



wwPDB EM Validation Summary Report ⓘ

Dec 14, 2024 – 03:21 PM EST

PDB ID : 8UPR
EMDB ID : EMD-42454
Title : Escherichia coli transcription-translation coupled complex class A (TTC-A) containing RfaH bound to ops signal, mRNA with a 21 nt long spacer, and fMet-tRNAs in E-site and P-site of the ribosome
Authors : Molodtsov, V.; Wang, C.; Ebright, R.H.
Deposited on : 2023-10-23
Resolution : 5.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

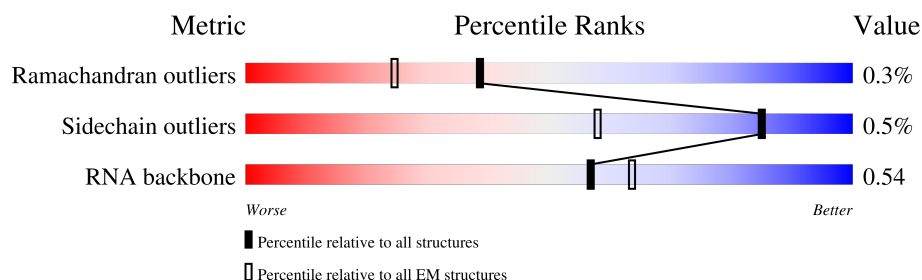
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.30 Å.

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






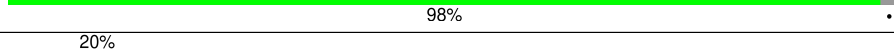
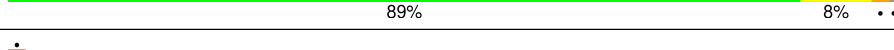
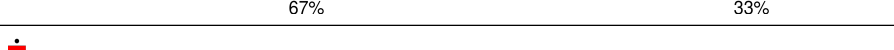
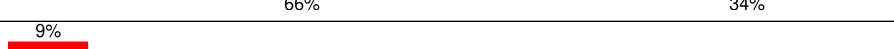
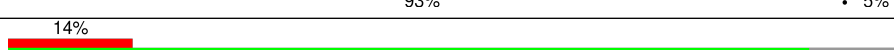
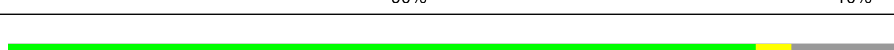


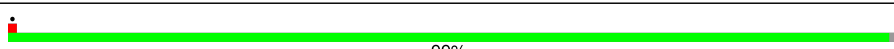



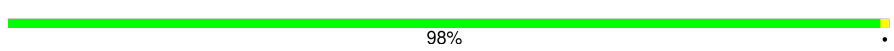
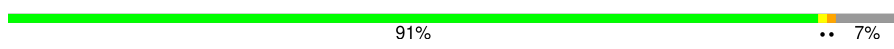


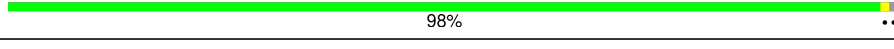
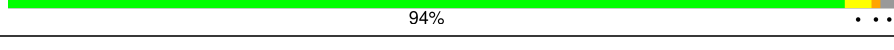
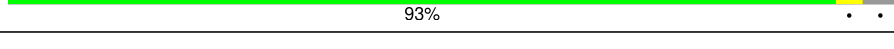
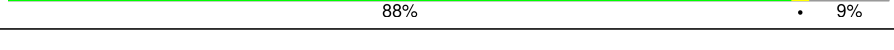
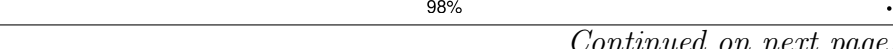

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	0	103	
2	1	110	
3	2	100	
4	3	104	
5	4	94	
6	5	38	
7	6	38	
8	7	38	

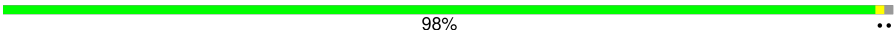
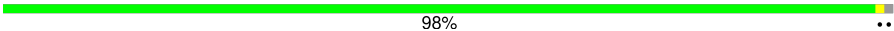
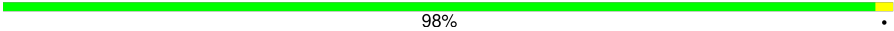
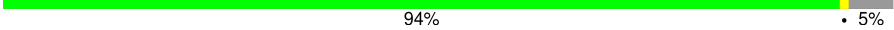

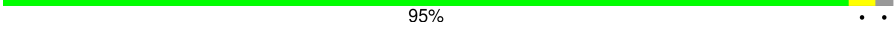
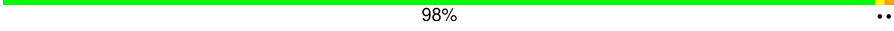



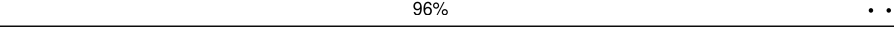
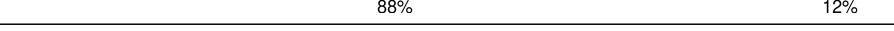
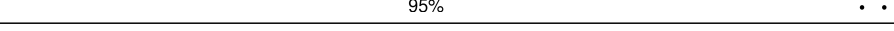
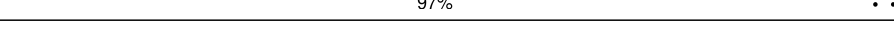
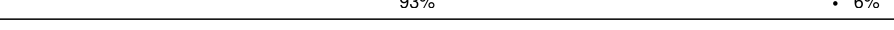
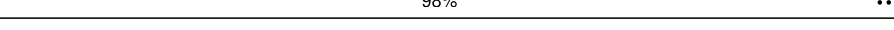
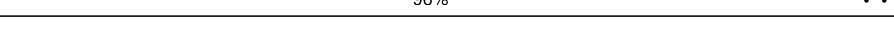
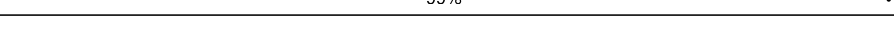
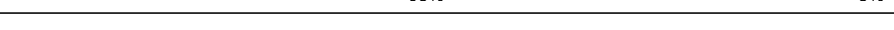
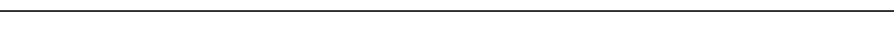

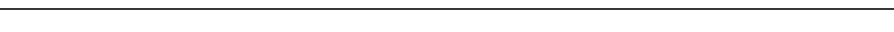
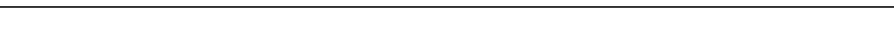


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Mol	Chain	Length	Quality of chain
9	9	165	
10	A	76	
10	B	76	
11	AA	1342	
12	AB	162	
13	AC	329	
13	AD	329	
14	AE	1407	
15	AF	91	
16	C	75	
17	D	1542	
18	E	87	
19	F	71	
20	G	241	
21	H	557	
22	I	233	
23	J	206	
24	K	167	
25	L	135	
26	M	179	
27	N	130	
28	O	130	
29	P	103	
30	Q	129	
31	R	124	

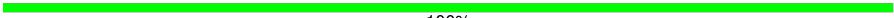








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Mol	Chain	Length	Quality of chain
32	S	101	 98% ..
33	T	89	 98% ..
34	U	82	 98% .
35	V	84	 94% • 5%
36	W	92	 87% • 10%
37	X	118	 95% ..
38	Y	142	 7% 98% ...
39	Z	121	 25% 75%
40	a	2904	 80% 19% ..
41	b	85	 89% 11%
42	c	78	 96% ..
43	d	120	 88% 12%
44	e	63	 95% ..
45	f	59	 97% ..
46	g	70	 93% • 6%
47	h	273	 98% ..
48	i	57	 96% ..
49	j	209	 99% .
50	k	55	 95% 5%
51	l	201	 99% .
52	m	46	 100%
53	n	179	 97% ..
54	o	65	 94% 5% .
55	p	177	 98% ..
56	q	38	 100%

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Mol	Chain	Length	Quality of chain
57	r	149	 100% ..
58	s	142	 97% ..
59	t	123	 97% .
60	u	144	 98% .
61	v	136	 99% .
62	w	127	 89% 5% 6% .
63	x	117	 99% .
64	y	115	 97% ..
65	z	118	 97% ..

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 276059 atoms, of which 98639 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	94	Total	C	H	N	O	S	0	0
			1557	470	811	140	134	2		

- Molecule 4 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	3	103	Total	C	H	N	O		0	0
			1632	498	844	148	142			

- Molecule 5 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 6 is a DNA chain called NT DNA ops.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	5	35	Total	C	N	O	P		0	0
			726	342	141	208	35			

- Molecule 7 is a DNA chain called T DNA ops.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	35	Total	C	N	O	P	0	0
			703	336	117	215	35		

- Molecule 8 is a RNA chain called mRNA with 21 nt long spacer.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	38	Total	C	N	O	P	0	0
			792	354	112	288	38		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 10 is a RNA chain called E-site and P-site tRNA (fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
10	A	76	Total 2446	C 723	H 826	N 295	O 527	P 75	0	0
10	B	76	Total 2434	C 723	H 814	N 295	O 527	P 75	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AA	1316	Total	C	N	O	S	0	0
			10381	6514	1810	2014	43		

- Molecule 12 is a protein called Transcription antitermination protein RfaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AB	161	Total	C	N	O	S	0	0
			1286	828	222	232	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AC	221	Total	C	N	O	S	0	0
			1698	1060	299	333	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	AD	218	Total	C	N	O	S	0	0
			1677	1048	297	326	6		

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AE	1337	Total	C	N	O	S	0	0
			10404	6535	1856	1963	50		

- Molecule 15 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AF	82	Total	C	N	O	S	0	0
			650	396	122	131	1		

- Molecule 16 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	66	Total	C	H	N	O	S	
			1103	344	559	102	97	1	0

- Molecule 17 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	1524	Total	C	H	N	O	P	
			49126	14585	16423	6003	10591	1524	0

- Molecule 18 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	86	Total	C	H	N	O	S	
			1388	414	719	138	114	3	0

- Molecule 19 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F	70	Total	C	H	N	O	S	
			1218	366	629	125	97	1	0

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	G	225	Total	C	H	N	O	S	0	0
			3545	1113	1785	316	323	8		

- Molecule 21 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	H	259	Total	C	H	N	O	S	0	0
			3184	1073	1454	305	349	3		

- Molecule 22 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	I	208	Total	C	H	N	O	S	0	0
			3346	1036	1710	307	290	3		

- Molecule 23 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	J	205	Total	C	H	N	O	S	0	0
			3350	1026	1707	315	298	4		

- Molecule 24 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	K	156	Total	C	H	N	O	S	0	0
			2348	717	1196	217	212	6		

- Molecule 25 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	L	104	Total	C	H	N	O	S	0	0
			1694	536	846	153	152	7		

- Molecule 26 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	M	151	Total	C	H	N	O	S	0	0
			2416	735	1235	227	215	4		

- Molecule 27 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	N	129	Total	C	H	N	O	S	0	0
			2010	616	1031	173	184	6		

- Molecule 28 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	O	127	Total	C	H	N	O	S	0	0
			2092	634	1070	206	179	3		

- Molecule 29 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	P	99	Total	C	H	N	O	S	0	0
			1621	495	831	151	143	1		

- Molecule 30 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	Q	117	Total	C	H	N	O	S	0	0
			1764	540	887	174	160	3		

- Molecule 31 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	R	121	Total	C	H	N	O	S	0	0
			1940	580	1001	194	161	4		

- Molecule 32 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	S	100	Total	C	H	N	O	S	0	0
			1649	499	844	164	139	3		

- Molecule 33 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	T	88	Total	C	H	N	O	S	0	0
			1448	439	734	144	130	1		

- Molecule 34 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	U	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 35 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	V	80	Total	C	H	N	O	S	0	0
			1339	411	691	121	113	3		

- Molecule 36 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	W	83	Total	C	H	N	O	S	0	0
			1351	424	688	126	111	2		

- Molecule 37 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	X	116	Total	C	H	N	O	S	0	0
			1864	558	964	181	158	3		

