wwPDB EM Validation Summary Report

May 27, 2024 – 08:03 AM EDT

PDB ID	:	7SSO
EMDB ID	:	EMD-25411
Title	:	Pre translocation 70S ribosome with A/A and P/E tRNA (Structure II-A)
Authors	:	Carbone, C.E.; Korostelev, A.A.
Deposited on	:	2021-11-11
Resolution	:	3.20 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:

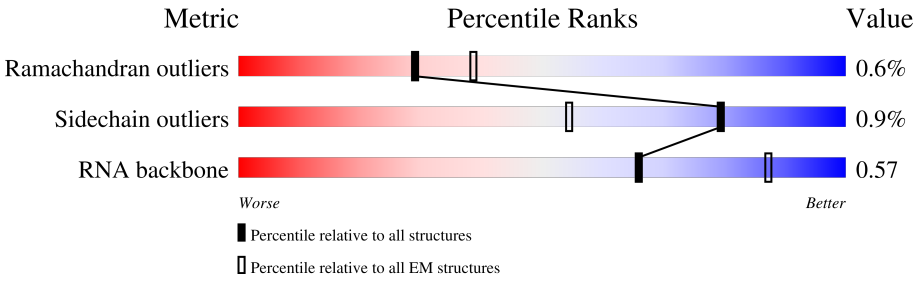
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3	1539	88% 12%
2	1	2903	84% 15%
3	2	120	86% 13%
4	5	77	77% 22%
5	b	271	99%
6	c	209	100%
7	d	201	5% 99%
8	e	177	97%

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Mol	Chain	Length	Quality of chain
9	f	176	98%
10	g	149	66% 96%
11	a	223	9% 59% 40%
12	h	131	95% 91% 8%
13	i	141	63% 97%
14	j	142	99%
15	k	122	98%
16	l	143	100%
17	m	136	98%
18	n	120	99%
19	o	116	100%
20	p	114	99%
21	q	117	99%
22	r	103	100%
23	s	110	99%
24	t	93	99%
25	u	102	100%
26	v	94	100%
27	w	75	100%
28	x	77	100%
29	y	63	5% 100%
30	z	58	98%
31	A	66	6% 67% 32%
32	B	56	100%
33	C	50	98%

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Mol	Chain	Length	Quality of chain
34	D	46	100%
35	E	64	97%
36	F	38	97%
37	4	35	6% 43% 11% 46%
38	6	77	82% 18%
39	G	225	12% 99%
40	H	206	99%
41	I	205	7% 99%
42	J	157	99%
43	K	100	98%
44	L	151	98%
45	M	129	100%
46	N	127	6% 95% 5%
47	O	98	17% 99%
48	P	116	97%
49	Q	123	98%
50	R	114	8% 98%
51	S	100	99%
52	T	88	98%
53	U	82	99%
54	V	80	96%
55	W	65	100%
56	X	79	8% 99%
57	Y	85	100%
58	Z	65	92% 6%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 148980 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	3	1539	33012	14725	6052	10697	1538	0	0

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1	2903	62317	27801	11468	20146	2902	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 802133627

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	2	120	2568	1145	471	833	119	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	insertion	GB 1266961702

- Molecule 4 is a RNA chain called tRNA Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	5	77	1647	733	295	542	77	0	0

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	c	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	d	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	e	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	f	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	g	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 11 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	134	Total	C	N	O	S	0	0
			1027	645	186	194	2		

- Molecule 12 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	h	131	Total	C	N	O	S	0	0
			989	625	175	184	5		

- Molecule 13 is a protein called 50S ribosomal protein L11.

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

- Molecule 14 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	j	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	k	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	l	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 17 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	m	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	n	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 19 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	o	116	Total 892	C 552	N 178	O 162	0	0

- Molecule 20 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	p	114	Total 917	C 574	N 179	O 163	S 1	0	0

- Molecule 21 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	q	117	Total 947	C 604	N 192	O 151	0	0

- Molecule 22 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	103	Total 816	C 516	N 153	O 145	S 2	0	0

- Molecule 23 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	s	110	Total 857	C 532	N 166	O 156	S 3	0	0

- Molecule 24 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	t	93	Total 739	C 466	N 139	O 132	S 2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	u	102	Total 780	C 492	N 146	O 142	0	0

- Molecule 26 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	v	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	w	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 28 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	x	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 30 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A	45	Total	C	N	O	S	0	0
			351	219	61	65	6		

- Molecule 32 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 33 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	C	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 34 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	D	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 35 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	E	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 36 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	F	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4	19	Total	C	N	O	P	0	0
			413	186	85	124	18		

- Molecule 38 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 39 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	G	225	Total	C	N	O	S	0	0
			1757	1111	315	323	8		

- Molecule 40 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	H	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 41 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	I	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 42 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	J	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 43 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	K	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 44 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 45 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	M	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 46 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	N	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 47 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	O	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 48 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	P	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 49 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Q	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	R	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 51 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 52 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	T	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 53 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	U	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 54 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	V	80	Total 649	C 411	N 121	O 114	S 3	0	0

- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	W	65	Total 536	C 339	N 100	O 96	S 1	0	0

- Molecule 56 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	X	79	Total 638	C 408	N 120	O 108	S 2	0	0

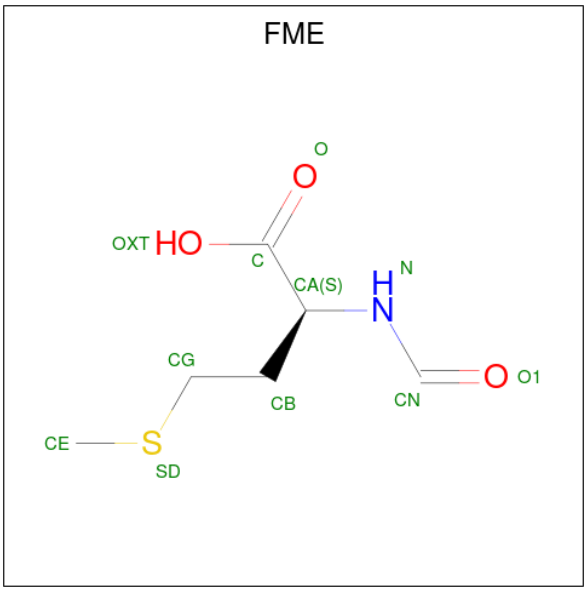
- Molecule 57 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Y	85	Total 665	C 411	N 137	O 114	S 3	0	0

- Molecule 58 is a protein called 30S ribosomal protein S21.

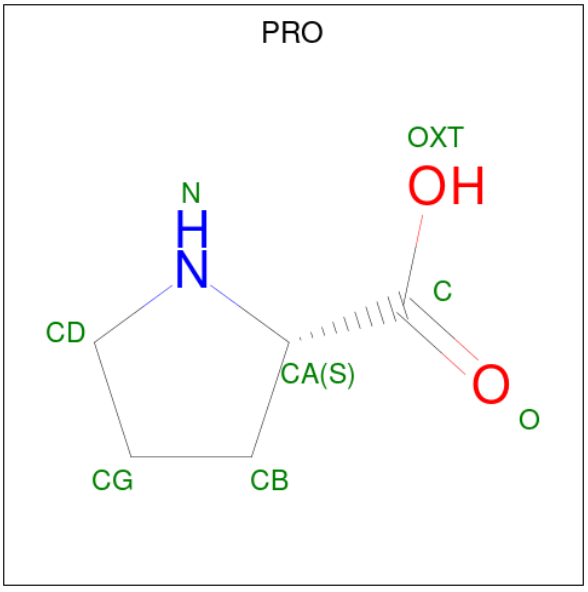
Mol	Chain	Residues	Atoms					AltConf	Trace
58	Z	65	Total 545	C 335	N 117	O 92	S 1	0	0

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
59	1	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 60 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



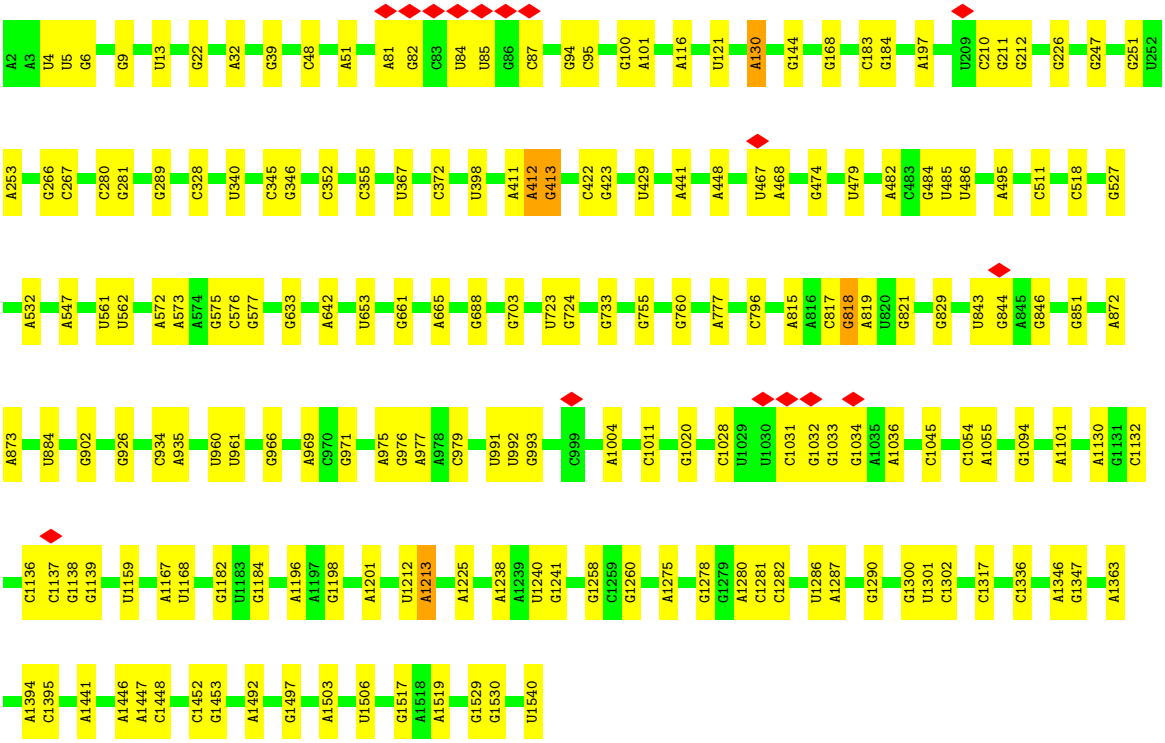
Mol	Chain	Residues	Atoms				AltConf
60	5	1	Total	C	N	O	0
			7	5	1	1	

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.

