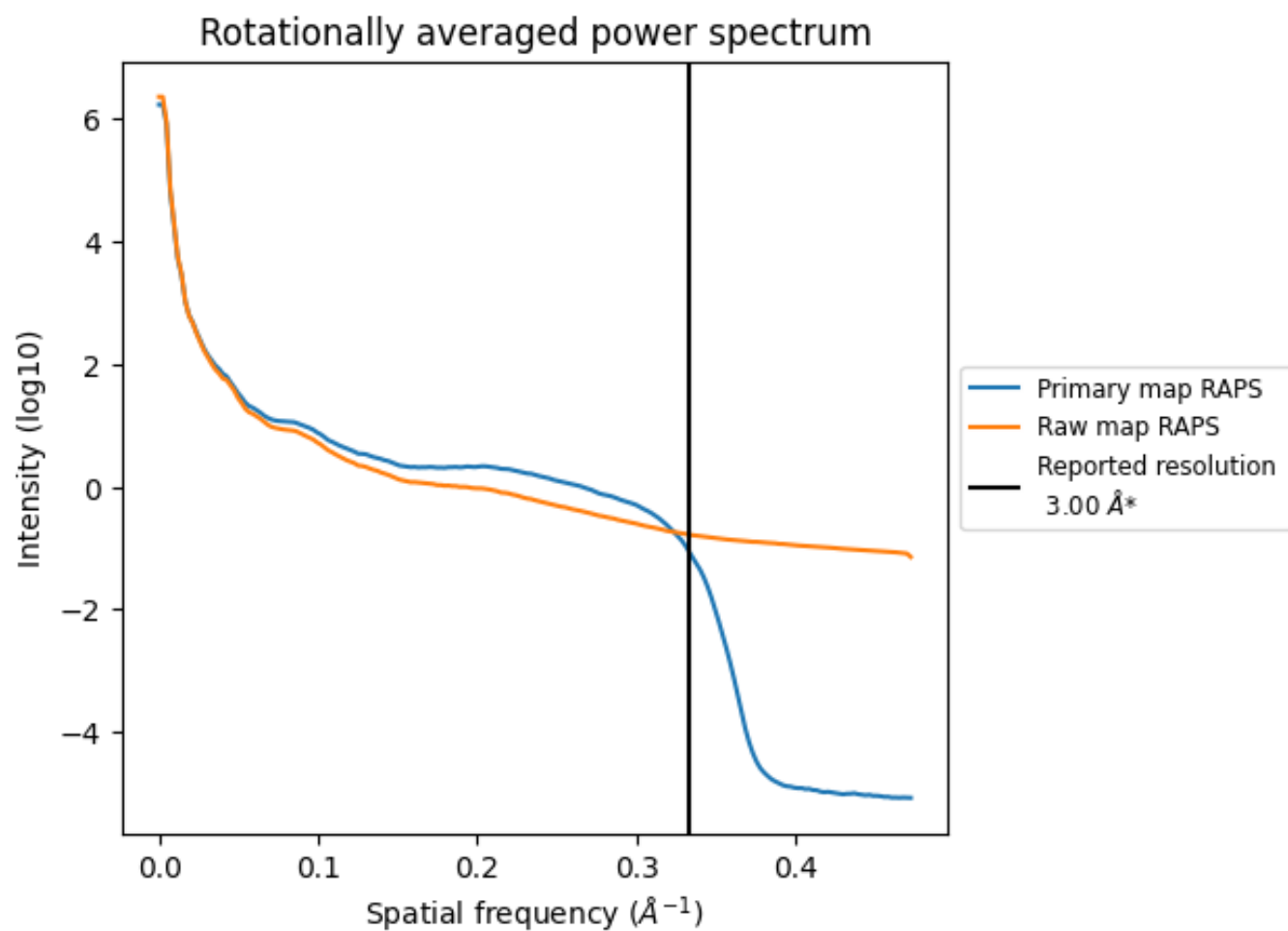
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1080 nm³; this corresponds to an approximate mass of 976 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 ⓘ