- Molecule 38 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Y	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 39 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Z	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 40 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	a	2880	Total	C	H	N	O	P	0	0
			92918	27587	31077	11398	19976	2880		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	conflict	GB 937521852

- Molecule 41 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	b	76	Total	C	H	N	O	S	0	0
			1181	360	599	117	104	1		

- Molecule 42 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	c	77	Total	C	H	N	O	S	0	0
			1277	388	652	129	106	2		

- Molecule 43 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	d	120	Total	C	H	N	O	P	0	0
			3870	1144	1301	468	837	120		

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	e	62	Total	C	H	N	O	S	0	0
			1032	308	531	98	94	1		

- Molecule 45 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	f	58	Total	C	H	N	O	S	0	0
			936	281	488	87	78	2		

- Molecule 46 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	g	66	Total	C	H	N	O	S	0	0
			1042	323	520	99	94	6		

- Molecule 47 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	h	271	Total	C	H	N	O	S	0	0
			4236	1288	2154	423	364	7		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	i	56	Total	C	H	N	O	S	0	0
			903	269	459	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	j	209	Total	C	H	N	O	S	0	0
			3182	979	1617	288	294	4		

- Molecule 50 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	k	52	Total	C	H	N	O		0	0
			890	275	464	78	73			

- Molecule 51 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	l	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	m	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 53 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	n	177	Total	C	H	N	O	S	0	0
			2853	899	1443	249	256	6		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	o	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	p	175	Total	C	H	N	O	S	0	0
			2671	826	1358	241	244	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	q	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 57 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	r	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 58 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	s	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 59 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	t	123	Total	C	H	N	O	S	0	0
			1969	593	1023	181	166	6		

- Molecule 60 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	u	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 61 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	v	136	Total	C	H	N	O	S	0	0
			2231	686	1157	205	177	6		

- Molecule 62 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	w	119	Total	C	H	N	O	S	0	0
			1945	588	994	195	163	5		

- Molecule 63 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	x	116	Total	C	H	N	O		0	0
			1815	552	923	178	162			

- Molecule 64 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	y	114	Total	C	H	N	O	S	0	0
			1879	574	962	179	163	1		

- Molecule 65 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	z	117	Total	C	H	N	O		0	0
			1967	604	1020	192	151			

- Molecule 66 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
66	AE	1	Total	Mg	0
			1	1	

- Molecule 67 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
67	AE	2	Total	Zn	0
			2	2	

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: Ribosomal protein L21

Chain 0:  100%

There are no outlier residues recorded for this chain.

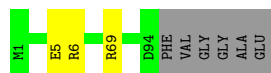
- Molecule 2: 50S ribosomal protein L22

Chain 1:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: 50S ribosomal protein L23

Chain 2:  91% 6%



- Molecule 4: 50S ribosomal protein L24

Chain 3:  99%



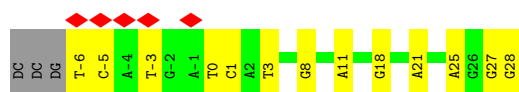
- Molecule 5: 50S ribosomal protein L25

Chain 4:  98%



- Molecule 6: NT DNA ops

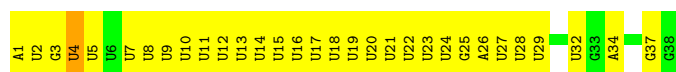
Chain 5:  13% 58% 34% 8%



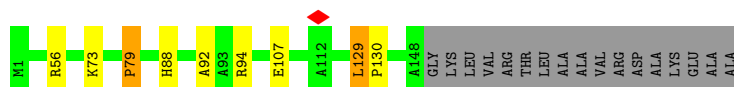
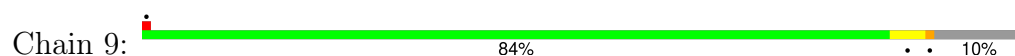
- Molecule 7: T DNA ops



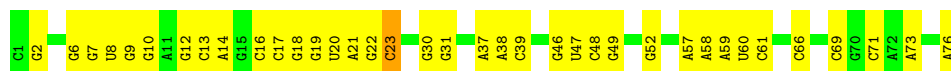
- Molecule 8: mRNA with 21 nt long spacer



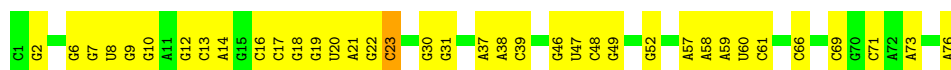
- Molecule 9: 50S ribosomal protein L10



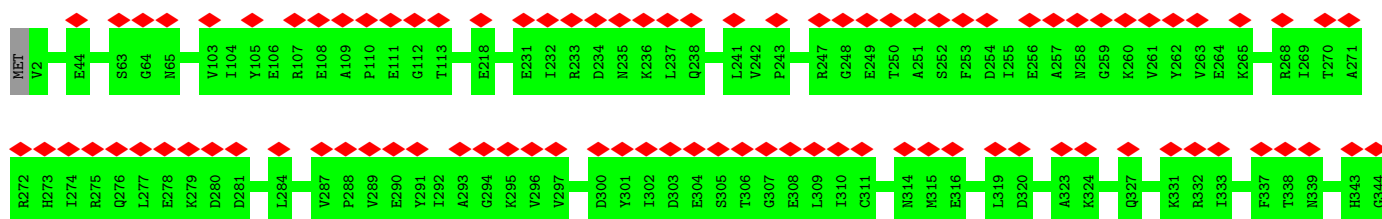
- Molecule 10: E-site and P-site tRNA (fMet)

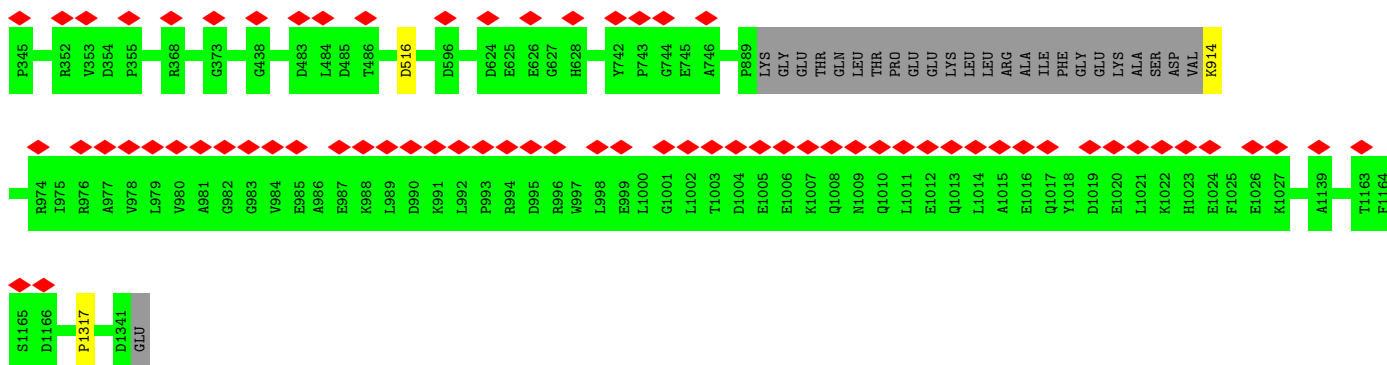


- Molecule 10: E-site and P-site tRNA (fMet)

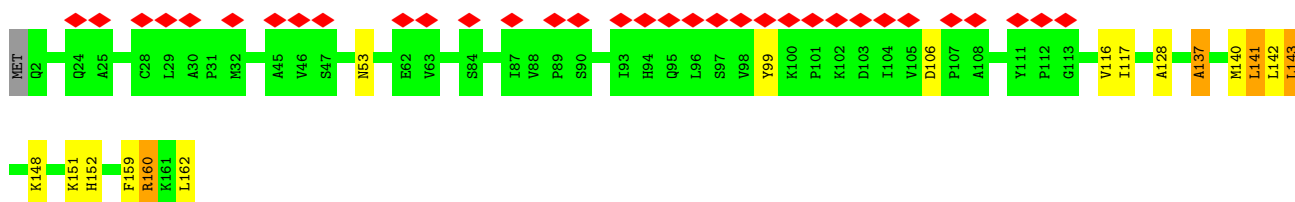
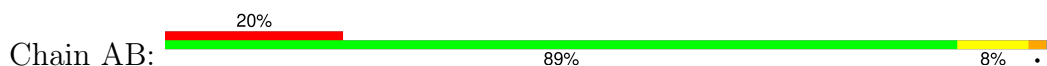


- Molecule 11: DNA-directed RNA polymerase subunit beta

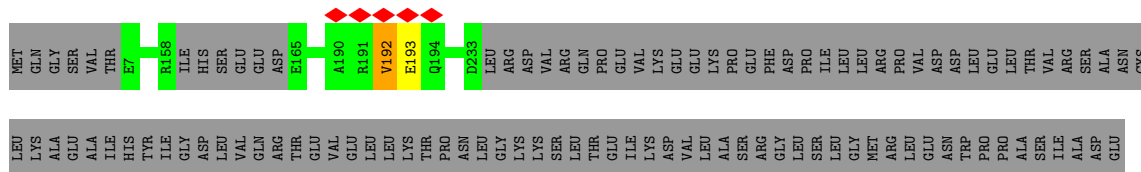




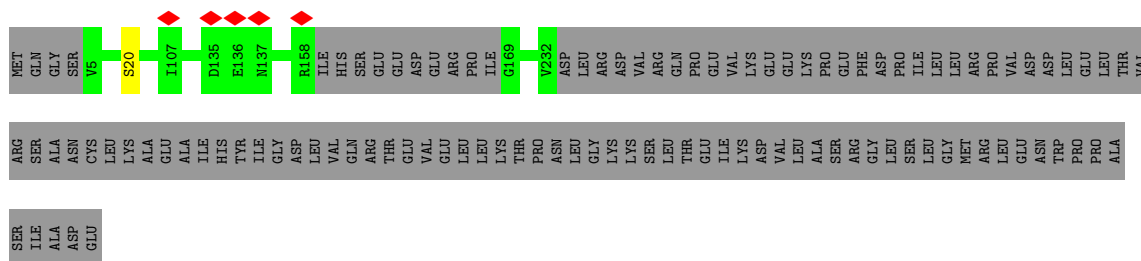
- Molecule 12: Transcription antitermination protein RfaH



- Molecule 13: DNA-directed RNA polymerase subunit alpha

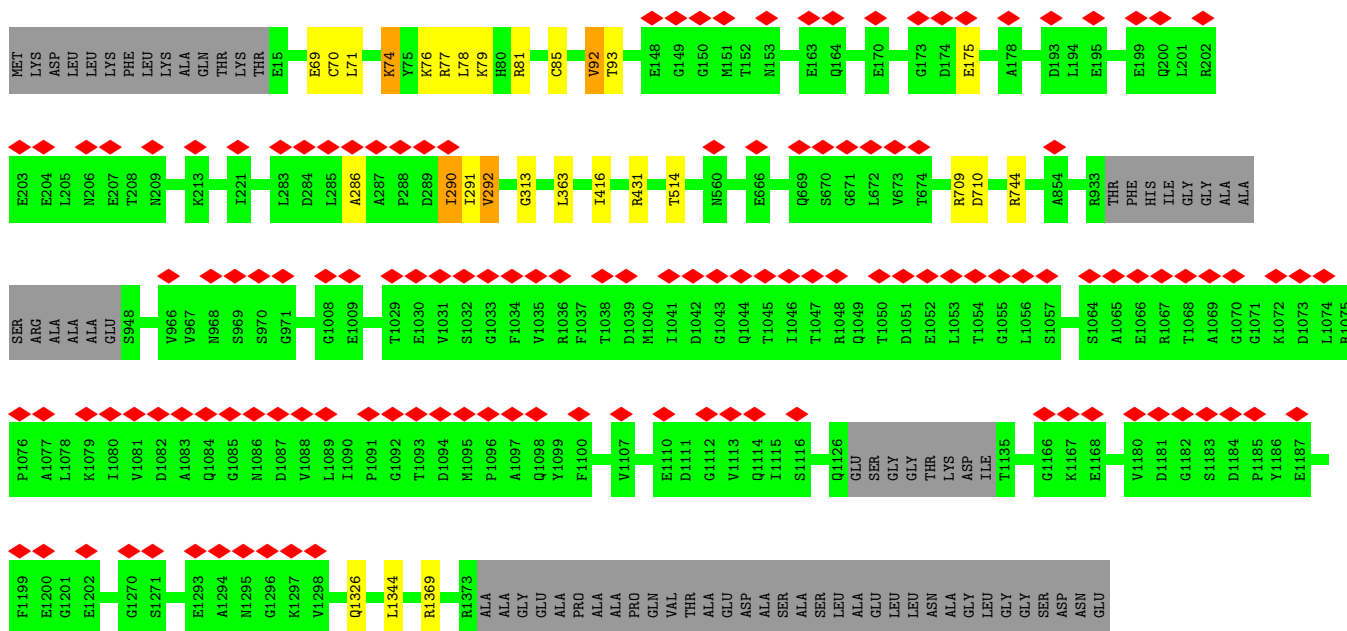


- Molecule 13: DNA-directed RNA polymerase subunit alpha

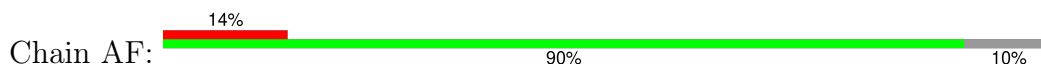


- Molecule 14: DNA-directed RNA polymerase subunit beta'