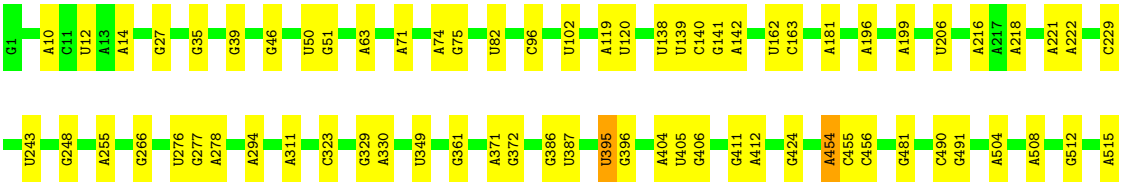
- Molecule 1: 16S rRNA

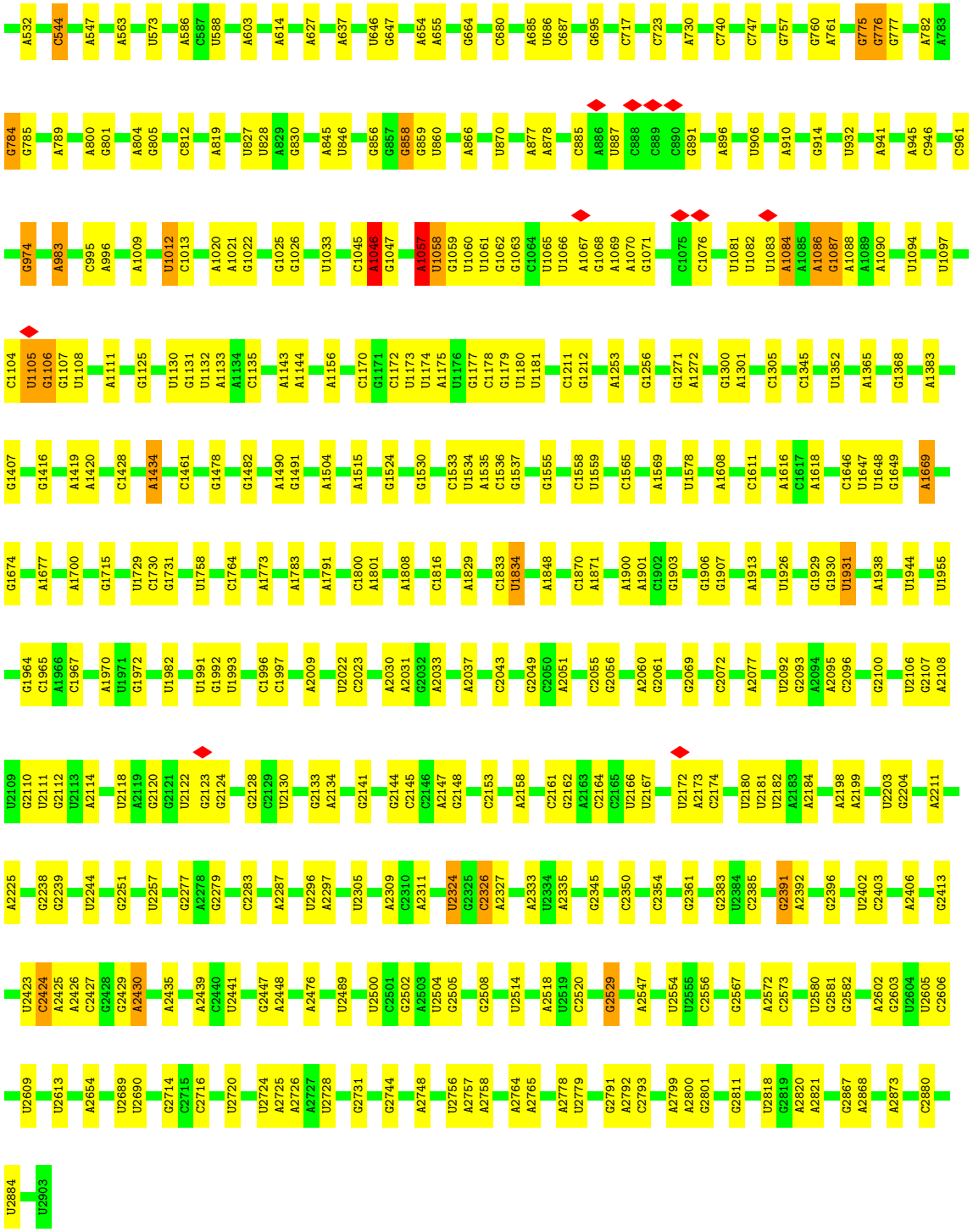
Chain 3:



- Molecule 2: 23S rRNA

Chain 1:





• Molecule 3: 5S rRNA

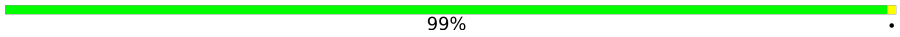
Chain 2:

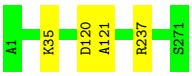
• Molecule 4: tRNA Pro

Chain 5:

• Molecule 5: 50S ribosomal protein L2

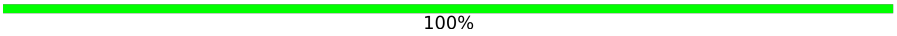
Chain b:





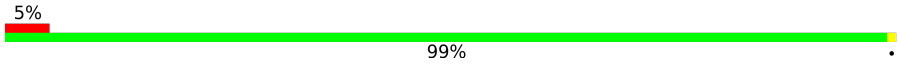
• Molecule 6: 50S ribosomal protein L3

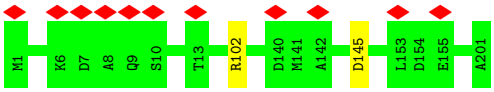
Chain c:



• Molecule 7: 50S ribosomal protein L4

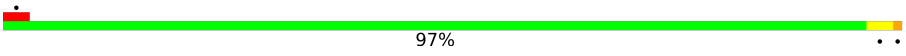
Chain d:

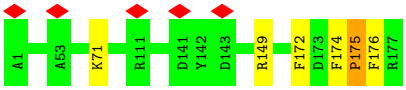




• Molecule 8: 50S ribosomal protein L5

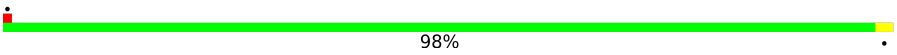
Chain e:

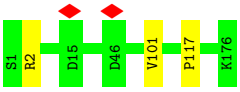




• Molecule 9: 50S ribosomal protein L6

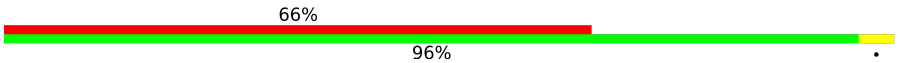
Chain f:

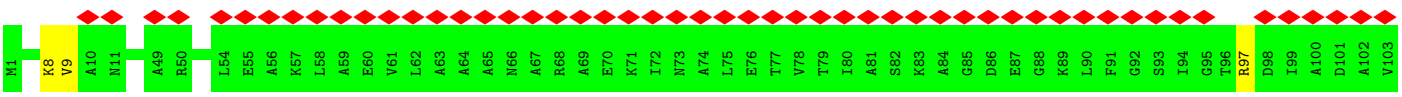


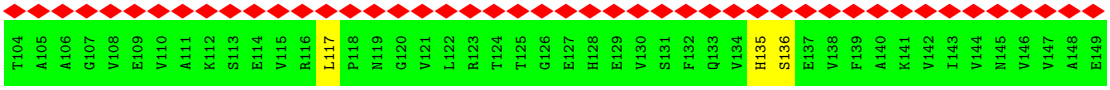


• Molecule 10: 50S ribosomal protein L9

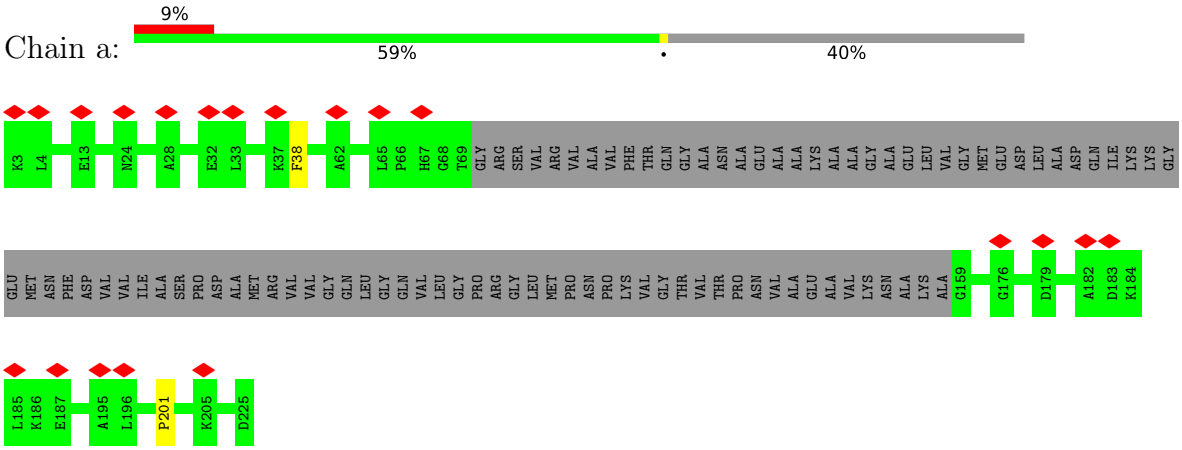
Chain g:



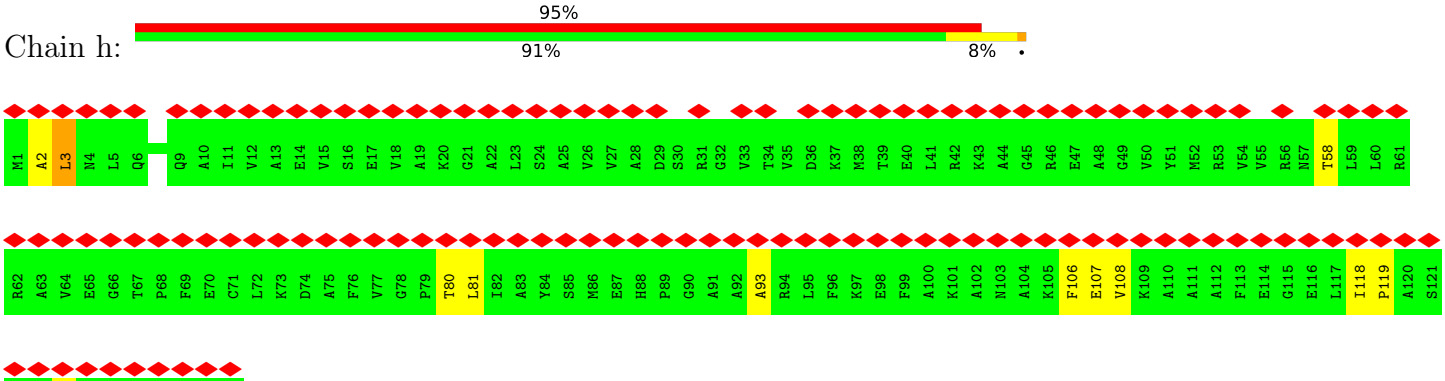




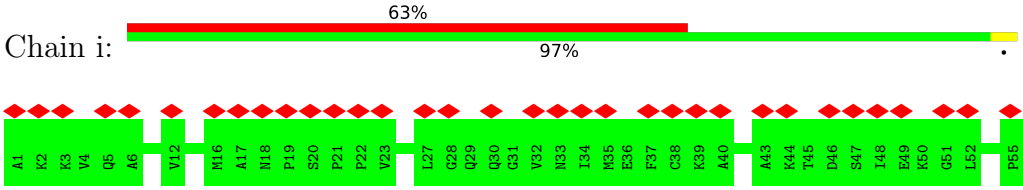
• Molecule 11: 50S ribosomal protein L1



• Molecule 12: 50S ribosomal protein L10



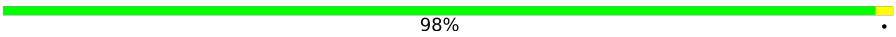
• Molecule 13: 50S ribosomal protein L11

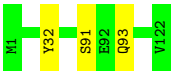


• Molecule 14: 50S ribosomal protein L13

• Molecule 15: 50S ribosomal protein L14

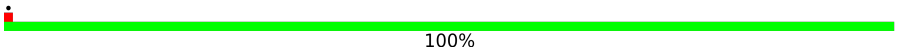
Chain k:





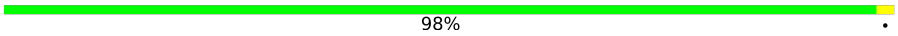
• Molecule 16: 50S ribosomal protein L15

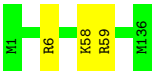
Chain l:



• Molecule 17: 50S ribosomal protein L16

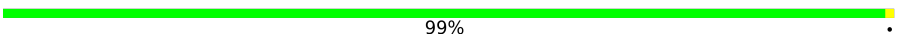
Chain m:





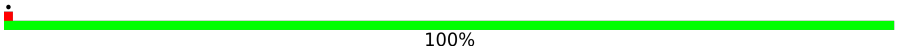
• Molecule 18: 50S ribosomal protein L17

Chain n:



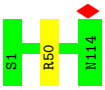
• Molecule 19: 50S ribosomal protein L18

Chain o:



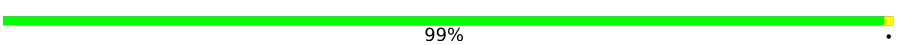
• Molecule 20: 50S ribosomal protein L19