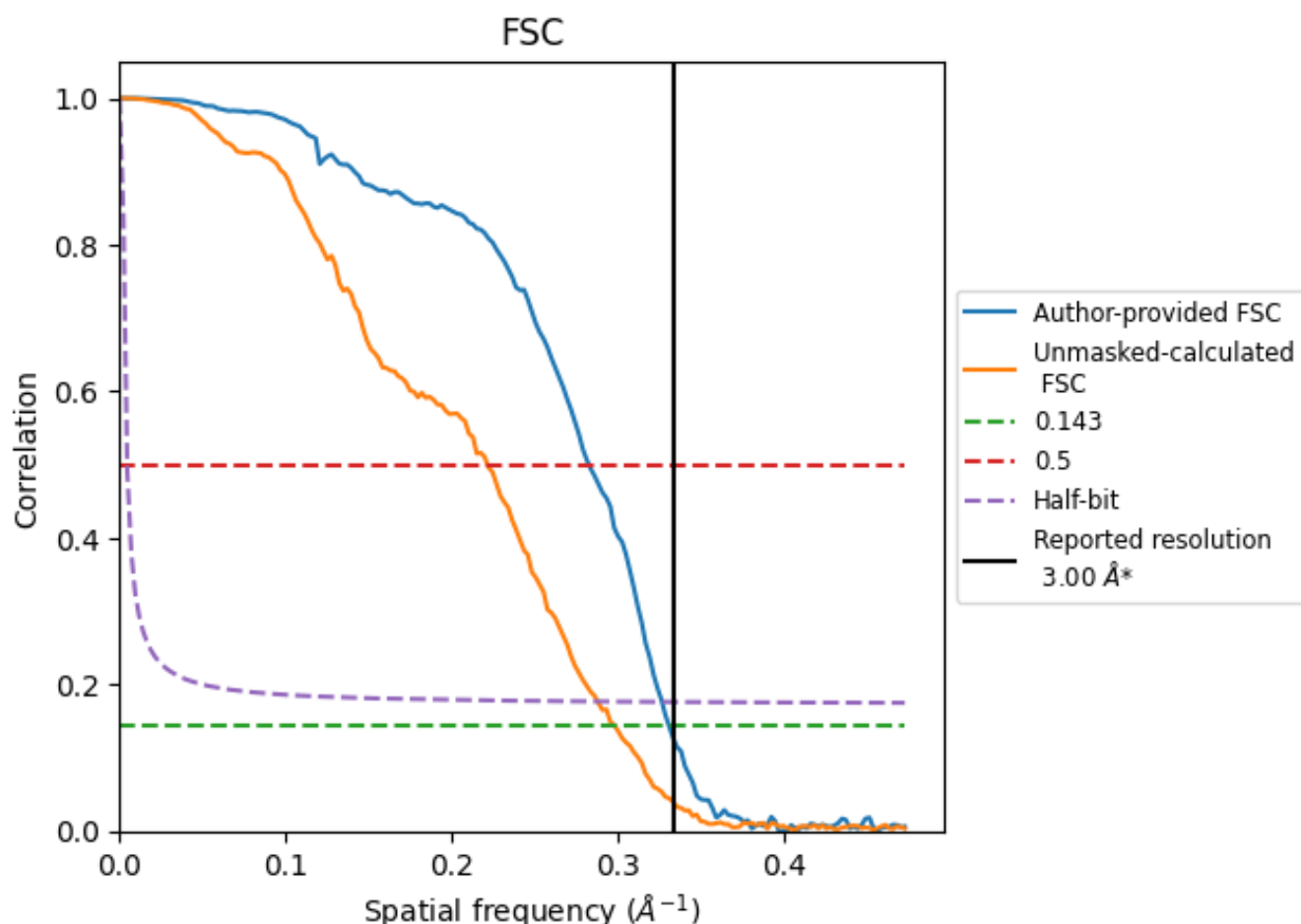


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

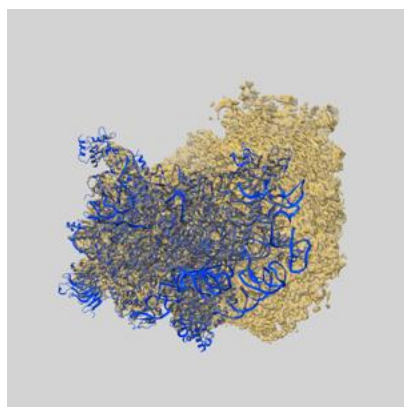
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.03	3.54	3.07
Unmasked-calculated*	3.36	4.52	3.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.36 differs from the reported value 3.0 by more than 10 %

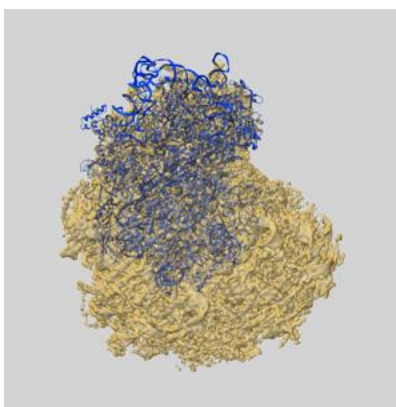
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11457 and PDB model 6ZVI. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