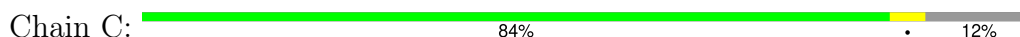




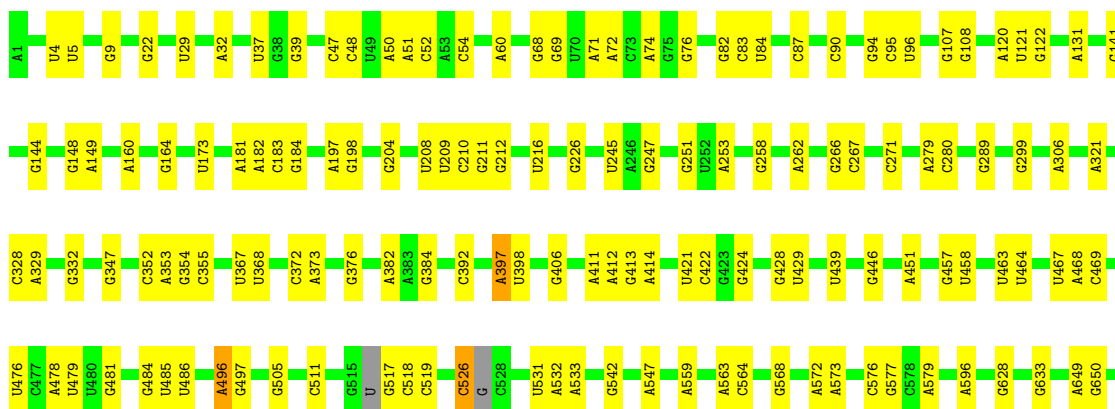
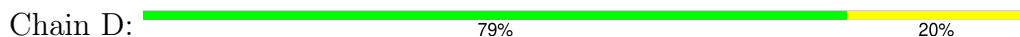
- Molecule 15: DNA-directed RNA polymerase subunit omega

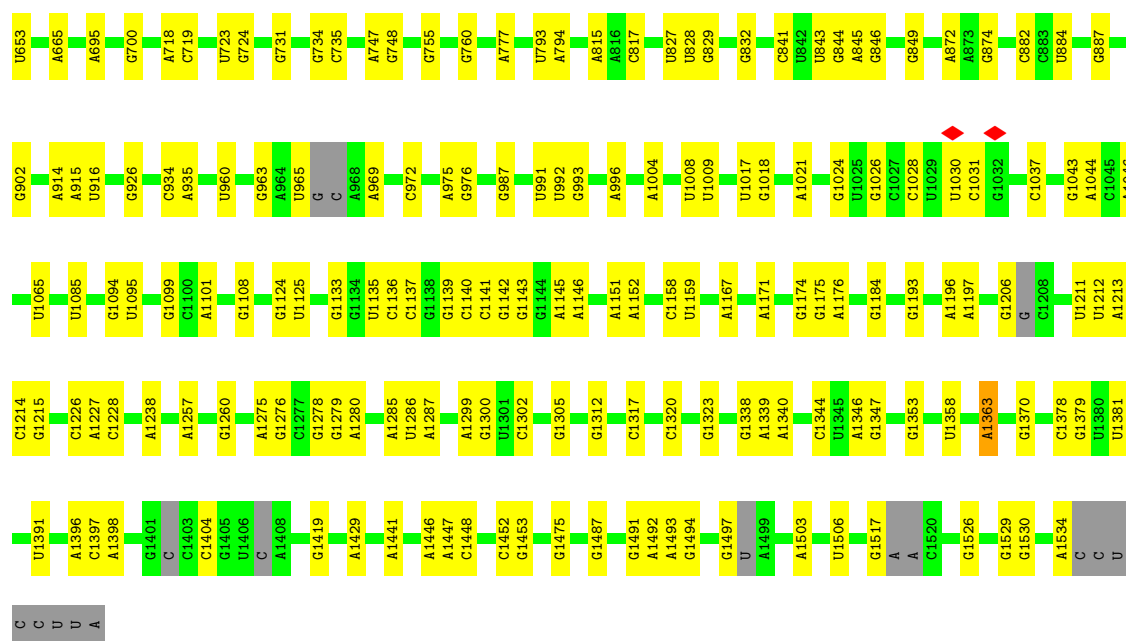


- Molecule 16: 30S ribosomal protein S18



- Molecule 17: 16S rRNA





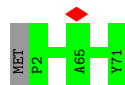
- Molecule 18: 30S ribosomal protein S20

Chain E: 99%



- Molecule 19: 30S ribosomal protein S21

Chain F: 99%



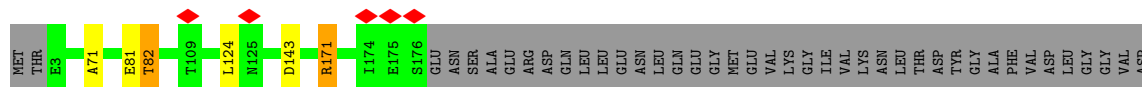
- Molecule 20: 30S ribosomal protein S2

Chain G: 90%



- Molecule 21: 30S ribosomal protein S1

Chain H: 45%



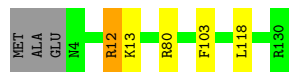
- Molecule 27: 30S ribosomal protein S8

Chain N:  98% ..



- Molecule 28: 30S ribosomal protein S9

Chain O:  94% ...




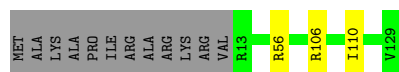
- Molecule 29: 30S ribosomal protein S10

Chain P:  93% . .



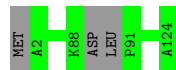
- Molecule 30: 30S ribosomal protein S11

Chain Q:  88% . 9%



- Molecule 31: 30S ribosomal protein S12

Chain R:  98% .



- Molecule 32: 30S ribosomal protein S14

Chain S:  98% ..



- Molecule 33: 30S ribosomal protein S15

Chain T:  98% ..



- Molecule 34: 30S ribosomal protein S16

```

graph LR
    M1[M1] --- R31[R31]
    R31 --- R35[R35]
    R35 --- A82[A82]

```

- MET
THR
ASP
K4
R27
V83
LEU

- | | | | | | | | | | | | | | |
|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | P2 | I40 | V62 | M66 | A84 | ALA | ASP | LYS | LYS | ALA | LYS | LYS | LYS |
|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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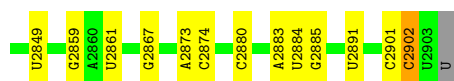
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- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | S1 | F30 | GLY | VAL | SER | ALA | ALA | ALA | VAL | VAL | VAL | ALA | ALA | GLY | PRO | VAL | GLU | ALA | ALA | GLU | GLU | LYS | THR | GLU | PHE | ASP | VAL | LEU | LEU | LYS | LYS | VAL | VAL | VAL | LEU | LEU | ARG | GLY | ALA | ALA | THR | GLY | LEU | GLY | LYS | ALA | ALA | ASP |
|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

VAL	GLU	SER	ALA	PRO	ALA	ALA	LEU	LYS	GLU	GLY	VAL	SER	LYS	ASP	ASP	ALA	GLU	ALA	LEU	LYS	LYS	ALA	LEU	GLU	GLU	ALA	GLY	ALA	GLU	VAL	GLU	VAL	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

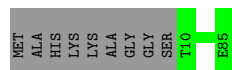
- G1 U4 A10 G15 G23 G27 U34 G35 G46 G58 U59 G60 G61 G62 U62 A63 U67 A71 A74 G75 A83 A84 G85 G96 A101 A101 U102 A103 G110 A118 A119 U120 U120 C130 A131 G136 U139 C140 G141 C163 C164 A165

U2609	G2458	A2322	G2162	C2055	U1758	U1554	C1345	G1107	C995	A819	A609	G411	A181
C2610	G2470	G2325	A2163	G2056	C1764	U1559	U1352	A1111	A996	U827	A613	A412	A196
C2612	U2474	C2326	C2164	A2060	C1773	U1566	A1365	G1112	U999	U828	A614	C420	G215
U2613	A2476	A2327	C2165	G2061	A1774	A1567	G1368	U1119	G1005	A845	A616	G424	A216
U2629	A2477	U2328	A2169	A2062	U1775	A1569	G1378	G1122	U1012	U846	A626	U461	A221
G2630	U2171	A1936	A2170	U2068	A1791	C1577	A1378	G1128	C1013	G888	A627	U451	A222
G2638	U2172	A1937	U2172	A2068	C1800	U1578	G1379	U1128	U1019	G889	A637	A457	C225
G2663	C2178	U	C2178	A2070	A1808	A1579	G1380	U1132	A1020	G869	A637	A457	C225
G2669	U2182	U1955	U2182	C2073	G1811	A1580	A1383	U1133	A1021	A878	C645	A477	G248
A2670	A2183	U	A2183	U	G1816	C1582	A1392	A1134	G1022	G881	U646	G461	C249
G2671	U2185	C1961	U2185	U2075	C1817	C1583	A1395	C1135	U1023	G882	A647	G491	C253
U2689	U2188	C	U2188	A2097	U1818	C1584	U1406	U1141	G1026	G883	A654	A501	G261
U2690	U2189	U2098	U2189	U2098	U1818	C1585	U1407	A1142	U1033	U884	A668	A501	C264
G2714	G2190	U2099	G2190	U2099	A1829	U1589	G1407	A1169	G1041	G885	U686	A503	A265
C2715	G2193	U2100	G2193	A2108	C1833	A1590	U1408	C1170	C1045	U888	G704	A504	G266
U2506	U2194	A1966	U2194	U2109	U1834	A1609	U1409	U1173	A1046	U891	U710	A505	C267
C2512	U2198	C1967	U2198	U2110	G	A1610	G1414	U1174	G1047	G892	U710	G509	G271
A2513	G2204	U1971	G2204	U2111	C1836	G1613	U1415	A1175	A1046	A893	U710	G520	A272
A2518	G2204	G1972	G2204	U2112	A1847	U1647	G1416	U1176	A1046	G894	U710	G520	C275
U2519	A2211	G1972	A2211	U2113	A1848	U1648	G1417	C1177	A1046	A895	U710	G520	C275
C2520	A2212	A1987	A2212	G2115	U1857	A	G1418	C1178	U1060	A896	G729	A522	U276
G2525	A2225	U1991	A2225	G2116	A1858	G1617	G1419	G1179	U1061	A897	A730	A522	G277
A2757	C2226	U1993	C2226	A2117	U1859	G1619	A1420	U1180	C888	A898	A730	A522	A278
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G2777	G2239	G2002	G2239	G2123	U1864	G1655	U1482	G1238	A1069	A910	U744	G637	A311
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C2793	G2252	A2020	G2252	G2128	U1872	U1674	U1490	G1266	A1073	U931	G757	U545	U373
U2796	G2252	G2021	G2252	U2131	G1873	G1674	U1497	C1257	G1074	A941	A764	U546	C353
U2797	A2268	C2022	A2268	U2132	G1906	A1677	U1497	G1266	C1079	G942	C765	G547	G361
U2798	A2278	G2027	A2278	G2133	G1907	G1703	A1503	G1266	A1080	A945	C765	G549	A362
A2799	C2283	U2028	C2283	A2134	U	U1714	A1508	G1271	U1082	A945	G775	G551	A371
G2801	A2287	A2031	A2287	U2139	A1912	G1715	A1509	U1273	A1083	G953	G776	G551	G372
U2818	A2288	A2032	A2288	G2140	A1913	U1729	A1515	A1276	A1085	U	A782	U569	A374
G2820	A2297	A2033	A2297	G2141	U	C1730	A1515	G1300	A1086	G956	G784	U573	G383
A2823	U2305	C2043	U2305	G2142	A1916	G1731	G1529	G1301	A1088	A960	A800	A575	C385
C2824	A2308	G2049	C2824	A2147	U	C1732	G1530	A1321	A1090	C961	A800	A575	G386
G2825	A2309	C2050	A2309	A2154	A1918	G1738	U1534	A1321	A1095	G974	G805	U588	G396
A2835	A2309	A2051	A2309	G2157	A1919	G1760	A1536	G1331	U1101	A953	C812	A603	U405
	A2309	A2052	A2309	G2159	G1922	G1760	A1536	G1334	U1101	A953	C812	A603	U405



- Molecule 41: 50S ribosomal protein L27

Chain b: 89% 11%



- Molecule 42: 50S ribosomal protein L28

Chain c: 96% ..