Chain p:

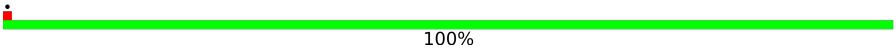


• Molecule 21: 50S ribosomal protein L20

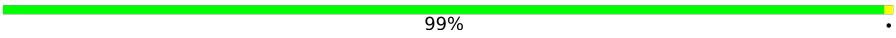
Chain q:



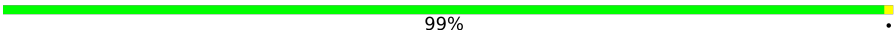
• Molecule 22: 50S ribosomal protein L21

Chain r: 

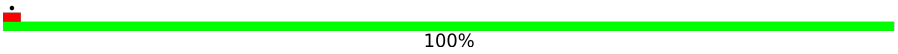
• Molecule 23: 50S ribosomal protein L22

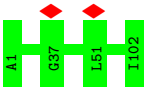
Chain s: 

• Molecule 24: 50S ribosomal protein L23

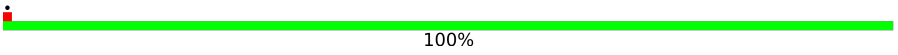
Chain t: 

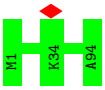
• Molecule 25: 50S ribosomal protein L24

Chain u: 

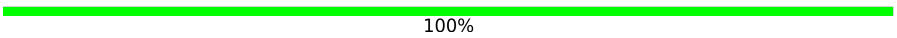


• Molecule 26: 50S ribosomal protein L25

Chain v: 

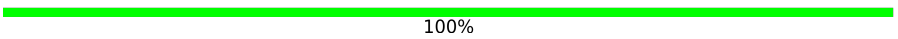


• Molecule 27: 50S ribosomal protein L27

Chain w: 

There are no outlier residues recorded for this chain.

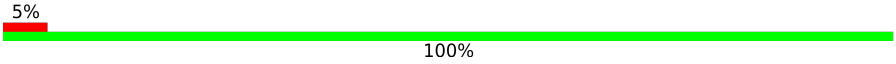
• Molecule 28: 50S ribosomal protein L28

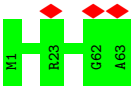
Chain x: 

There are no outlier residues recorded for this chain.

• Molecule 29: 50S ribosomal protein L29

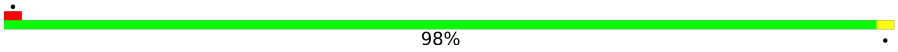
Chain y:

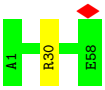




• Molecule 30: 50S ribosomal protein L30

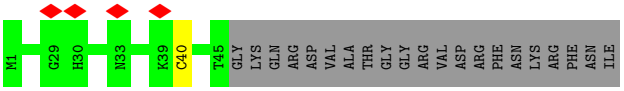
Chain z:





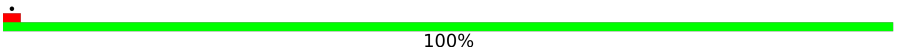
• Molecule 31: 50S ribosomal protein L31

Chain A:



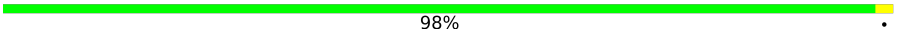
• Molecule 32: 50S ribosomal protein L32

Chain B:



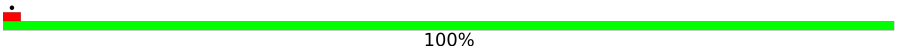
• Molecule 33: 50S ribosomal protein L33

Chain C:



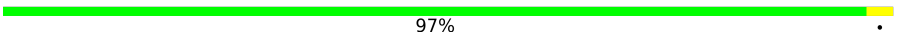
• Molecule 34: 50S ribosomal protein L34

Chain D:



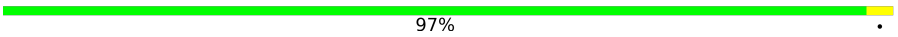
• Molecule 35: 50S ribosomal protein L35

Chain E:



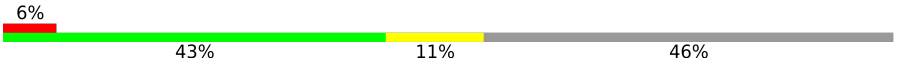
• Molecule 36: 50S ribosomal protein L36

Chain F:



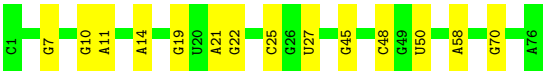
• Molecule 37: mRNA

Chain 4:



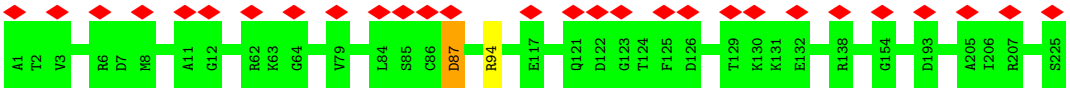
• Molecule 38: tRNA fMet

Chain 6:



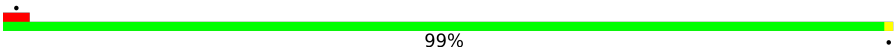
• Molecule 39: 30S ribosomal protein S2

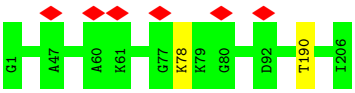
Chain G:



• Molecule 40: 30S ribosomal protein S3

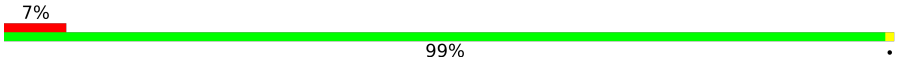
Chain H:

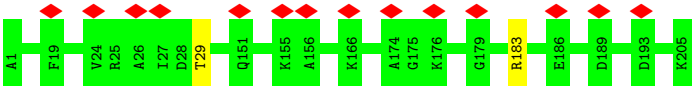




• Molecule 41: 30S ribosomal protein S4

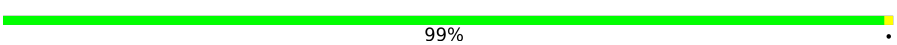
Chain I:





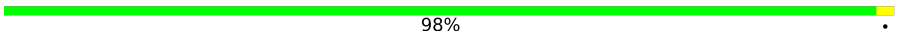
• Molecule 42: 30S ribosomal protein S5

Chain J:



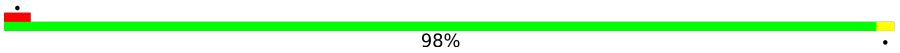
• Molecule 43: 30S ribosomal protein S6

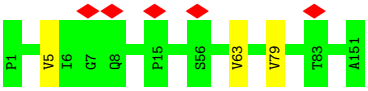
Chain K:



• Molecule 44: 30S ribosomal protein S7

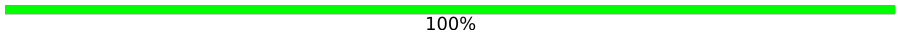
Chain L:





• Molecule 45: 30S ribosomal protein S8

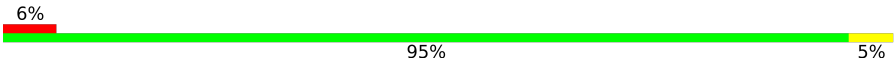
Chain M:

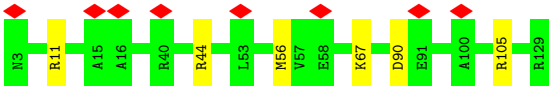


There are no outlier residues recorded for this chain.

• Molecule 46: 30S ribosomal protein S9

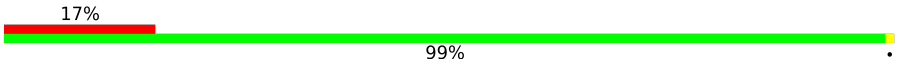
Chain N:

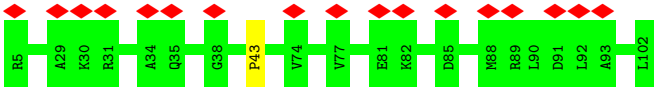




• Molecule 47: 30S ribosomal protein S10

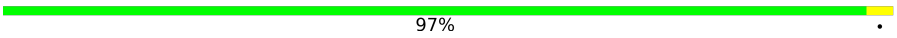
Chain O:

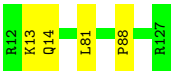




• Molecule 48: 30S ribosomal protein S11

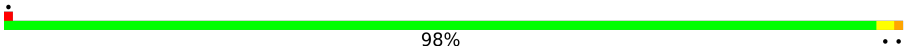
Chain P:

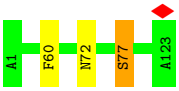




• Molecule 49: 30S ribosomal protein S12

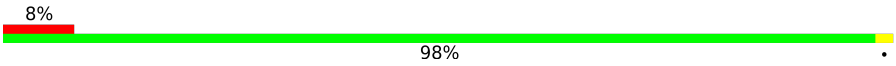
Chain Q:

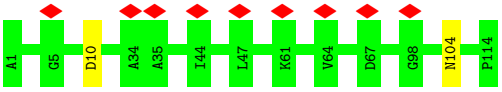




• Molecule 50: 30S ribosomal protein S13

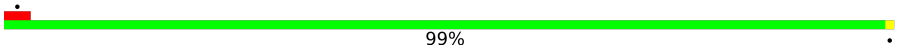
Chain R:

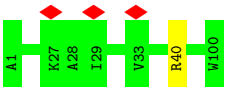




• Molecule 51: 30S ribosomal protein S14

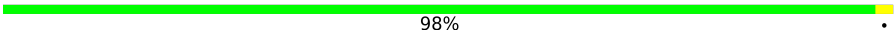
Chain S:





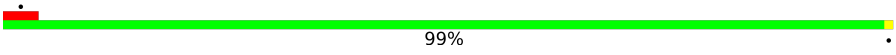
• Molecule 52: 30S ribosomal protein S15

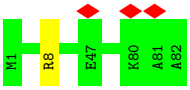
Chain T:



• Molecule 53: 30S ribosomal protein S16

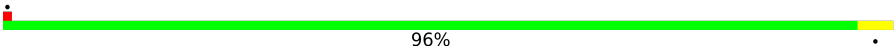
Chain U:

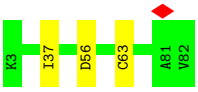




• Molecule 54: 30S ribosomal protein S17

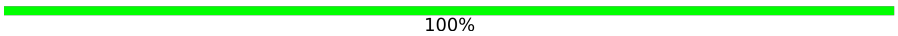
Chain V:





• Molecule 55: 30S ribosomal protein S18

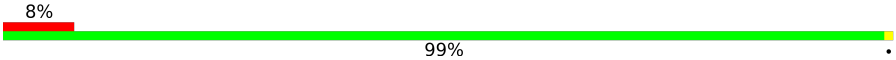
Chain W:

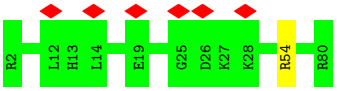


There are no outlier residues recorded for this chain.