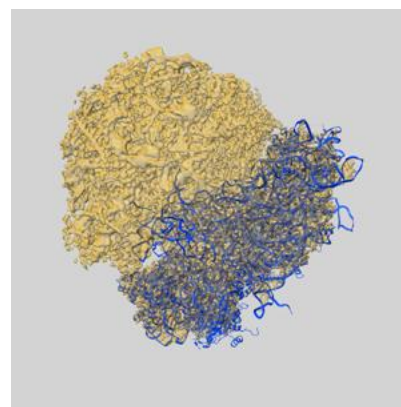
9.1 Map-model overlay [i](#)



X



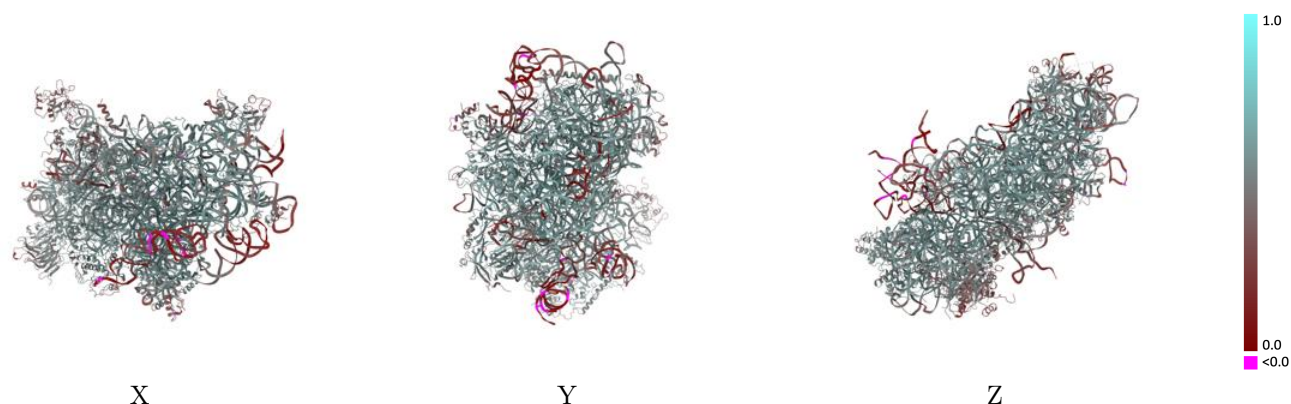
Y



Z

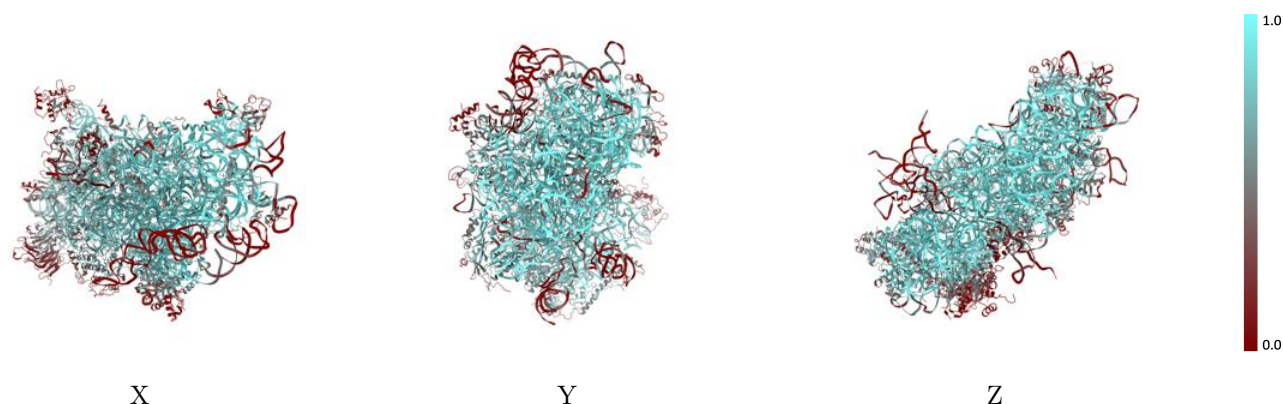
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