- Molecule 43: 5S rRNA

Chain d: 88% 12%



- Molecule 44: 50S ribosomal protein L29

Chain e: 95% ..



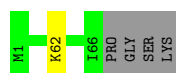
- Molecule 45: 50S ribosomal protein L30

Chain f: 97% ..



- Molecule 46: 50S ribosomal protein L31

Chain g: 93% • 6%



- Molecule 47: 50S ribosomal protein L2

Chain h: 98% ..



- Molecule 48: 50S ribosomal protein L32

Chain i: 96% ..



- Molecule 49: 50S ribosomal protein L3

Chain j: 99% .



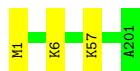
- Molecule 50: 50S ribosomal protein L33

Chain k: 95% 5%



- Molecule 51: 50S ribosomal protein L4

Chain l: 99% .



- Molecule 52: 50S ribosomal protein L34

Chain m: 100%

There are no outlier residues recorded for this chain.

- Molecule 53: 50S ribosomal protein L5

Chain n: 97% ..



- Molecule 54: 50S ribosomal protein L35

Chain o: 94% 5% .



- Molecule 55: 50S ribosomal protein L6

Chain p:  98% ..



- Molecule 56: 50S ribosomal protein L36

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L9

Chain r:  100%

There are no outlier residues recorded for this chain.

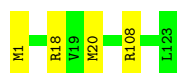
- Molecule 58: 50S ribosomal protein L13

Chain s:  97% ..



- Molecule 59: 50S ribosomal protein L14

Chain t:  97% .



- Molecule 60: 50S ribosomal protein L15

Chain u:  98% .



- Molecule 61: 50S ribosomal protein L16

Chain v:  99% .



- Molecule 62: 50S ribosomal protein L17

Chain w:  89% 5% 6%



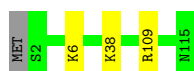
- Molecule 63: 50S ribosomal protein L18

Chain x: 99%



- Molecule 64: 50S ribosomal protein L19

Chain y: 97%



- Molecule 65: 50S ribosomal protein L20

Chain z: 97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10509	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0025	Depositor
Map size (Å)	531.968, 531.968, 531.968	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.039, 1.039, 1.039	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	0	0.47	0/829	0.60	0/1107
2	1	0.58	0/864	0.69	0/1156
3	2	0.67	1/752 (0.1%)	0.72	1/1005 (0.1%)
4	3	0.41	0/796	0.55	0/1062
5	4	0.65	2/766 (0.3%)	0.69	0/1025
6	5	1.14	11/816 (1.3%)	1.12	2/1259 (0.2%)
7	6	1.12	8/783 (1.0%)	1.10	0/1203
8	7	0.53	2/879 (0.2%)	0.87	3/1364 (0.2%)
9	9	0.36	0/1131	0.66	2/1524 (0.1%)
10	A	0.55	1/1810 (0.1%)	1.26	12/2821 (0.4%)
10	B	0.55	1/1810 (0.1%)	1.26	11/2821 (0.4%)
11	AA	0.43	0/10547	0.61	1/14232 (0.0%)
12	AB	0.42	0/1317	0.85	5/1786 (0.3%)
13	AC	0.41	0/1718	0.62	0/2328
13	AD	0.36	0/1696	0.62	0/2298
14	AE	0.42	0/10561	0.63	3/14258 (0.0%)
15	AF	0.33	0/652	0.57	0/879
16	C	0.70	0/553	0.92	4/743 (0.5%)
17	D	0.59	13/36610 (0.0%)	1.03	67/57091 (0.1%)
18	E	0.57	0/675	0.71	0/895
19	F	0.62	0/597	0.59	0/792
20	G	0.66	2/1791 (0.1%)	0.83	7/2413 (0.3%)
21	H	0.43	0/1746	0.70	0/2382
22	I	0.62	2/1663 (0.1%)	0.71	4/2241 (0.2%)
23	J	0.54	2/1665 (0.1%)	0.59	0/2227
24	K	0.69	1/1165 (0.1%)	0.86	4/1568 (0.3%)
25	L	0.79	3/867 (0.3%)	0.82	3/1171 (0.3%)
26	M	0.54	0/1195	0.69	2/1602 (0.1%)
27	N	0.52	0/989	0.63	1/1326 (0.1%)
28	O	0.67	4/1034 (0.4%)	0.82	4/1375 (0.3%)
29	P	0.52	0/800	0.70	2/1082 (0.2%)
30	Q	0.71	1/893 (0.1%)	0.81	4/1205 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	R	0.56	0/952	0.65	0/1274
32	S	0.64	1/817 (0.1%)	0.64	0/1088
33	T	0.56	0/722	0.72	1/964 (0.1%)
34	U	0.45	0/659	0.65	1/884 (0.1%)
35	V	0.57	0/657	0.70	0/881
36	W	0.56	1/680 (0.1%)	0.69	3/915 (0.3%)
37	X	0.48	0/909	0.72	1/1215 (0.1%)
38	Y	0.42	1/1046 (0.1%)	0.57	2/1410 (0.1%)
39	Z	0.23	0/227	0.38	0/304
40	a	0.61	14/69247 (0.0%)	1.03	129/107985 (0.1%)
41	b	0.47	0/589	0.57	0/779
42	c	0.56	1/635 (0.2%)	0.66	1/848 (0.1%)
43	d	0.50	0/2872	0.95	0/4478
44	e	0.81	2/502 (0.4%)	0.66	0/667
45	f	0.53	0/452	0.72	2/605 (0.3%)
46	g	0.50	1/531 (0.2%)	0.67	1/709 (0.1%)
47	h	0.53	2/2121 (0.1%)	0.67	6/2852 (0.2%)
48	i	0.42	0/450	0.65	1/599 (0.2%)
49	j	0.53	0/1586	0.64	2/2134 (0.1%)
50	k	0.51	0/433	0.67	0/576
51	l	0.54	1/1571 (0.1%)	0.64	1/2113 (0.0%)
52	m	0.43	0/380	0.61	0/498
53	n	0.51	0/1434	0.68	2/1926 (0.1%)
54	o	0.51	0/513	0.86	1/676 (0.1%)
55	p	0.50	0/1333	0.68	3/1805 (0.2%)
56	q	0.46	0/303	0.61	0/397
57	r	0.34	0/1122	0.52	0/1515
58	s	0.83	5/1152 (0.4%)	0.81	5/1551 (0.3%)
59	t	0.55	1/955 (0.1%)	0.89	5/1279 (0.4%)
60	u	0.47	1/1062 (0.1%)	0.63	0/1413
61	v	0.61	1/1093 (0.1%)	0.75	1/1460 (0.1%)
62	w	0.90	5/964 (0.5%)	0.95	9/1289 (0.7%)
63	x	0.42	0/902	0.57	0/1209
64	y	0.46	0/929	0.58	1/1242 (0.1%)
65	z	0.63	1/960 (0.1%)	0.59	0/1278
All	All	0.58	92/190730 (0.0%)	0.92	320/281059 (0.1%)

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
9	9	0	3
12	AB	0	10
13	AC	0	1
13	AD	0	1
14	AE	0	4
20	G	0	1
21	H	0	5
22	I	0	1
24	K	0	2
28	O	0	1
37	X	0	1
38	Y	0	1
53	n	0	1
54	o	0	1
58	s	0	1
60	u	0	2
All	All	0	36

The worst 5 of 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	w	35	LYS	CE-NZ	-15.21	1.11	1.49
25	L	42	TRP	CB-CG	-12.38	1.27	1.50
3	2	5	GLU	CG-CD	-11.53	1.34	1.51
44	e	46	VAL	CB-CG1	-11.32	1.29	1.52
62	w	42	LYS	CD-CE	-10.77	1.24	1.51

The worst 5 of 320 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	1019	U	C5-C4-O4	30.71	144.33	125.90
40	a	1141	U	C5-C4-O4	29.52	143.61	125.90
17	D	37	U	C5-C4-O4	29.43	143.56	125.90
17	D	1358	U	C5-C4-O4	29.20	143.42	125.90
17	D	827	U	C5-C4-O4	28.66	143.10	125.90

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	9	107	GLU	Peptide
9	9	79	PRO	Peptide

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Mol	Chain	Res	Type	Group
9	9	92	ALA	Peptide
12	AB	106	ASP	Peptide
12	AB	116	VAL	Peptide

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	
1	0	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
2	1	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
3	2	92/100 (92%)	87 (95%)	5 (5%)	0	100	100
4	3	101/104 (97%)	98 (97%)	3 (3%)	0	100	100
5	4	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
9	9	146/165 (88%)	101 (69%)	42 (29%)	3 (2%)	5	29
11	AA	1312/1342 (98%)	1199 (91%)	112 (8%)	1 (0%)	48	83
12	AB	159/162 (98%)	109 (69%)	45 (28%)	5 (3%)	3	21
13	AC	217/329 (66%)	203 (94%)	12 (6%)	2 (1%)	14	51
13	AD	214/329 (65%)	198 (92%)	16 (8%)	0	100	100
14	AE	1331/1407 (95%)	1210 (91%)	115 (9%)	6 (0%)	25	64
15	AF	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
16	C	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
18	E	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
19	F	68/71 (96%)	68 (100%)	0	0	100	100
20	G	223/241 (92%)	212 (95%)	10 (4%)	1 (0%)	30	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	H	255/557 (46%)	182 (71%)	66 (26%)	7 (3%)	4	25
22	I	206/233 (88%)	193 (94%)	13 (6%)	0	100	100
23	J	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
24	K	154/167 (92%)	145 (94%)	8 (5%)	1 (1%)	22	60
25	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	13	49
26	M	149/179 (83%)	140 (94%)	8 (5%)	1 (1%)	19	56
27	N	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
28	O	125/130 (96%)	116 (93%)	8 (6%)	1 (1%)	16	54
29	P	97/103 (94%)	89 (92%)	8 (8%)	0	100	100
30	Q	115/129 (89%)	107 (93%)	8 (7%)	0	100	100
31	R	117/124 (94%)	112 (96%)	5 (4%)	0	100	100
32	S	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
33	T	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
34	U	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
35	V	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
36	W	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
37	X	114/118 (97%)	103 (90%)	9 (8%)	2 (2%)	7	33
38	Y	139/142 (98%)	101 (73%)	38 (27%)	0	100	100
39	Z	28/121 (23%)	22 (79%)	6 (21%)	0	100	100
41	b	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
42	c	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
44	e	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
45	f	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
46	g	64/70 (91%)	62 (97%)	2 (3%)	0	100	100
47	h	269/273 (98%)	255 (95%)	14 (5%)	0	100	100
48	i	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
49	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
50	k	50/55 (91%)	50 (100%)	0	0	100	100
51	l	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
52	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
53	n	175/179 (98%)	161 (92%)	13 (7%)	1 (1%)	22	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	o	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	8	37
55	p	173/177 (98%)	162 (94%)	11 (6%)	0	100	100
56	q	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
57	r	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
58	s	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
59	t	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
60	u	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
61	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
62	w	117/127 (92%)	112 (96%)	5 (4%)	0	100	100
63	x	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
64	y	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
65	z	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
All	All	9486/10558 (90%)	8740 (92%)	713 (8%)	33 (0%)	38	72