• Molecule 56: 30S ribosomal protein S19

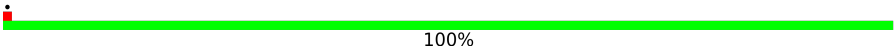
Chain X:





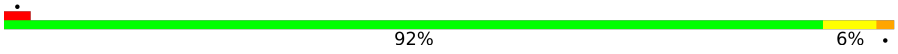
• Molecule 57: 30S ribosomal protein S20

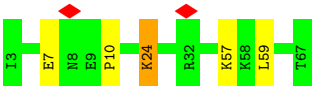
Chain Y:



• Molecule 58: 30S ribosomal protein S21

Chain Z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7257	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	19.960	Depositor
Minimum map value	-7.347	Depositor
Average map value	-0.020	Depositor
Map value standard deviation	1.142	Depositor
Recommended contour level	2.3	Depositor
Map size (Å)	381.8, 381.8, 381.8	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

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	3	0.67	0/36963	0.70	2/57662 (0.0%)
2	1	0.67	8/69796 (0.0%)	0.72	26/108888 (0.0%)
3	2	0.70	0/2872	0.70	1/4479 (0.0%)
4	5	0.79	1/1840 (0.1%)	0.77	1/2868 (0.0%)
5	b	0.55	0/2122	0.62	0/2852
6	c	0.47	0/1586	0.64	1/2134 (0.0%)
7	d	0.44	0/1571	0.59	0/2113
8	e	0.36	0/1435	0.56	0/1926
9	f	0.39	0/1343	0.59	0/1816
10	g	0.33	0/1122	0.71	2/1515 (0.1%)
11	a	0.32	0/1034	0.64	0/1387
12	h	0.32	0/1002	0.70	0/1350
13	i	0.34	0/1046	0.71	0/1410
14	j	0.49	0/1152	0.55	0/1551
15	k	0.53	0/948	0.64	0/1268
16	l	0.44	0/1054	0.66	0/1403
17	m	0.48	0/1093	0.58	0/1460
18	n	0.46	0/974	0.57	0/1301
19	o	0.36	0/902	0.58	0/1209
20	p	0.46	0/929	0.59	0/1242
21	q	0.53	0/960	0.51	0/1278
22	r	0.47	0/829	0.58	0/1107
23	s	0.43	0/864	0.57	0/1156
24	t	0.44	0/745	0.59	0/994
25	u	0.38	0/788	0.60	0/1051
26	v	0.44	0/766	0.59	0/1025
27	w	0.46	0/582	0.53	0/769
28	x	0.48	0/635	0.58	0/848
29	y	0.30	0/510	0.54	0/677
30	z	0.38	0/453	0.55	0/605
31	A	0.29	0/358	0.55	0/480
32	B	0.41	0/450	0.57	0/599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	C	0.41	0/417	0.57	0/554
34	D	0.52	0/380	0.57	0/498
35	E	0.48	0/513	0.59	0/676
36	F	0.47	0/303	0.57	0/397
37	4	0.73	0/465	0.67	0/725
38	6	0.81	0/1832	0.71	0/2855
39	G	0.35	0/1788	0.58	1/2408 (0.0%)
40	H	0.37	0/1652	0.56	0/2225
41	I	0.36	0/1665	0.60	0/2227
42	J	0.46	0/1170	0.68	0/1573
43	K	0.41	0/836	0.66	0/1128
44	L	0.42	0/1196	0.62	0/1602
45	M	0.43	0/989	0.57	0/1326
46	N	0.36	0/1034	0.62	0/1375
47	O	0.31	0/797	0.64	0/1077
48	P	0.43	0/886	0.62	0/1195
49	Q	0.46	0/969	0.69	0/1300
50	R	0.32	0/893	0.61	0/1193
51	S	0.36	0/817	0.54	0/1088
52	T	0.37	0/722	0.57	0/964
53	U	0.38	0/659	0.56	0/884
54	V	0.38	0/658	0.61	1/881 (0.1%)
55	W	0.43	0/545	0.53	0/731
56	X	0.37	0/653	0.59	0/877
57	Y	0.34	0/671	0.54	0/888
58	Z	0.40	0/551	0.81	1/728 (0.1%)
All	All	0.61	9/161785 (0.0%)	0.69	36/241798 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	3	0	6
2	1	0	43
3	2	0	1
4	5	0	2
5	b	0	1
8	e	0	3
10	g	0	2
11	a	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	i	0	1
15	k	0	2
17	m	0	2
35	E	0	1
36	F	0	1
42	J	0	1
43	K	0	1
44	L	0	1
46	N	0	1
47	O	0	1
48	P	0	1
49	Q	0	1
58	Z	0	1
All	All	0	74

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	870	U	O3'-P	10.84	1.74	1.61
2	1	870	U	C3'-O3'	9.59	1.55	1.42
2	1	906	U	O3'-P	7.27	1.69	1.61
2	1	1057	A	C3'-O3'	5.89	1.50	1.42
2	1	1105	U	O3'-P	-5.82	1.54	1.61

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	974	G	N9-C1'-C2'	7.89	124.26	114.00
10	g	117	LEU	CA-CB-CG	7.46	132.45	115.30
2	1	1058	U	O5'-P-OP1	-7.15	99.26	105.70
2	1	1057	A	OP1-P-O3'	7.04	120.69	105.20
2	1	1105	U	C5'-C4'-O4'	6.90	117.38	109.10

There are no chirality outliers.

5 of 74 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3	1167	A	Sidechain
1	3	130	A	Sidechain
1	3	760	G	Sidechain
1	3	818	G	Sidechain

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Mol	Chain	Res	Type	Group
1	3	884	U	Sidechain

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
5	b	269/271 (99%)	235 (87%)	33 (12%)	1 (0%)	34 69
6	c	207/209 (99%)	188 (91%)	19 (9%)	0	100 100
7	d	199/201 (99%)	184 (92%)	15 (8%)	0	100 100
8	e	175/177 (99%)	158 (90%)	15 (9%)	2 (1%)	14 51
9	f	174/176 (99%)	156 (90%)	17 (10%)	1 (1%)	25 64
10	g	147/149 (99%)	121 (82%)	24 (16%)	2 (1%)	11 46
11	a	130/223 (58%)	109 (84%)	20 (15%)	1 (1%)	19 58
12	h	129/131 (98%)	92 (71%)	27 (21%)	10 (8%)	1 6
13	i	139/141 (99%)	116 (84%)	22 (16%)	1 (1%)	22 61
14	j	140/142 (99%)	126 (90%)	13 (9%)	1 (1%)	22 61
15	k	120/122 (98%)	99 (82%)	21 (18%)	0	100 100
16	l	141/143 (99%)	120 (85%)	21 (15%)	0	100 100
17	m	134/136 (98%)	120 (90%)	14 (10%)	0	100 100
18	n	118/120 (98%)	104 (88%)	14 (12%)	0	100 100
19	o	114/116 (98%)	105 (92%)	9 (8%)	0	100 100
20	p	112/114 (98%)	104 (93%)	8 (7%)	0	100 100
21	q	115/117 (98%)	111 (96%)	4 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	r	101/103 (98%)	85 (84%)	16 (16%)	0	100	100
23	s	108/110 (98%)	104 (96%)	3 (3%)	1 (1%)	17	56
24	t	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
25	u	100/102 (98%)	88 (88%)	12 (12%)	0	100	100
26	v	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
27	w	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
28	x	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
29	y	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
30	z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
31	A	43/66 (65%)	34 (79%)	9 (21%)	0	100	100
32	B	54/56 (96%)	49 (91%)	5 (9%)	0	100	100
33	C	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
34	D	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
35	E	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	9	43
36	F	36/38 (95%)	27 (75%)	9 (25%)	0	100	100
39	G	223/225 (99%)	207 (93%)	16 (7%)	0	100	100
40	H	204/206 (99%)	185 (91%)	19 (9%)	0	100	100
41	I	203/205 (99%)	174 (86%)	28 (14%)	1 (0%)	29	67
42	J	155/157 (99%)	133 (86%)	21 (14%)	1 (1%)	25	64
43	K	98/100 (98%)	71 (72%)	26 (26%)	1 (1%)	15	54
44	L	149/151 (99%)	134 (90%)	14 (9%)	1 (1%)	22	61
45	M	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
46	N	125/127 (98%)	108 (86%)	16 (13%)	1 (1%)	19	58
47	O	96/98 (98%)	81 (84%)	15 (16%)	0	100	100
48	P	114/116 (98%)	97 (85%)	15 (13%)	2 (2%)	8	41
49	Q	121/123 (98%)	100 (83%)	20 (16%)	1 (1%)	19	58
50	R	112/114 (98%)	98 (88%)	13 (12%)	1 (1%)	17	56
51	S	98/100 (98%)	84 (86%)	14 (14%)	0	100	100
52	T	86/88 (98%)	77 (90%)	8 (9%)	1 (1%)	13	49
53	U	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
54	V	78/80 (98%)	65 (83%)	13 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
55	W	63/65 (97%)	61 (97%)	2 (3%)	0	100 100
56	X	77/79 (98%)	72 (94%)	5 (6%)	0	100 100
57	Y	83/85 (98%)	81 (98%)	2 (2%)	0	100 100
58	Z	63/65 (97%)	40 (64%)	21 (33%)	2 (3%)	4 26
All	All	5962/6178 (96%)	5252 (88%)	677 (11%)	33 (1%)	29 64

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	h	80	THR
12	h	108	VAL
12	h	118	ILE
50	R	104	ASN
52	T	46	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	b	216/216 (100%)	214 (99%)	2 (1%)	78 91
6	c	164/164 (100%)	164 (100%)	0	100 100
7	d	165/165 (100%)	163 (99%)	2 (1%)	71 88
8	e	148/148 (100%)	146 (99%)	2 (1%)	67 86
9	f	137/137 (100%)	135 (98%)	2 (2%)	65 85
10	g	114/114 (100%)	114 (100%)	0	100 100
11	a	110/174 (63%)	110 (100%)	0	100 100
12	h	100/100 (100%)	97 (97%)	3 (3%)	41 73
13	i	109/109 (100%)	107 (98%)	2 (2%)	59 82
14	j	116/116 (100%)	116 (100%)	0	100 100
15	k	103/103 (100%)	102 (99%)	1 (1%)	76 90
16	l	102/102 (100%)	102 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	m	109/109 (100%)	108 (99%)	1 (1%)	78 91
18	n	100/100 (100%)	99 (99%)	1 (1%)	76 90
19	o	86/86 (100%)	86 (100%)	0	100 100
20	p	99/99 (100%)	98 (99%)	1 (1%)	76 90
21	q	89/89 (100%)	88 (99%)	1 (1%)	73 88
22	r	84/84 (100%)	84 (100%)	0	100 100
23	s	93/93 (100%)	93 (100%)	0	100 100
24	t	80/80 (100%)	79 (99%)	1 (1%)	69 87
25	u	83/83 (100%)	83 (100%)	0	100 100
26	v	78/78 (100%)	78 (100%)	0	100 100
27	w	57/57 (100%)	57 (100%)	0	100 100
28	x	67/67 (100%)	67 (100%)	0	100 100
29	y	55/55 (100%)	55 (100%)	0	100 100
30	z	48/48 (100%)	47 (98%)	1 (2%)	53 79
31	A	42/59 (71%)	41 (98%)	1 (2%)	49 77
32	B	47/47 (100%)	47 (100%)	0	100 100
33	C	45/45 (100%)	44 (98%)	1 (2%)	52 79
34	D	38/38 (100%)	38 (100%)	0	100 100
35	E	51/51 (100%)	51 (100%)	0	100 100
36	F	34/34 (100%)	34 (100%)	0	100 100
39	G	186/186 (100%)	184 (99%)	2 (1%)	73 88
40	H	170/170 (100%)	168 (99%)	2 (1%)	71 88
41	I	172/172 (100%)	171 (99%)	1 (1%)	86 94
42	J	119/119 (100%)	119 (100%)	0	100 100
43	K	87/87 (100%)	87 (100%)	0	100 100
44	L	124/124 (100%)	123 (99%)	1 (1%)	81 93
45	M	104/104 (100%)	104 (100%)	0	100 100
46	N	105/105 (100%)	101 (96%)	4 (4%)	33 67
47	O	86/86 (100%)	86 (100%)	0	100 100
48	P	89/89 (100%)	88 (99%)	1 (1%)	73 88
49	Q	103/103 (100%)	101 (98%)	2 (2%)	57 81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
50	R	92/92 (100%)	91 (99%)	1 (1%)	73 88
51	S	83/83 (100%)	82 (99%)	1 (1%)	71 88
52	T	76/76 (100%)	75 (99%)	1 (1%)	69 87
53	U	65/65 (100%)	64 (98%)	1 (2%)	65 85
54	V	74/74 (100%)	72 (97%)	2 (3%)	44 75
55	W	56/56 (100%)	56 (100%)	0	100 100
56	X	70/70 (100%)	69 (99%)	1 (1%)	67 86
57	Y	65/65 (100%)	65 (100%)	0	100 100
58	Z	55/55 (100%)	53 (96%)	2 (4%)	35 69
All	All	4950/5031 (98%)	4906 (99%)	44 (1%)	79 91