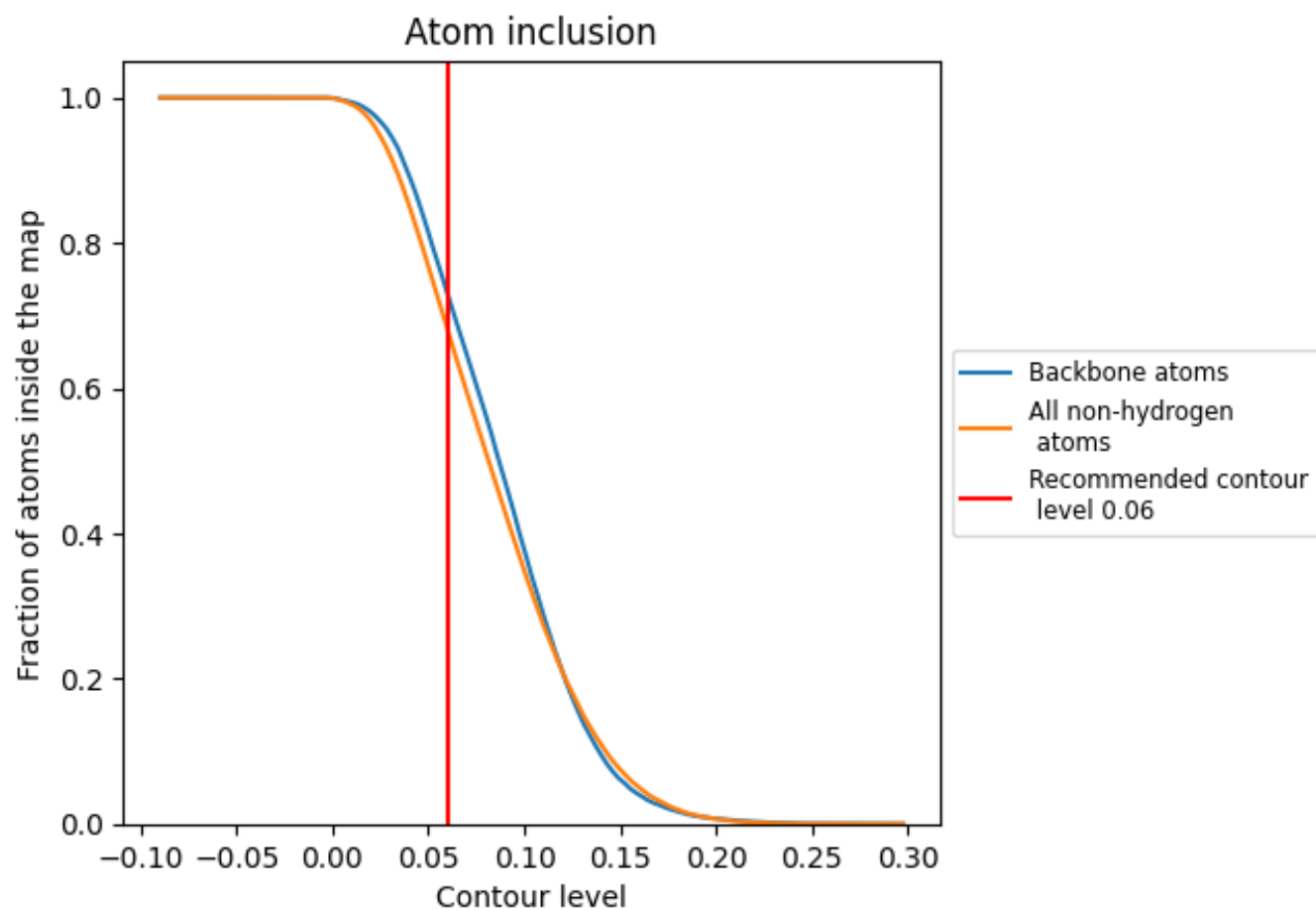
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 73% of all backbone atoms, 68% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6799	 0.5110
A	 0.6248	 0.5280
B	 0.6586	 0.5490
C	 0.5038	 0.4940
D	 0.6431	 0.5620
E	 0.8848	 0.6060
H	 0.8473	 0.5930
I	 0.5793	 0.5260
J	 0.5166	 0.5120
K	 0.8051	 0.5720
L	 0.5947	 0.5380
N	 0.5933	 0.5240
O	 0.9057	 0.6000
P	 0.6145	 0.5020
Q	 0.1952	 0.3810
R	 0.2825	 0.4860
T	 0.1611	 0.4210
d	 0.2642	 0.2940
e	 0.2524	 0.1280
f	 0.3260	 0.3330
h	 0.8078	 0.5230
i	 0.5934	 0.5490
j	 0.5910	 0.5260
k	 0.7544	 0.5790
l	 0.5891	 0.5310
m	 0.7284	 0.5680
n	 0.6372	 0.5320
o	 0.5264	 0.5000
p	 0.3892	 0.4780
q	 0.7214	 0.5450
r	 0.6422	 0.5240
s	 0.5777	 0.5110
t	 0.8039	 0.5770
u	 0.1000	 0.3290
v	 0.7913	 0.5780



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Chain	Atom inclusion	Q-score
w	 0.6877	 0.5460
x	 0.5686	 0.5170
y	 0.6923	 0.5570
z	 0.4995	 0.5140