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	AB	141	LEU
12	AB	152	HIS
20	G	127	ASP
21	H	304	VAL
26	M	56	LYS

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	
1	0	84/84 (100%)	84 (100%)	0	100	100
2	1	93/93 (100%)	93 (100%)	0	100	100
3	2	81/84 (96%)	80 (99%)	1 (1%)	67	79
4	3	84/85 (99%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4	78/78 (100%)	78 (100%)	0	100	100
9	9	112/123 (91%)	109 (97%)	3 (3%)	40	59
11	AA	1135/1157 (98%)	1134 (100%)	1 (0%)	92	95
12	AB	141/142 (99%)	140 (99%)	1 (1%)	81	87
13	AC	186/286 (65%)	186 (100%)	0	100	100
13	AD	185/286 (65%)	185 (100%)	0	100	100
14	AE	1122/1168 (96%)	1103 (98%)	19 (2%)	56	72
15	AF	70/75 (93%)	70 (100%)	0	100	100
16	C	57/65 (88%)	57 (100%)	0	100	100
18	E	65/66 (98%)	65 (100%)	0	100	100
19	F	60/61 (98%)	60 (100%)	0	100	100
20	G	187/199 (94%)	186 (100%)	1 (0%)	86	89
21	H	137/461 (30%)	137 (100%)	0	100	100
22	I	171/190 (90%)	170 (99%)	1 (1%)	84	88
23	J	172/173 (99%)	171 (99%)	1 (1%)	84	88
24	K	119/126 (94%)	119 (100%)	0	100	100
25	L	91/116 (78%)	91 (100%)	0	100	100
26	M	124/147 (84%)	124 (100%)	0	100	100
27	N	104/105 (99%)	104 (100%)	0	100	100
28	O	105/107 (98%)	104 (99%)	1 (1%)	73	82
29	P	86/90 (96%)	85 (99%)	1 (1%)	67	79
30	Q	90/99 (91%)	90 (100%)	0	100	100
31	R	101/104 (97%)	101 (100%)	0	100	100
32	S	83/84 (99%)	83 (100%)	0	100	100
33	T	76/77 (99%)	76 (100%)	0	100	100
34	U	65/65 (100%)	64 (98%)	1 (2%)	60	75
35	V	74/78 (95%)	73 (99%)	1 (1%)	62	76
36	W	72/79 (91%)	72 (100%)	0	100	100
37	X	94/96 (98%)	94 (100%)	0	100	100
38	Y	109/110 (99%)	108 (99%)	1 (1%)	75	83
39	Z	26/85 (31%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	b	58/63 (92%)	58 (100%)	0	100	100
42	c	67/68 (98%)	67 (100%)	0	100	100
44	e	54/55 (98%)	54 (100%)	0	100	100
45	f	48/49 (98%)	48 (100%)	0	100	100
46	g	59/62 (95%)	59 (100%)	0	100	100
47	h	216/218 (99%)	216 (100%)	0	100	100
48	i	47/48 (98%)	47 (100%)	0	100	100
49	j	164/164 (100%)	164 (100%)	0	100	100
50	k	47/49 (96%)	47 (100%)	0	100	100
51	l	165/165 (100%)	164 (99%)	1 (1%)	84	88
52	m	38/38 (100%)	38 (100%)	0	100	100
53	n	148/150 (99%)	148 (100%)	0	100	100
54	o	51/52 (98%)	51 (100%)	0	100	100
55	p	136/138 (99%)	136 (100%)	0	100	100
56	q	34/34 (100%)	34 (100%)	0	100	100
57	r	114/114 (100%)	114 (100%)	0	100	100
58	s	116/116 (100%)	115 (99%)	1 (1%)	75	83
59	t	104/104 (100%)	103 (99%)	1 (1%)	73	82
60	u	103/103 (100%)	103 (100%)	0	100	100
61	v	109/109 (100%)	109 (100%)	0	100	100
62	w	99/103 (96%)	98 (99%)	1 (1%)	73	82
63	x	86/87 (99%)	86 (100%)	0	100	100
64	y	99/100 (99%)	97 (98%)	2 (2%)	50	68
65	z	89/90 (99%)	88 (99%)	1 (1%)	70	80
All	All	7890/8723 (90%)	7850 (100%)	40 (0%)	85	89

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	O	12	ARG
59	t	108	ARG
29	P	5	ARG
38	Y	44	LYS
64	y	6	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
51	l	92	HIS
65	z	72	ASN
53	n	5	HIS
62	w	18	GLN
14	AE	777	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	75/76 (98%)	29 (38%)	8 (10%)
10	B	75/76 (98%)	29 (38%)	8 (10%)
17	D	1514/1542 (98%)	290 (19%)	20 (1%)
40	a	2859/2904 (98%)	508 (17%)	0
43	d	119/120 (99%)	15 (12%)	0
8	7	37/38 (97%)	28 (75%)	5 (13%)
All	All	4679/4756 (98%)	899 (19%)	41 (0%)

5 of 899 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	3	G
8	7	4	U
8	7	5	U
8	7	7	U
8	7	8	U

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
17	D	517	G
17	D	1213	A
17	D	991	U
17	D	1196	A
17	D	1447	A

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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](#)

There are no chain breaks in this entry.

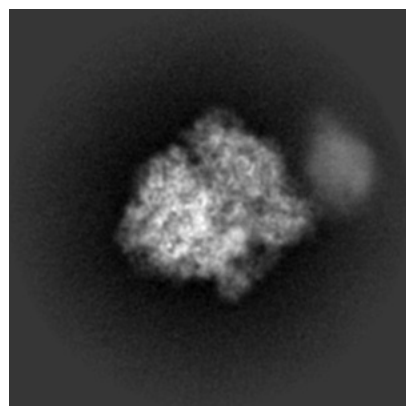
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42454. These allow visual inspection of the internal detail of the map and identification of artifacts.

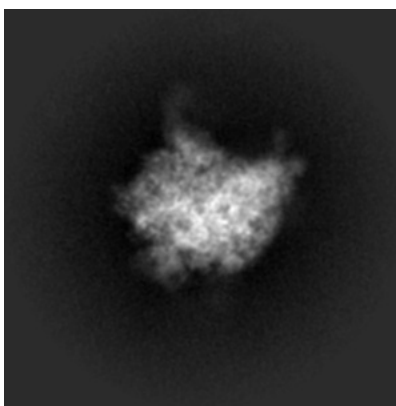
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

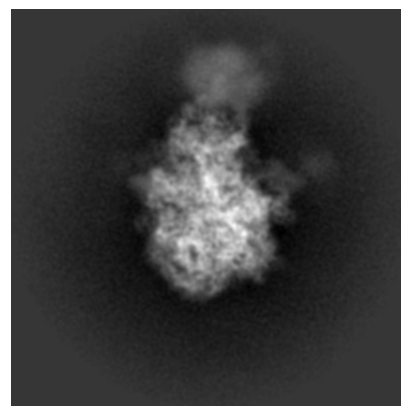
6.1.1 Primary map



X

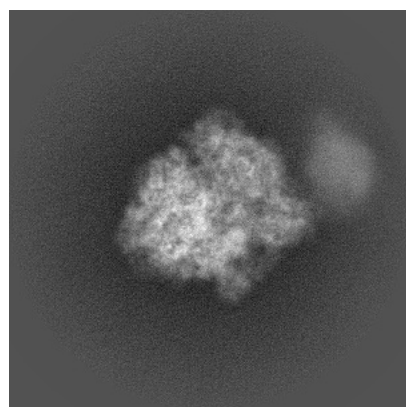


Y

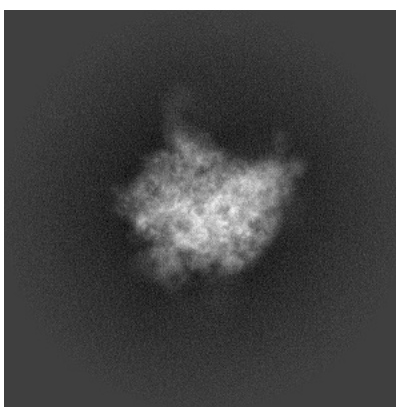


Z

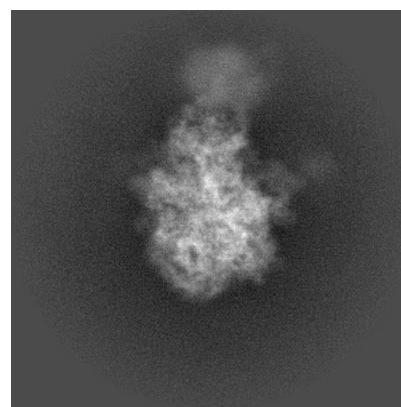
6.1.2 Raw map



X



Y

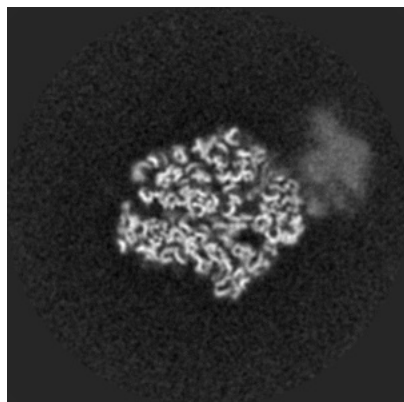


Z

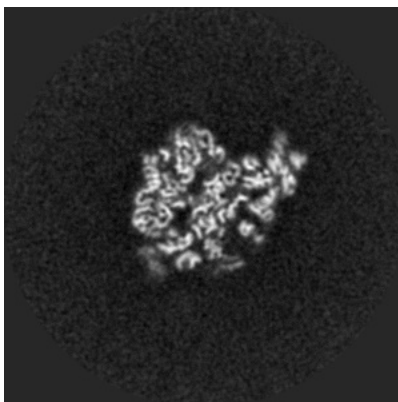
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

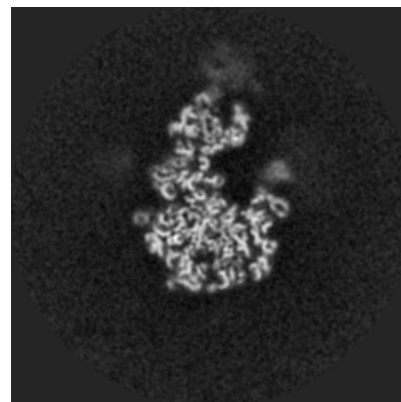
6.2.1 Primary map



X Index: 256

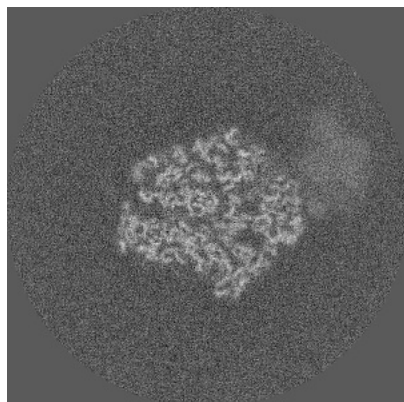


Y Index: 256

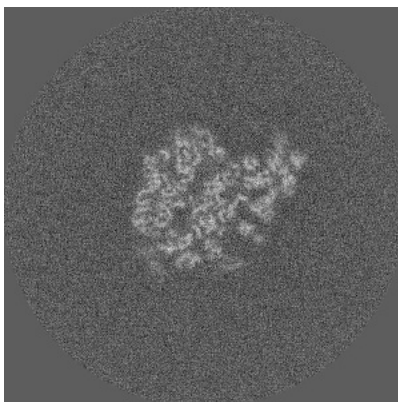


Z Index: 256

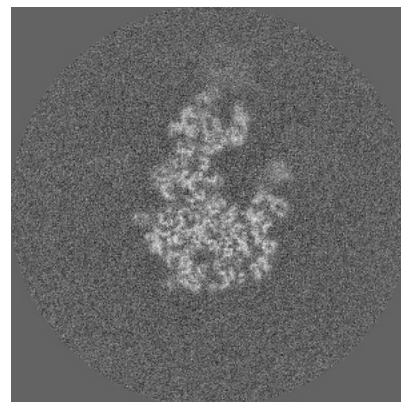
6.2.2 Raw map



X Index: 256



Y Index: 256

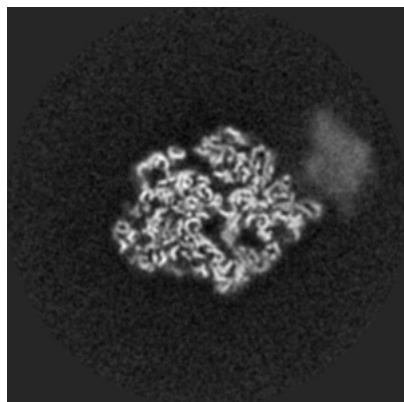


Z Index: 256

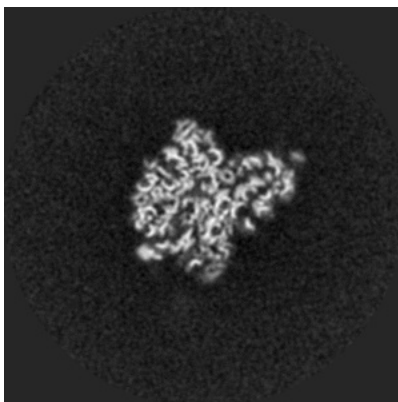
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