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	N	11	ARG
50	R	10	ASP
46	N	44	ARG
48	P	81	LEU
52	T	88	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
43	K	63	ASN
57	Y	20	ASN
45	M	3	GLN
50	R	13	HIS
18	n	9	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	1538/1539 (99%)	184 (11%)	4 (0%)
2	1	2902/2903 (99%)	418 (14%)	19 (0%)
3	2	119/120 (99%)	16 (13%)	1 (0%)
37	4	18/35 (51%)	4 (22%)	0
38	6	76/77 (98%)	14 (18%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	5	76/77 (98%)	15 (19%)	0
All	All	4729/4751 (99%)	651 (13%)	24 (0%)

5 of 651 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	4	U
1	3	5	U
1	3	6	G
1	3	9	G
1	3	13	U

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	1	1156	A
2	1	2311	A
2	1	2296	U
2	1	2326	C
2	1	760	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
59	FME	1	3001	60	6,7,10	0.83	0	2,7,11	1.96	1 (50%)
60	PRO	5	101	4,59	5,7,8	3.55	3 (60%)	7,8,10	1.53	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	FME	1	3001	60	-	4/5/6/11	-
60	PRO	5	101	4,59	-	0/0/9/11	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	5	101	PRO	CD-N	-5.38	1.29	1.49
60	5	101	PRO	O-C	4.96	1.39	1.19
60	5	101	PRO	CB-CA	-2.55	1.31	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	5	101	PRO	O-C-CA	-3.46	115.71	124.78
59	1	3001	FME	CE-SD-CG	2.76	109.88	100.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1	3001	FME	N-CA-CB-CG
59	1	3001	FME	C-CA-CB-CG
59	1	3001	FME	O-C-CA-CB
59	1	3001	FME	CA-CB-CG-SD

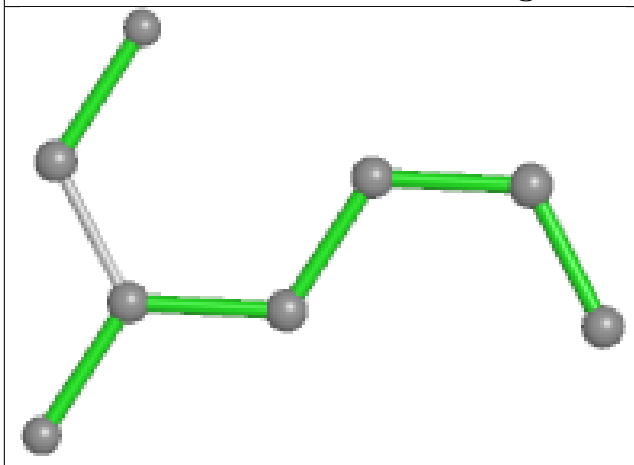
There are no ring outliers.

No monomer is involved in short contacts.

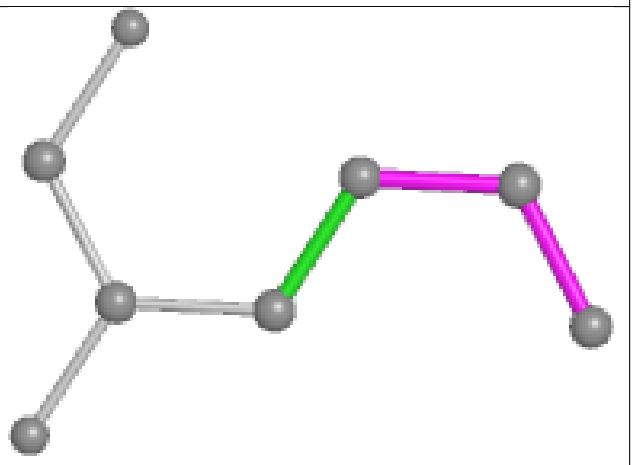
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

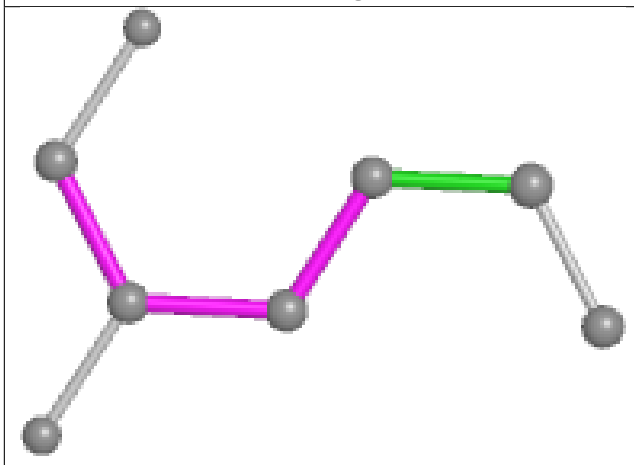
Ligand FME 1 3001



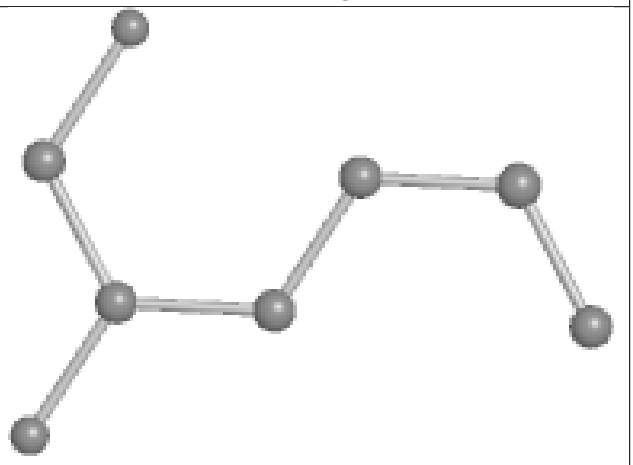
Bond lengths



Bond angles



Torsions



Rings

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.

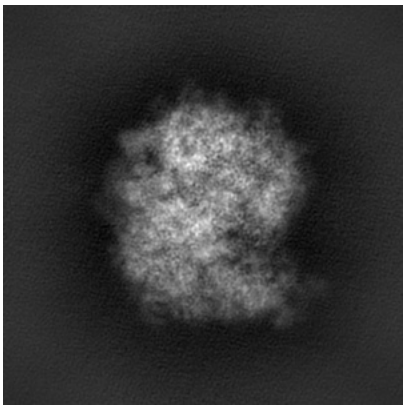
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25411. These allow visual inspection of the internal detail of the map and identification of artifacts.

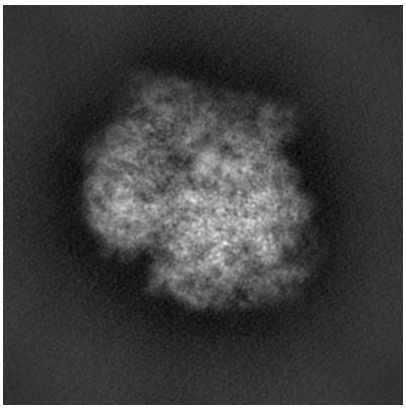
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

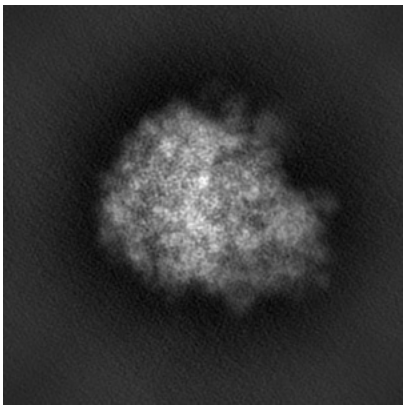
6.1.1 Primary map



X

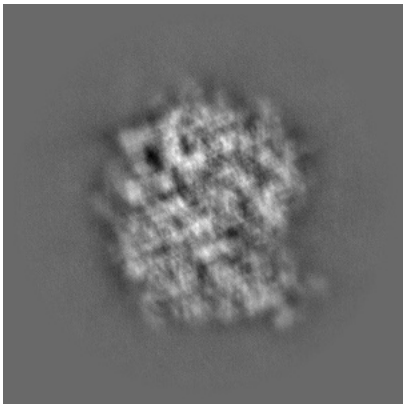


Y

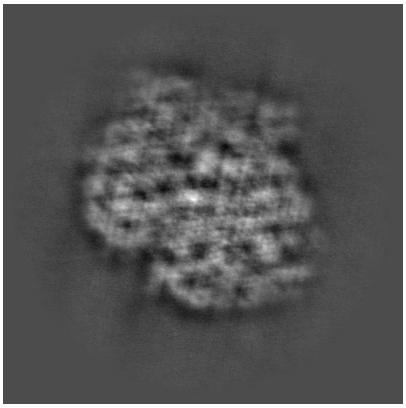


Z

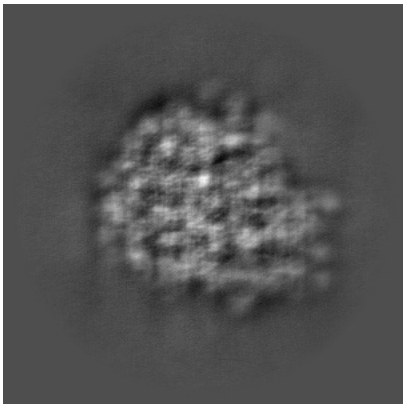
6.1.2 Raw map



X



Y

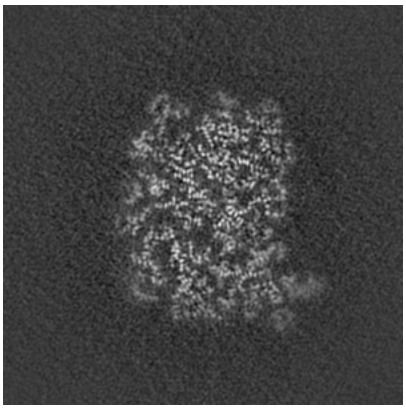


Z

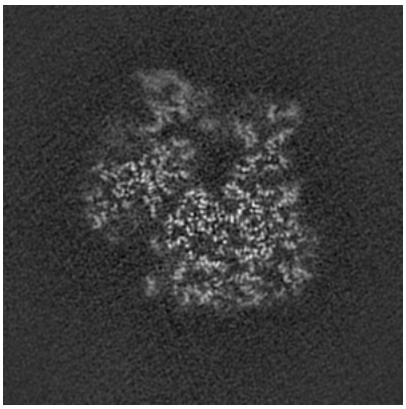
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