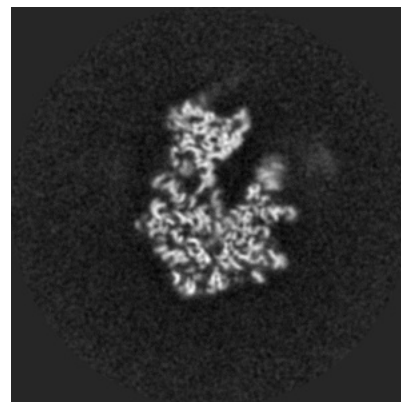
6.3.1 Primary map



X Index: 248

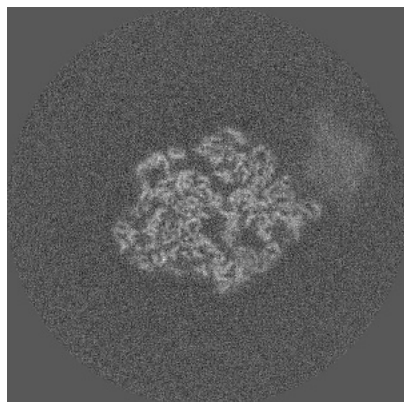


Y Index: 249

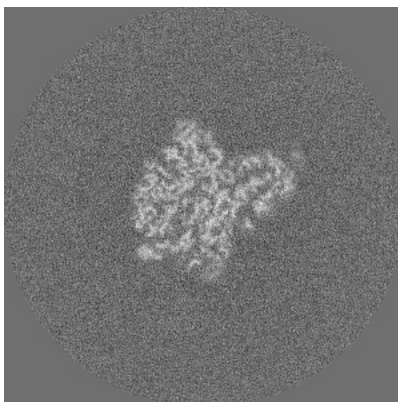


Z Index: 241

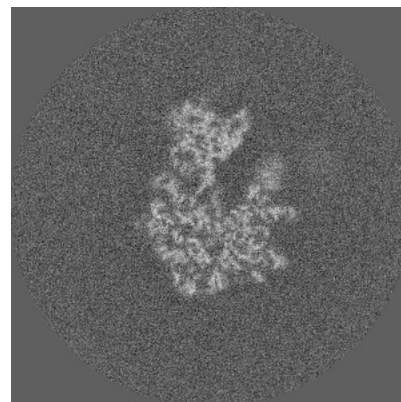
6.3.2 Raw map



X Index: 248



Y Index: 249

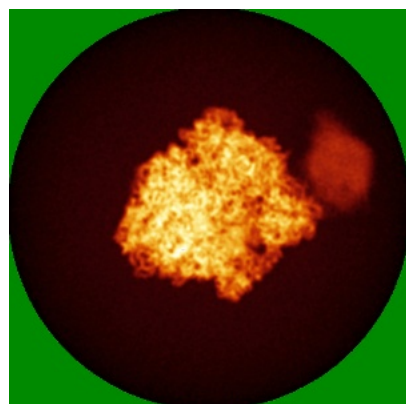


Z Index: 241

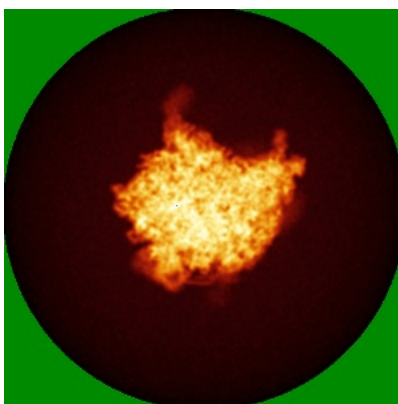
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X

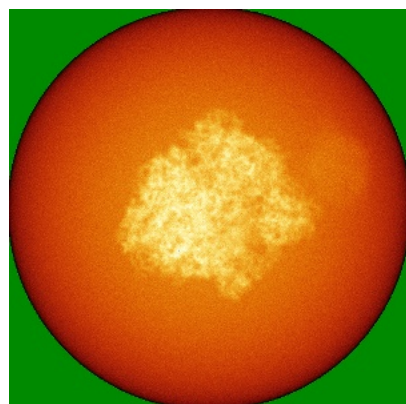


Y

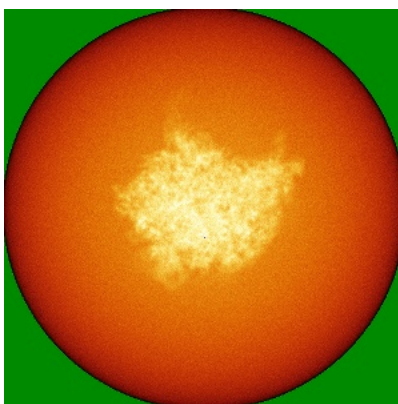


Z

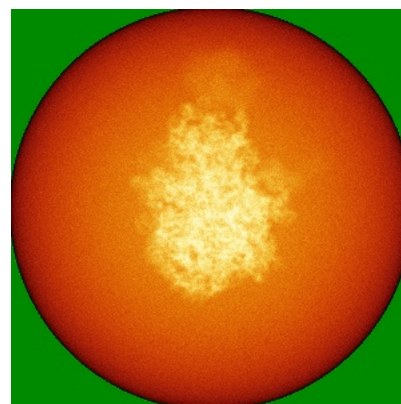
6.4.2 Raw map



X



Y

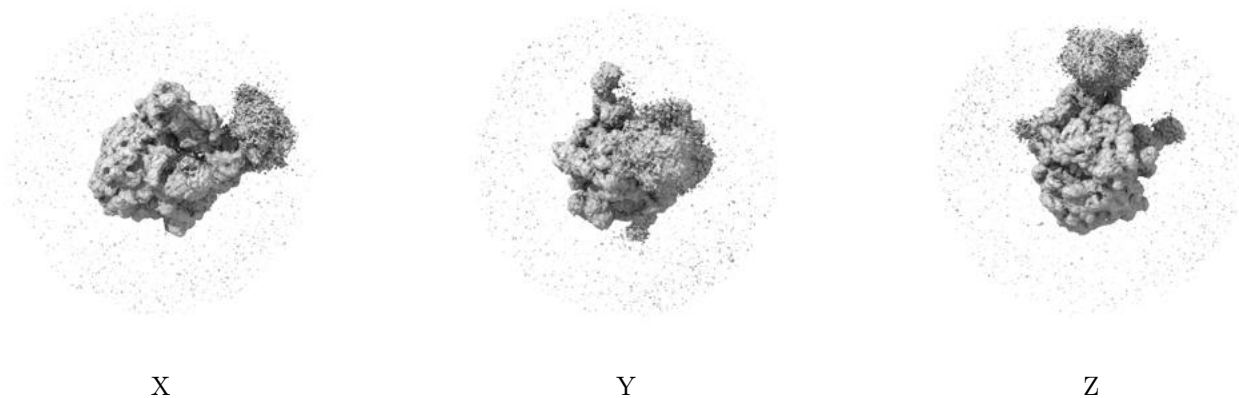


Z

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

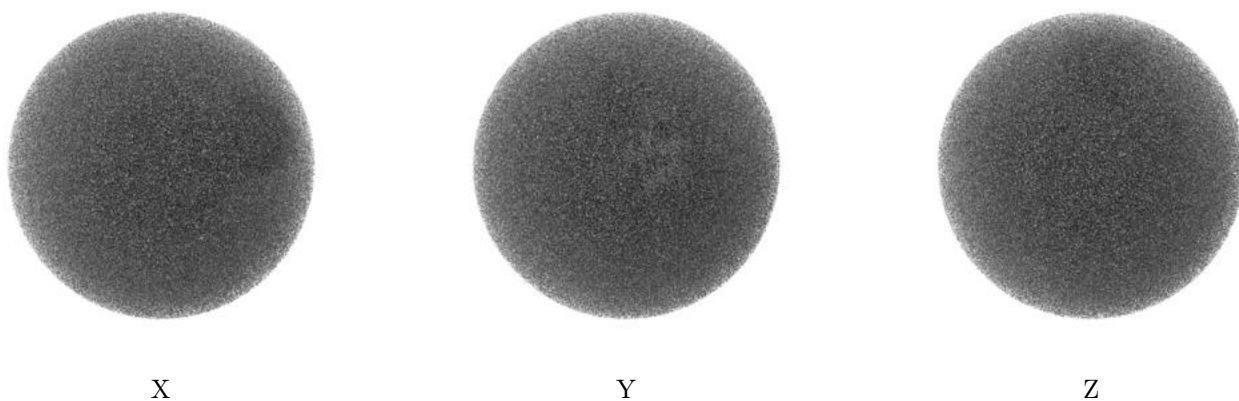
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

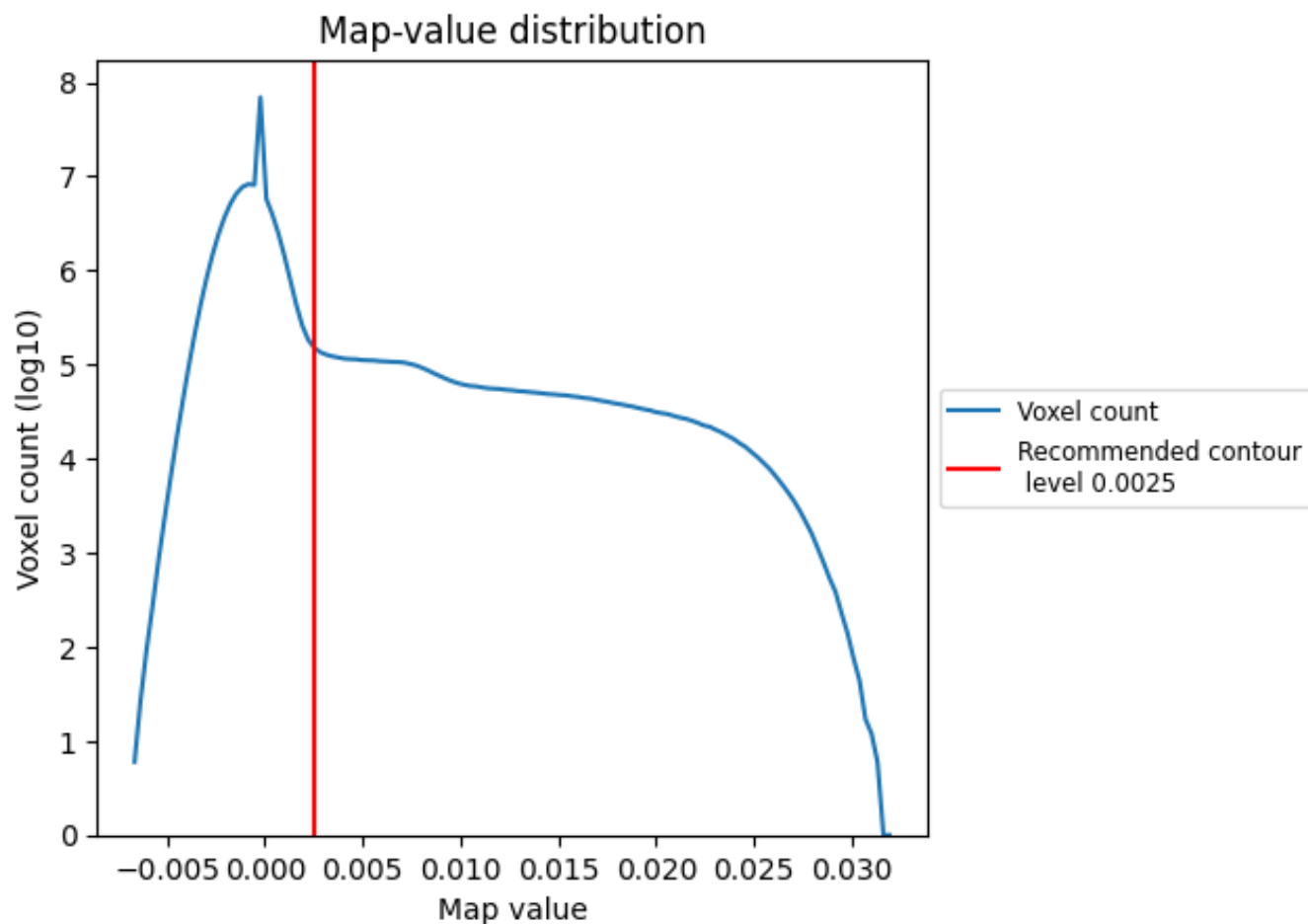
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

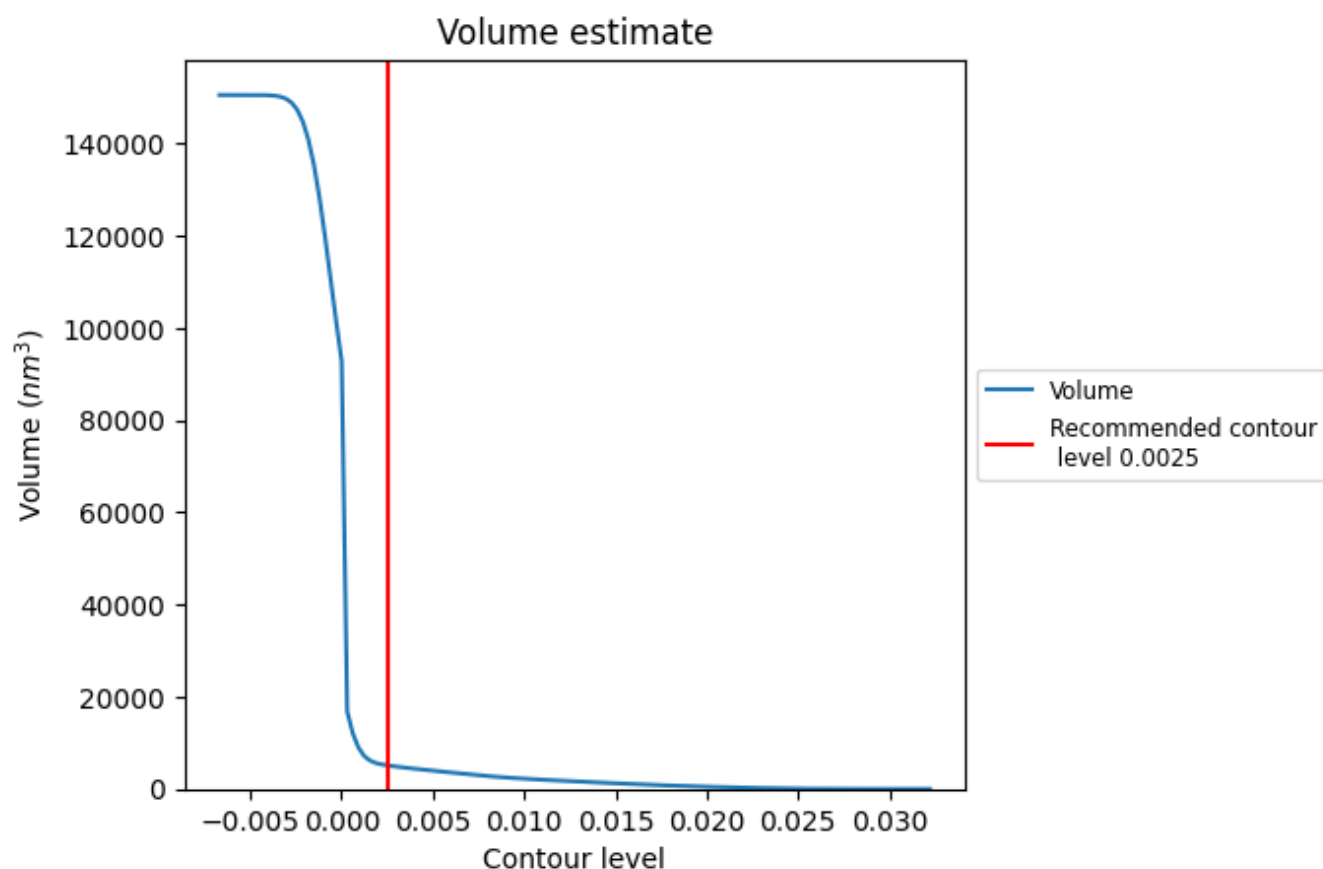
This section contains the results of statistical analysis of the map.

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.

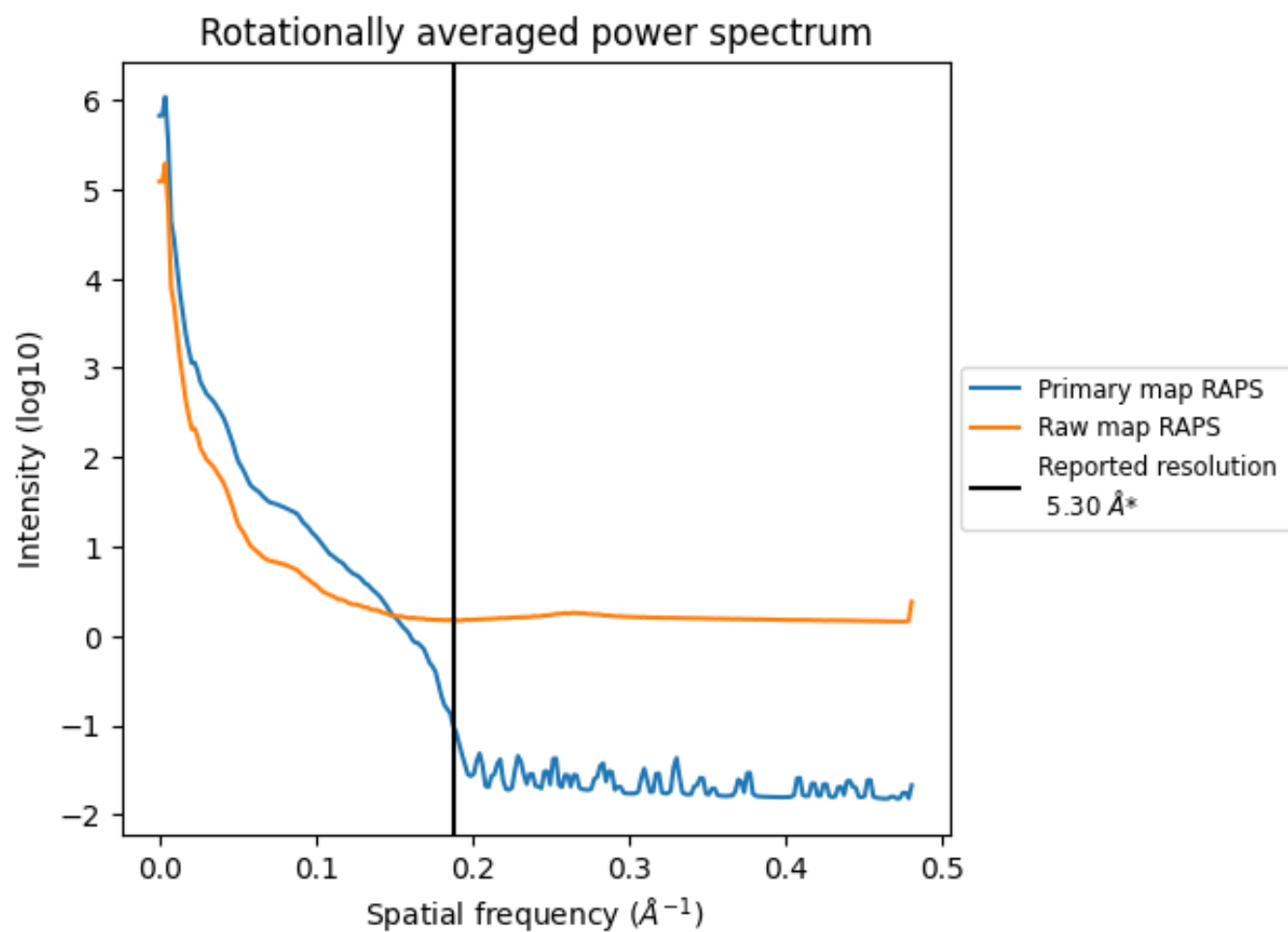
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5120 nm^3 ; this corresponds to an approximate mass of 4625 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 ⓘ