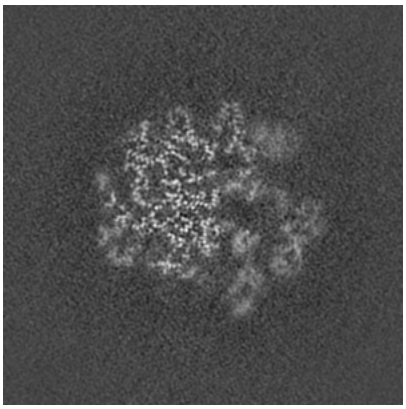
6.2.1 Primary map



X Index: 230

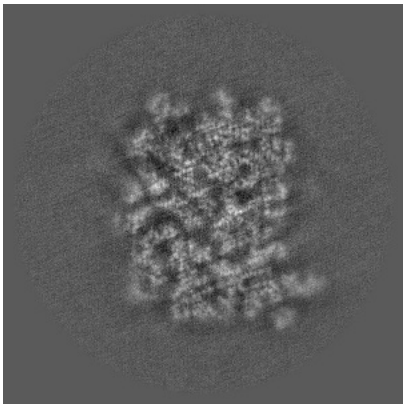


Y Index: 230

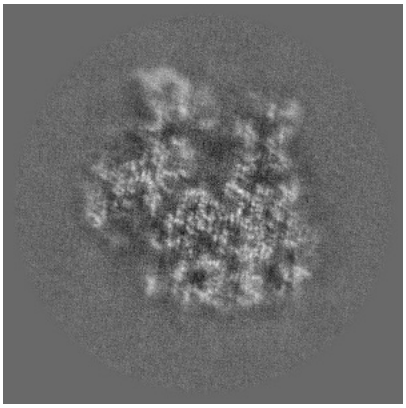


Z Index: 230

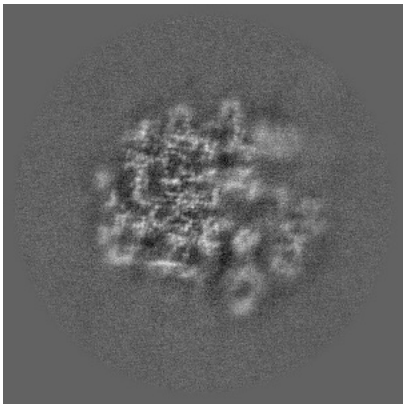
6.2.2 Raw map



X Index: 230



Y Index: 230

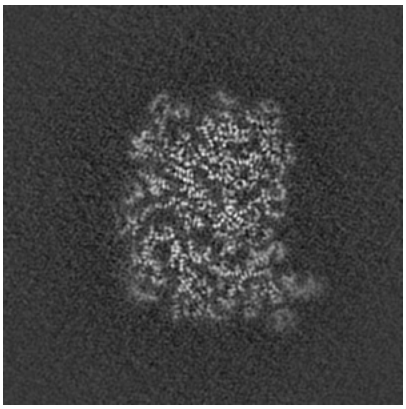


Z Index: 230

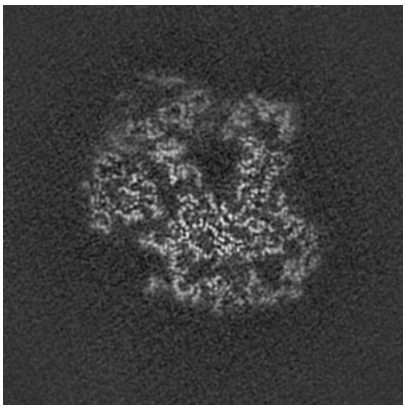
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

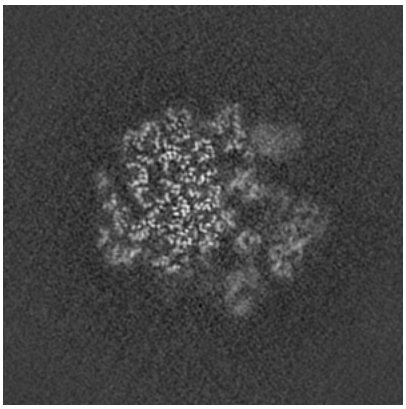
6.3.1 Primary map



X Index: 229

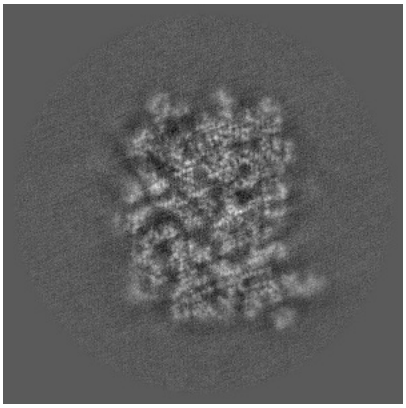


Y Index: 222

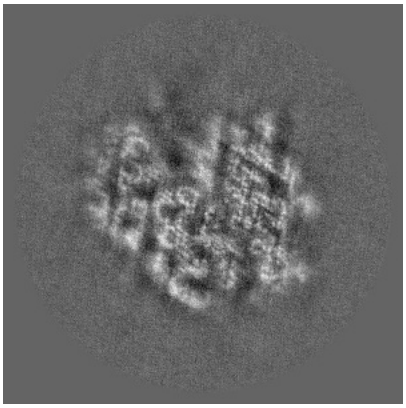


Z Index: 227

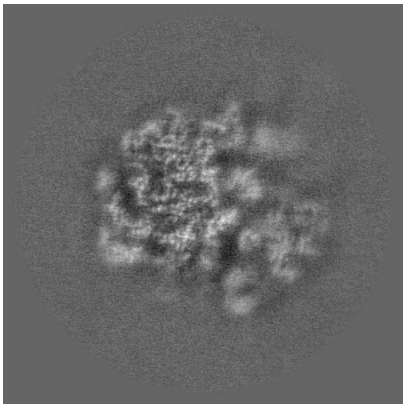
6.3.2 Raw map



X Index: 230



Y Index: 253

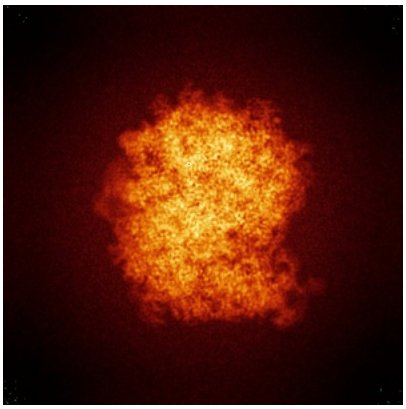


Z Index: 224

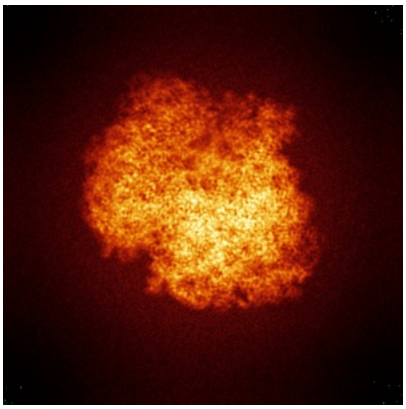
The images above show the largest variance slices of the map in three orthogonal directions.

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

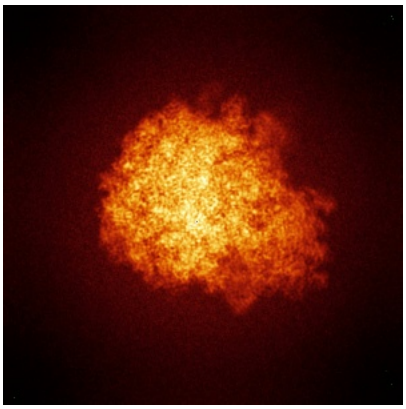
6.4.1 Primary map



X

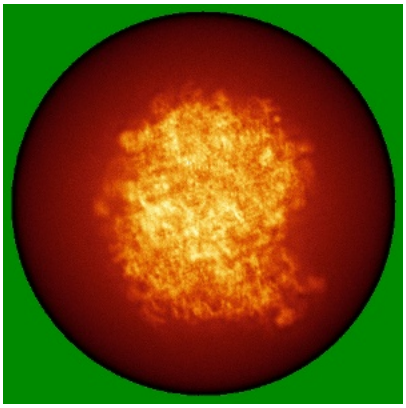


Y

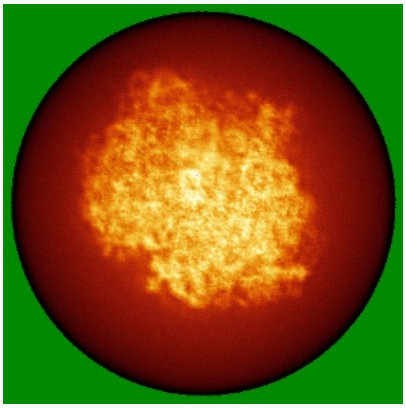


Z

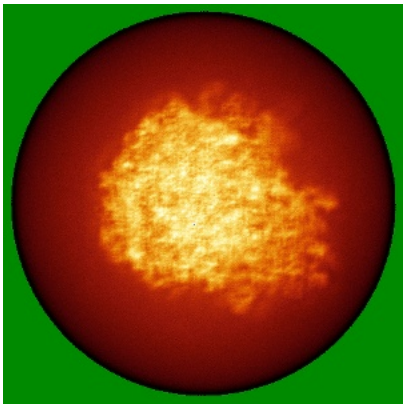
6.4.2 Raw map



X



Y

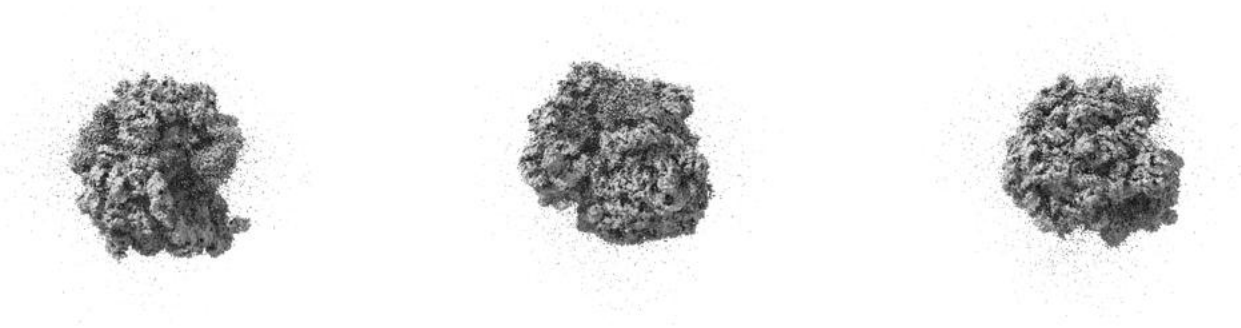


Z

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

6.5 Orthogonal surface views (i)

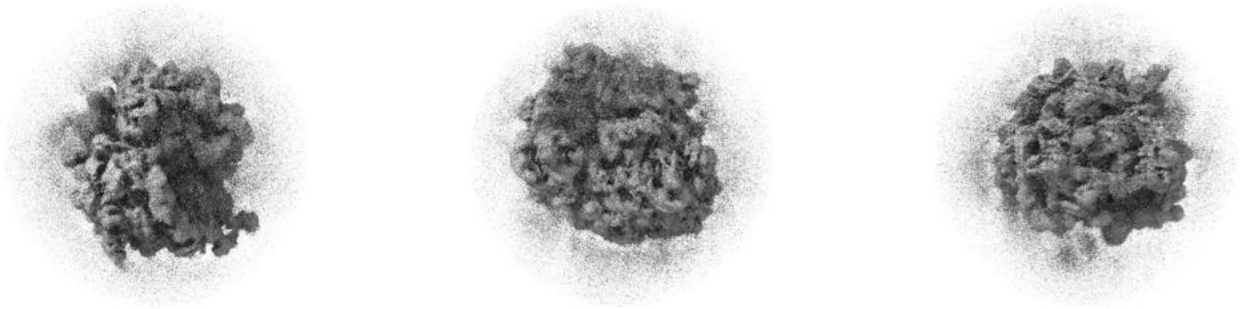
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

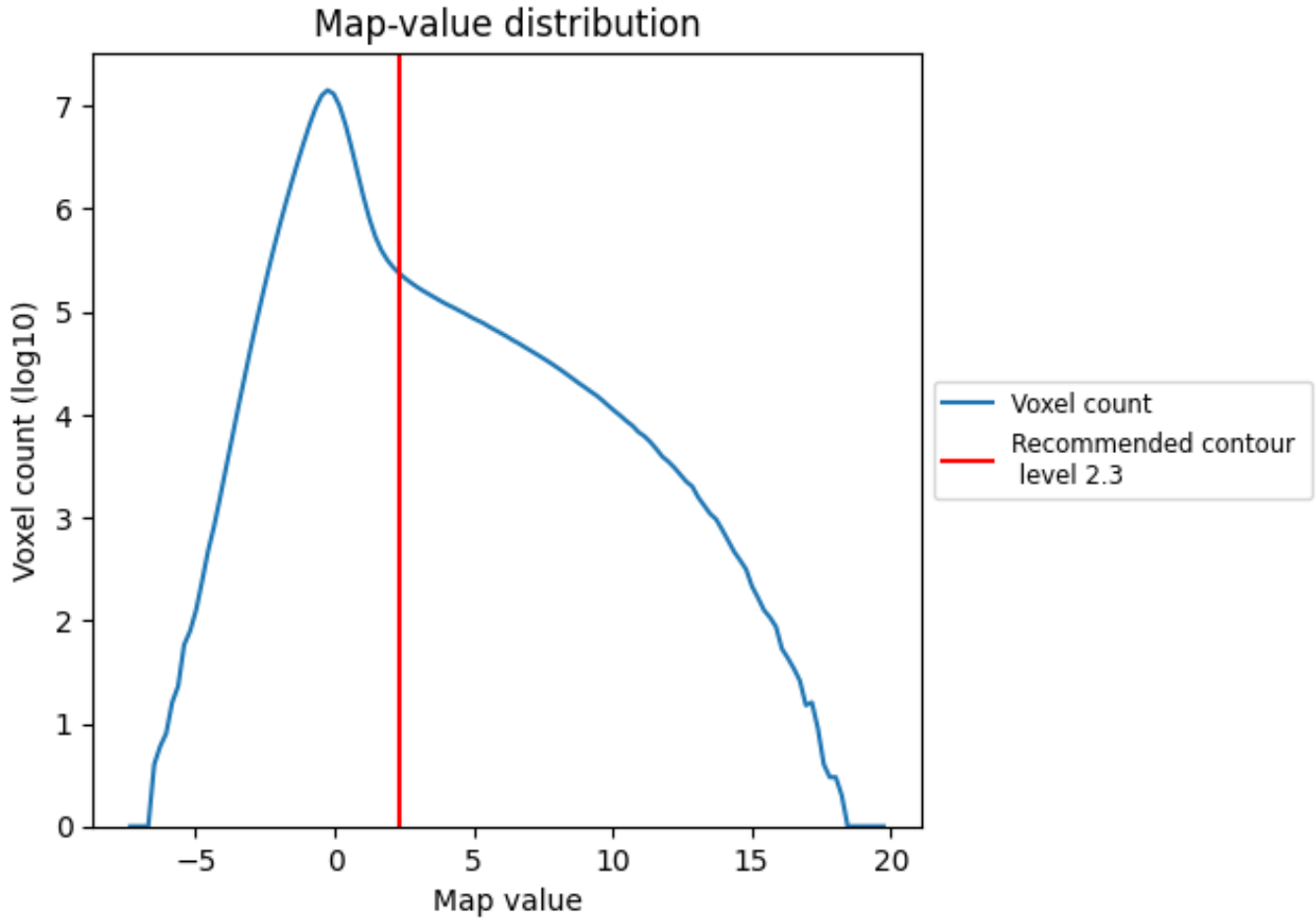
6.6 Mask visualisation (i)

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

7 Map analysis

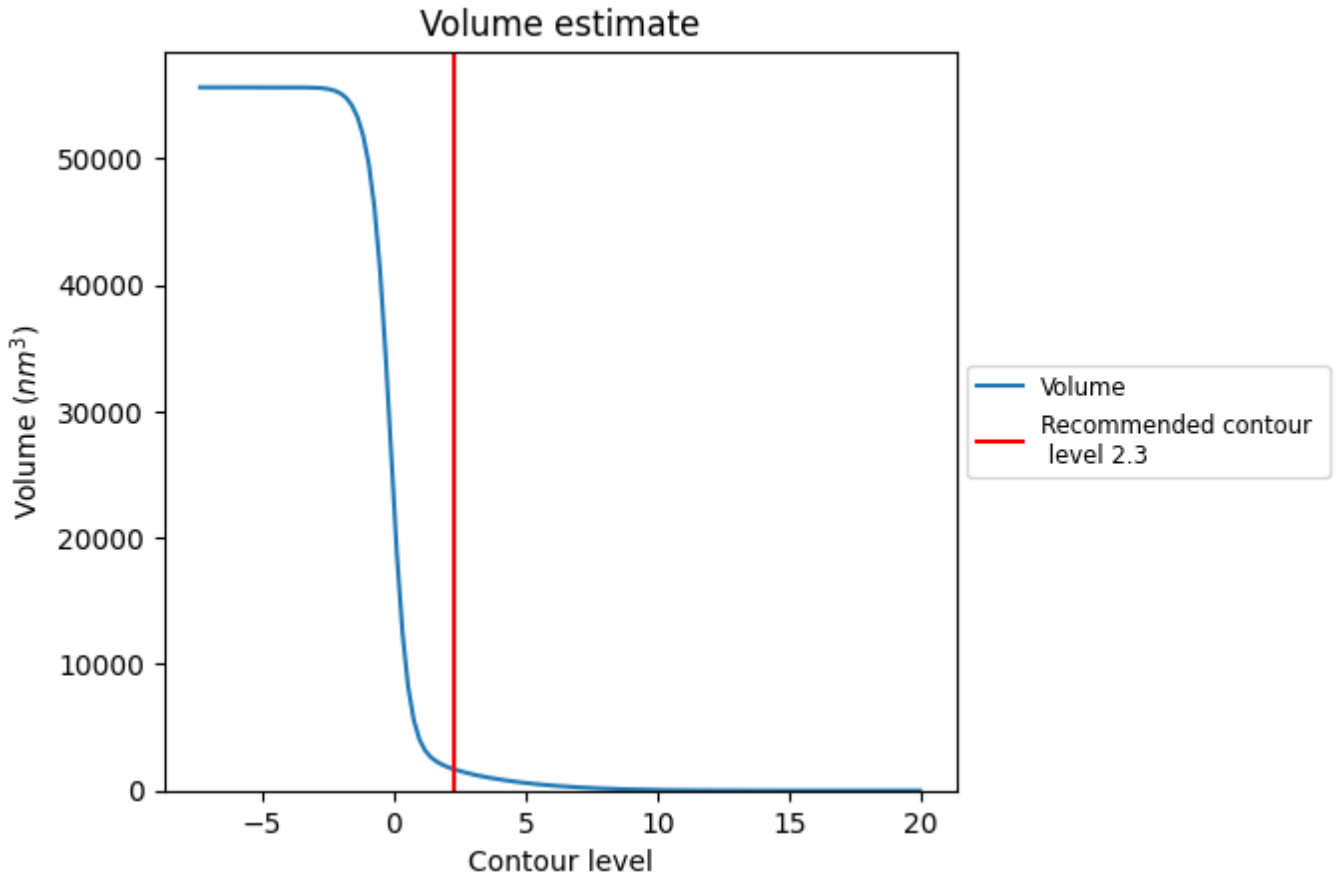
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

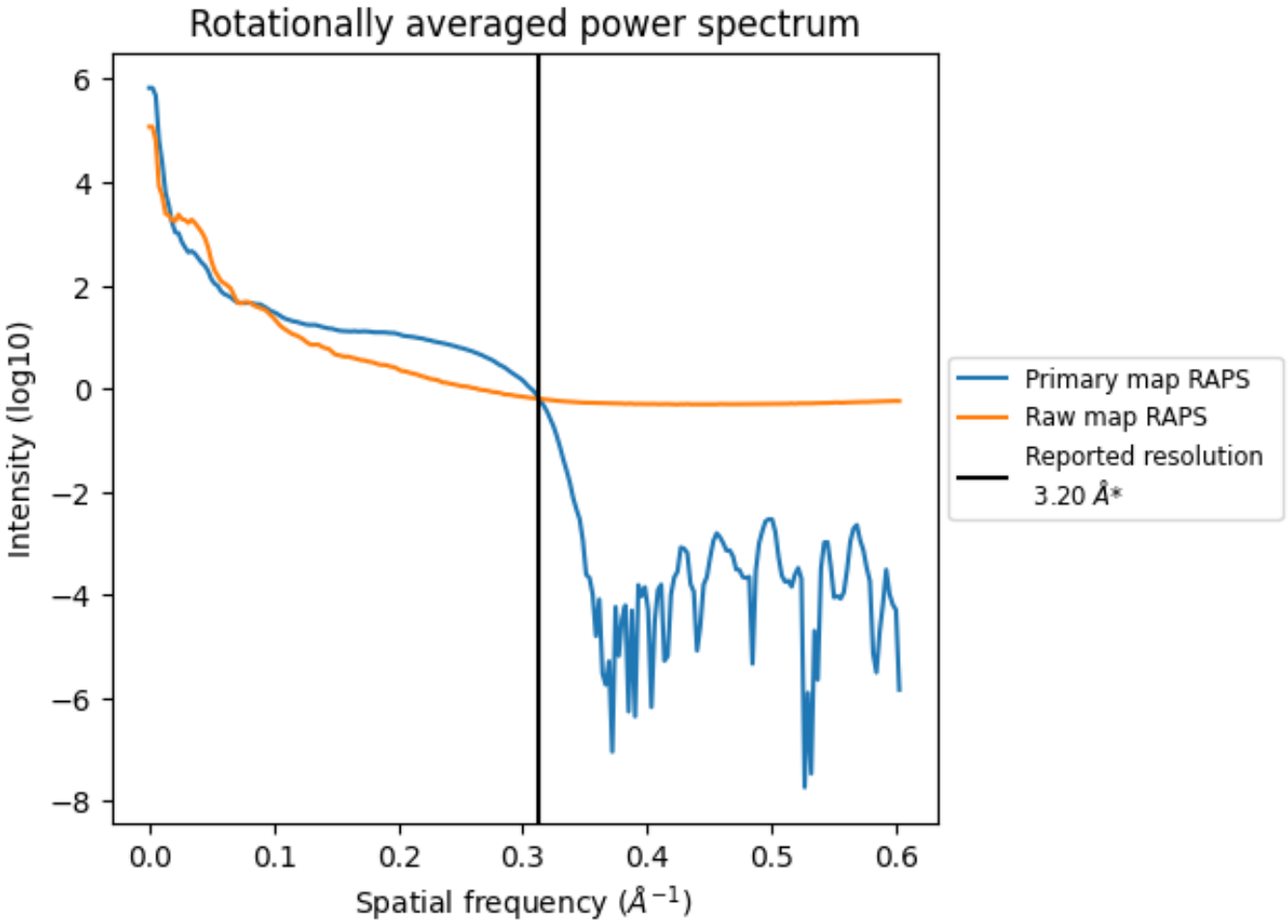
7.2 Volume estimate (i)



The volume at the recommended contour level is 1677 nm^3; this corresponds to an approximate mass of 1515 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