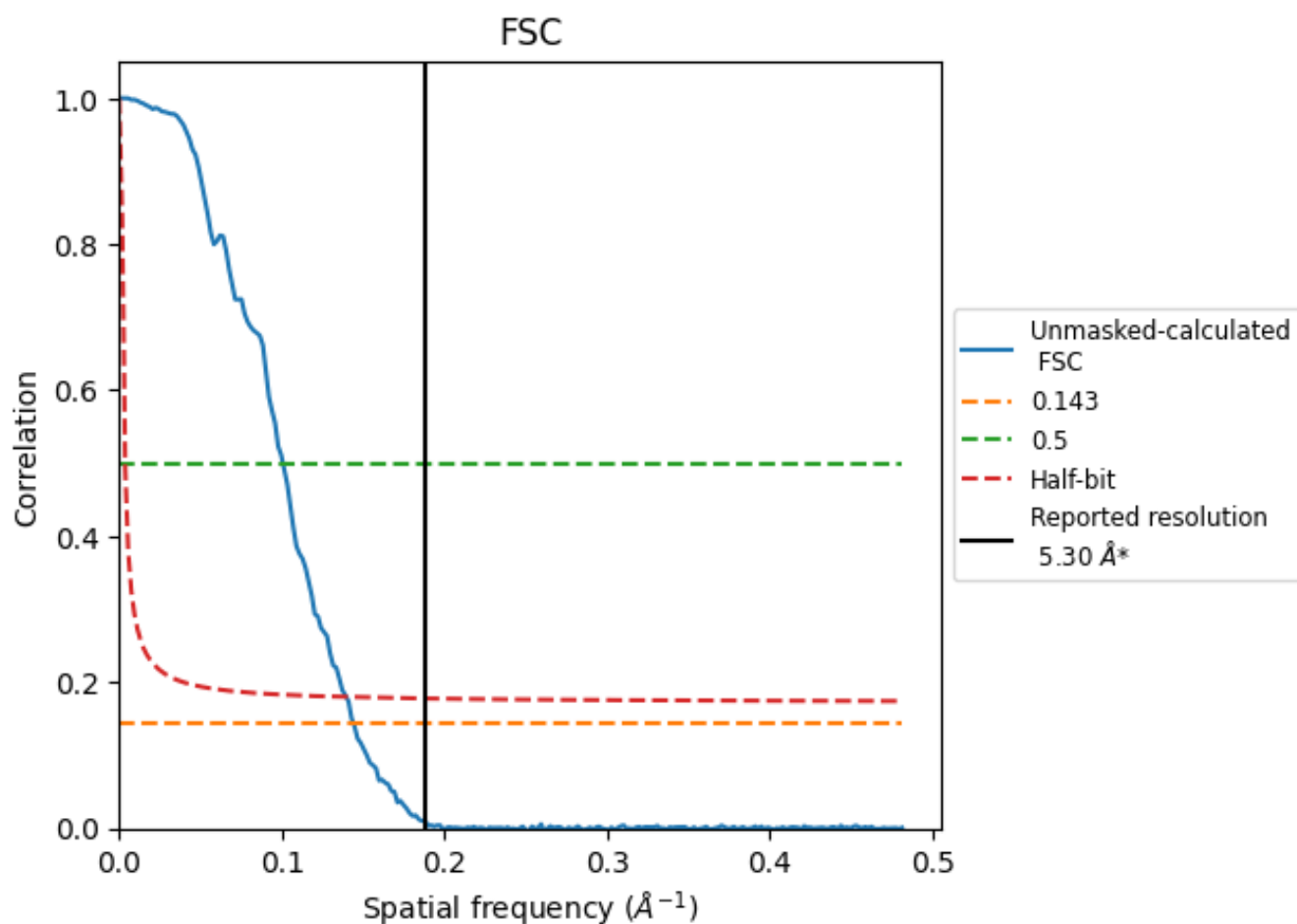


*Reported resolution corresponds to spatial frequency of 0.189 \AA^{-1}

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 0.189 Å⁻¹

8.2 Resolution estimates [i](#)

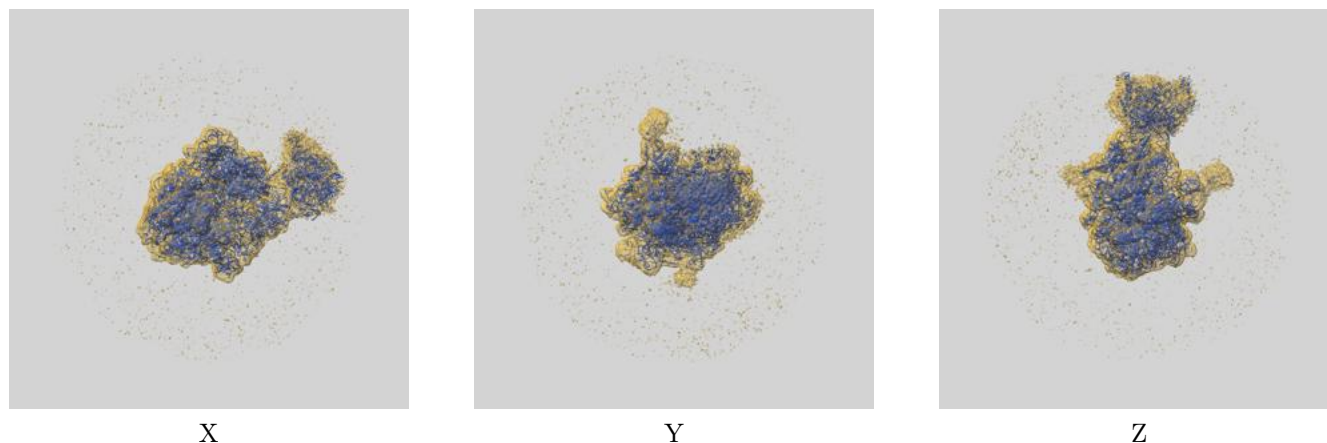
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.94	9.93	7.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.94 differs from the reported value 5.3 by more than 10 %

9 Map-model fit [i](#)

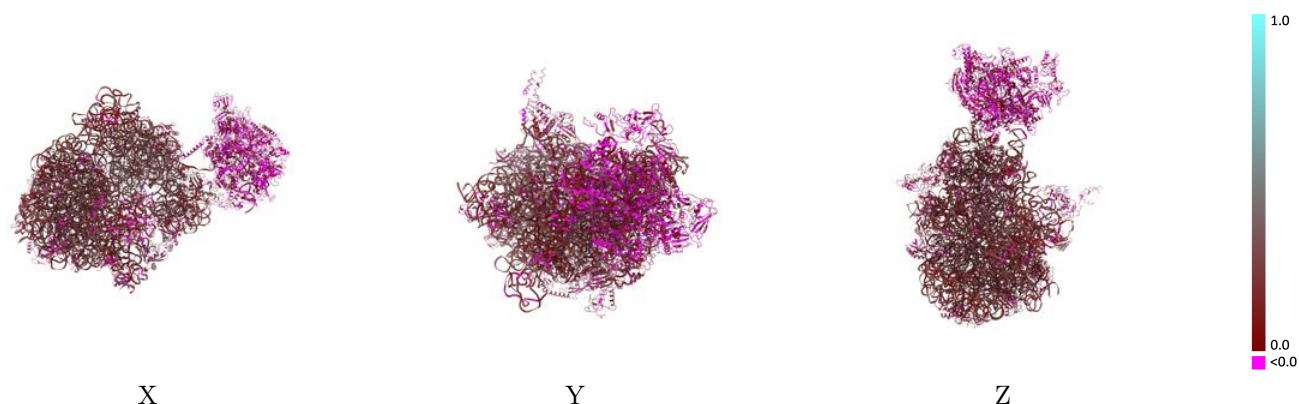
This section contains information regarding the fit between EMDB map EMD-42454 and PDB model 8UPR. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



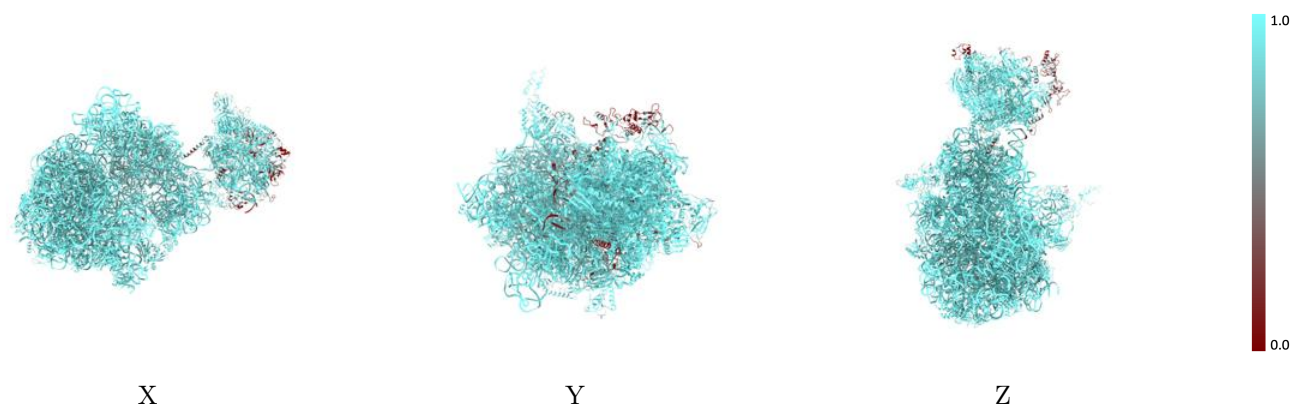
The images above show the 3D surface view of the map at the recommended contour level 0.0025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



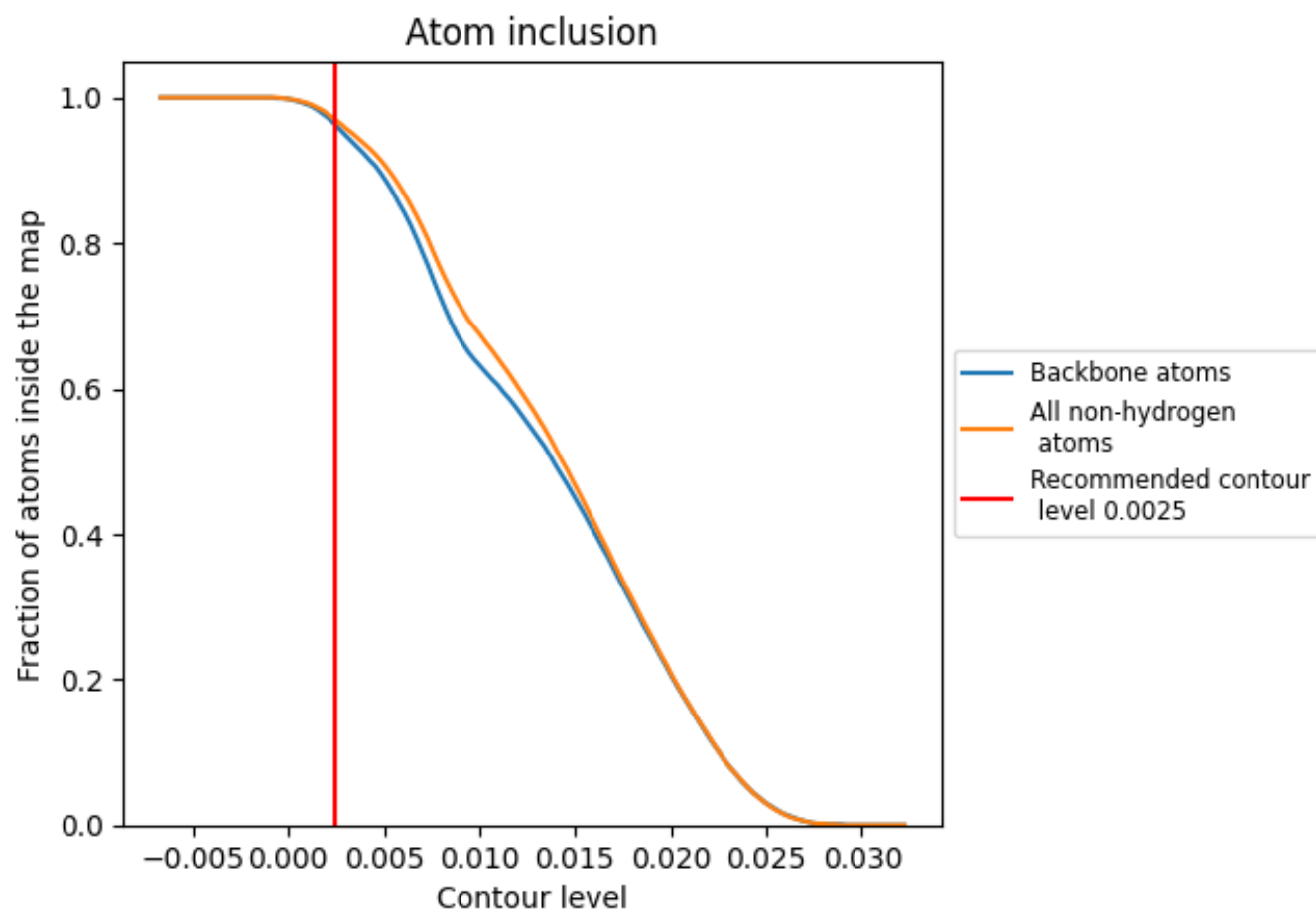
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0025).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 97% 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 (0.0025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9690	 0.1640
0	 0.9940	 0.1470
1	 0.9960	 0.1770
2	 0.9840	 0.1390
3	 0.9960	 0.1320
4	 0.9950	 0.1550
5	 0.8440	 0.0630
6	 0.8950	 0.0530
7	 0.9820	 0.0800
9	 0.9740	 0.0970
A	 1.0000	 0.1790
AA	 0.8530	 0.0180
AB	 0.7320	 0.0520
AC	 0.9780	 0.0280
AD	 0.9450	 0.0160
AE	 0.8920	 0.0320
AF	 0.7900	 0.0190
B	 0.9800	 0.1100
C	 0.9980	 0.1530
D	 0.9980	 0.2210
E	 0.9990	 0.1540
F	 0.9820	 0.1740
G	 0.9850	 0.1580
H	 0.9140	 0.0630
I	 0.9920	 0.1870
J	 0.9980	 0.1730
K	 0.9970	 0.2020
L	 1.0000	 0.1540
M	 0.9930	 0.1490
N	 0.9870	 0.1750
O	 0.9910	 0.1280
P	 1.0000	 0.1580
Q	 0.9970	 0.1510
R	 0.9980	 0.2050
S	 0.9970	 0.1650



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Chain	Atom inclusion	Q-score
T	 1.0000	 0.1490
U	 0.9980	 0.1610
V	 0.9910	 0.1670
W	 0.9750	 0.1230
X	 0.9930	 0.1390
Y	 0.9010	 0.0550
Z	 0.9690	 0.0340
a	 0.9990	 0.2090
b	 0.9970	 0.1270
c	 0.9920	 0.1580
d	 1.0000	 0.1810
e	 0.9920	 0.1320
f	 0.9930	 0.1740
g	 0.9940	 0.1140
h	 0.9930	 0.1500
i	 0.9910	 0.1870
j	 0.9960	 0.1550
k	 1.0000	 0.1360
l	 0.9890	 0.1340
m	 0.9940	 0.1680
n	 0.9880	 0.1240
o	 1.0000	 0.1240
p	 0.9980	 0.1480
q	 0.9970	 0.1410
r	 0.9660	 0.1120
s	 0.9960	 0.1710
t	 0.9900	 0.1740
u	 0.9940	 0.1280
v	 0.9920	 0.1800
w	 0.9950	 0.1510
x	 0.9820	 0.0900
y	 0.9940	 0.1690
z	 0.9970	 0.1390