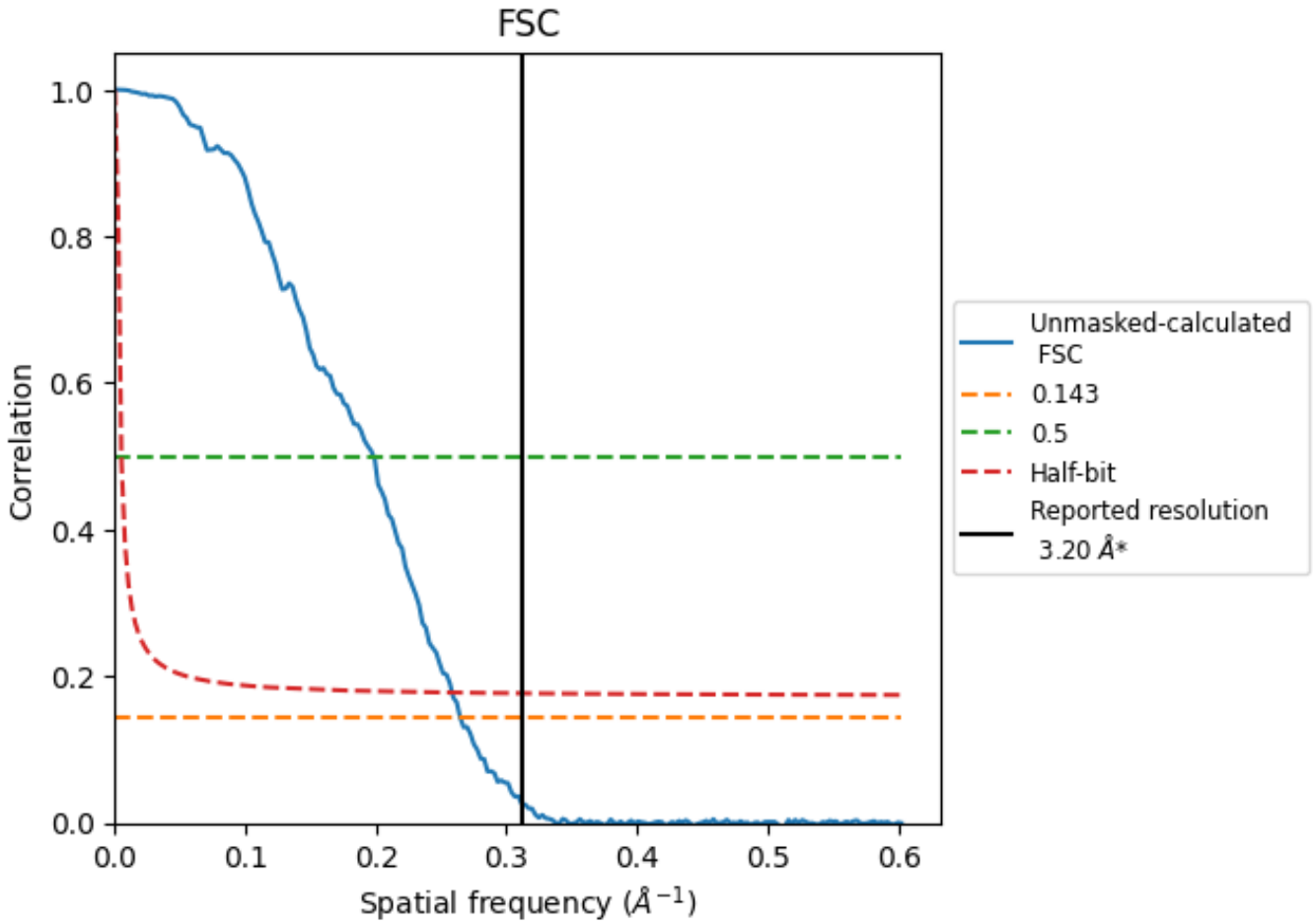


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

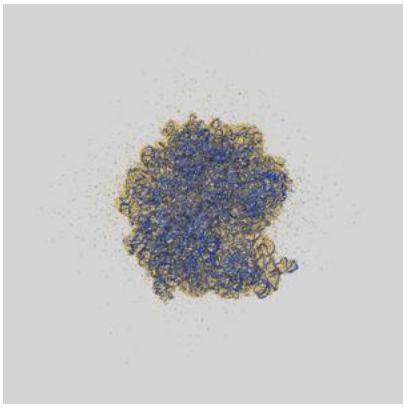
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	5.05	3.87

*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 3.78 differs from the reported value 3.2 by more than 10 %

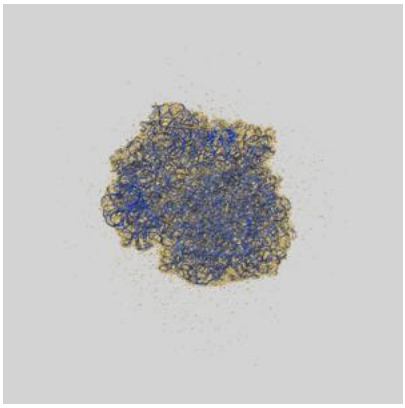
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25411 and PDB model 7SSO. Per-residue inclusion information can be found in section 3 on page 15.

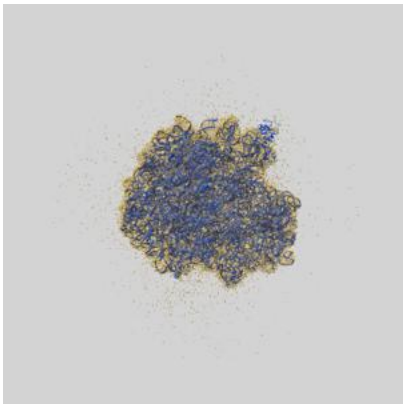
9.1 Map-model overlay



X



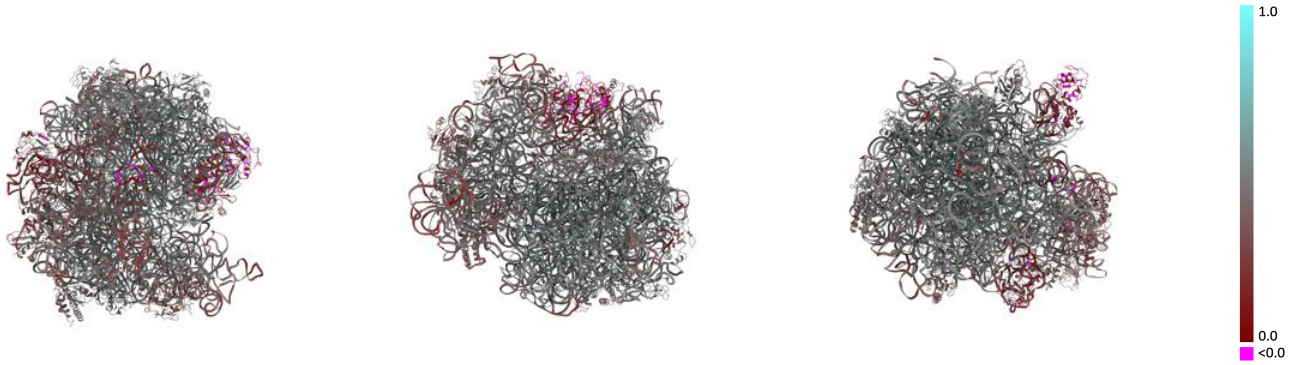
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.3 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.

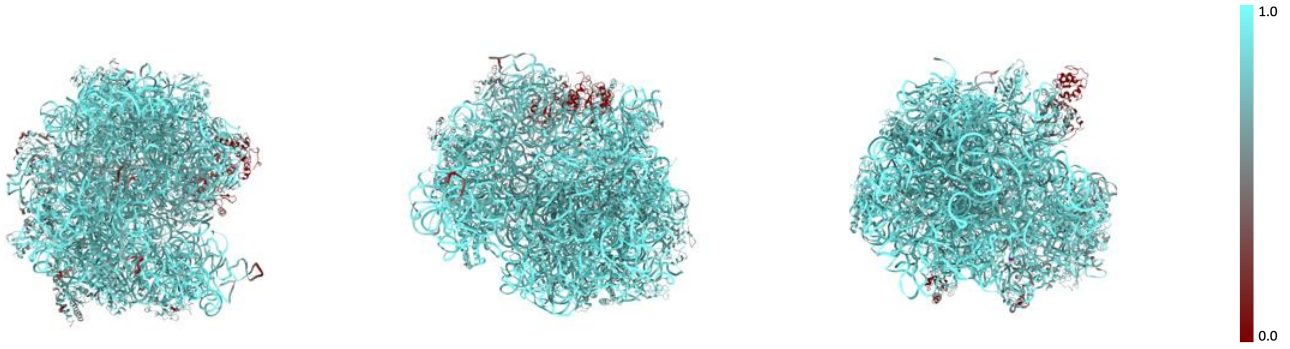
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

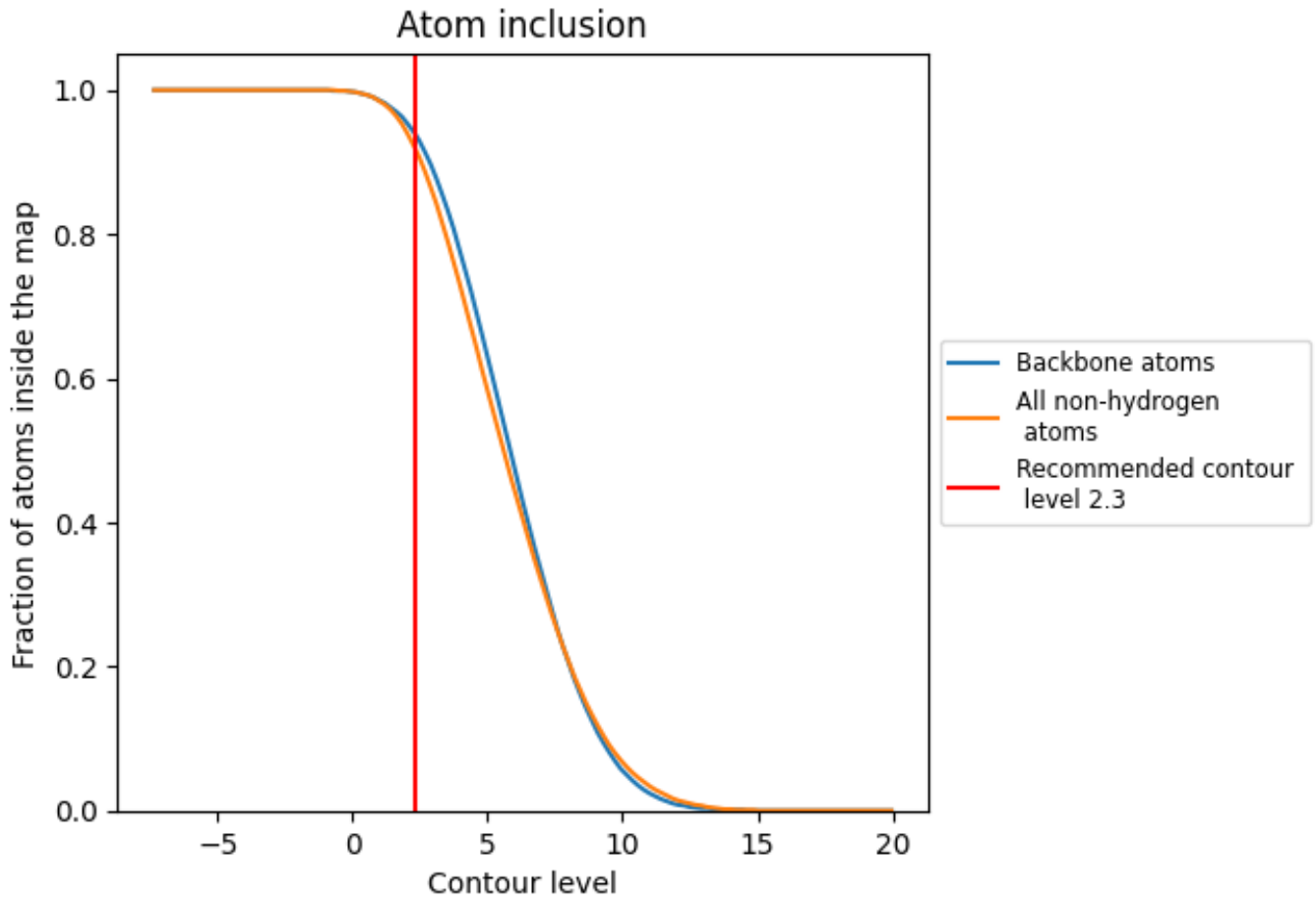
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.3).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (2.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9200	0.4460
1	0.9760	0.4670
2	0.9680	0.4370
3	0.9550	0.4360
4	0.8230	0.2980
5	0.9760	0.3960
6	0.9620	0.3490
A	0.7440	0.2950
B	0.9230	0.4840
C	0.8560	0.4700
D	0.9470	0.5180
E	0.9530	0.5220
F	0.9280	0.5100
G	0.6860	0.4110
H	0.8120	0.4430
I	0.7650	0.3900
J	0.8980	0.4730
K	0.8720	0.4210
L	0.7720	0.3560
M	0.8810	0.4840
N	0.7840	0.4140
O	0.6430	0.4050
P	0.9080	0.4570
Q	0.9070	0.4620
R	0.7660	0.3600
S	0.8050	0.4070
T	0.9260	0.4640
U	0.8880	0.4600
V	0.8880	0.4480
W	0.9130	0.4730
X	0.7880	0.3620
Y	0.8450	0.4010
Z	0.7720	0.3790
a	0.6600	0.3070
b	0.9630	0.5200

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Chain	Atom inclusion	Q-score
c	0.9170	0.4980
d	0.8220	0.4620
e	0.8060	0.3520
f	0.8690	0.4380
g	0.3140	0.3340
h	0.0900	0.0500
i	0.3540	0.2350
j	0.9290	0.4990
k	0.9400	0.5110
l	0.9050	0.4880
m	0.9190	0.4980
n	0.9200	0.4940
o	0.8670	0.4370
p	0.8960	0.4880
q	0.9440	0.5130
r	0.8780	0.4950
s	0.9130	0.5020
t	0.8750	0.4710
u	0.8270	0.4530
v	0.8710	0.4780
w	0.9520	0.5230
x	0.9420	0.5080
y	0.8110	0.4110
z	0.8830	0.4910