wwPDB EM Validation Summary Report

Sep 16, 2026 – 01:20 AM EDT

PDB ID	:	5WFK / pdb_00005wfk
EMDB ID	:	EMD-8828
Title	:	70S ribosome-EF-Tu H84A complex with GTP and near-cognate tRNA (Complex C3)
Authors	:	Fislage, M.; Frank, J.
Deposited on	:	2017-07-12
Resolution	:	3.40 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:

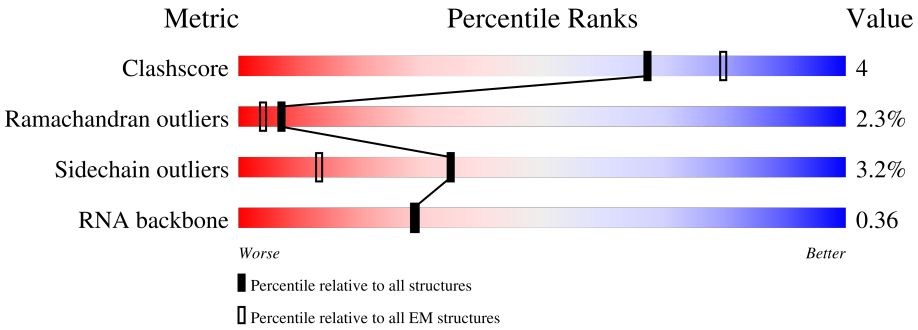
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

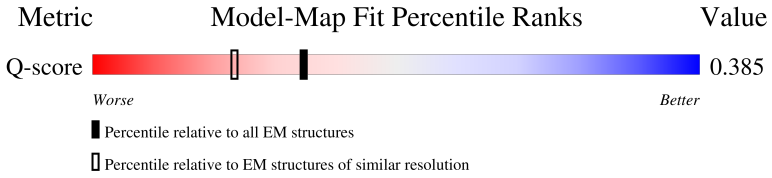
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	A	2903	67% 28% 5%
2	B	120	72% 27% .
3	C	271	92% 7%

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Mol	Chain	Length	Quality of chain
4	D	208	92% 6%
5	E	200	94% 6%
6	F	177	96%
7	G	174	95% 5%
8	H	149	8% 96%
9	I	141	19% 83% 15%
10	J	141	91% 9%
11	K	122	85% 13%
12	L	143	92% 8%
13	M	136	96%
14	N	119	94% 5%
15	O	116	97%
16	P	114	95% 5%
17	Q	115	95% 5%
18	R	102	90% 8%
19	S	109	94% 6%
20	T	92	93% 7%
21	U	102	96%
22	V	92	95% 5%
23	W	75	91% 9%
24	X	77	100%
25	Y	60	97%
26	Z	56	100%
27	0	55	91% 9%
28	1	51	96%

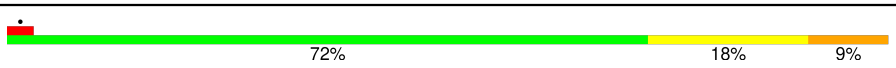
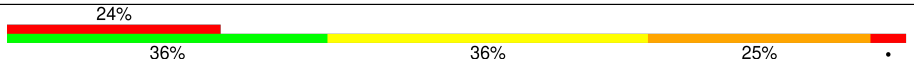
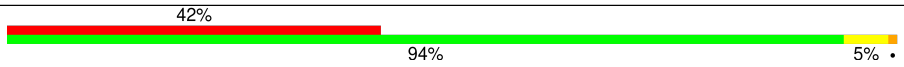
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Mol	Chain	Length	Quality of chain
29	2	45	87% 13%
30	3	64	97%
31	4	38	100%
32	5	131	72% 85% 15%
33	6	66	95% 5%
34	a	1540	56% 35% 9%
35	b	218	96%
36	c	206	96%
37	d	205	96%
38	e	157	91% 8%
39	f	100	89% 9%
40	g	151	94% 6%
41	h	129	94% 5%
42	i	127	85% 12%
43	j	98	86% 10%
44	k	116	91% 7%
45	l	121	85% 13%
46	m	115	94% 5%
47	n	101	92% 8%
48	o	88	90% 7%
49	p	82	94% 6%
50	q	80	90% 9%
51	r	65	83% 14%
52	s	79	90% 10%
53	t	85	88% 12%

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Mol	Chain	Length	Quality of chain
54	u	65	
55	v	77	
55	w	77	
56	x	12	
57	y	76	
58	z	393	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	6MZ	A	2030	-	-	X	-
57	MIA	y	37	-	-	X	-

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 154325 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2900	62277	27788	11459	20130	2900	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	120	2572	1145	471	836	120	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	-	expression tag	GB 1324665466

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	271	2082	1288	423	364	7	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	208	1557	974	287	293	3	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	200	1544	969	282	289	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	174	Total	C	N	O	S	0	0
			1304	820	239	243	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L11.

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

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	141	Total	C	N	O	S	0	0
			1120	708	211	197	4		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	115	Total	C	N	O	0	0
			933	595	190	148		

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	102	Total	C	N	O	S	0	0
			810	513	152	143	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	92	Total	C	N	O	S	0	0
			730	461	138	130	1		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	92	Total	C	N	O	S	0	0
			739	471	135	131	2		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	75	Total	C	N	O	S	0	0
			572	355	116	100	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	60	Total	C	N	O	S	0	0
			494	305	96	91	2		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	56	Total	C	N	O	S	0	0
			434	273	85	74	2		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	1	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total	C	N	O	P	2	0
			33095	14768	6067	10718	1542		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	1	0
			1164	724	221	213	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	121	Total	C	N	O	S	0	0
			940	581	193	162	4		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			810	502	165	140	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

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

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 55 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		
55	w	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	12	Total	C	N	O	P	0	0
			252	113	43	84	12		

- Molecule 57 is a RNA chain called Phe-tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	y	76	Total	C	N	O	P	S	0	0
			1632	731	290	533	76	2		

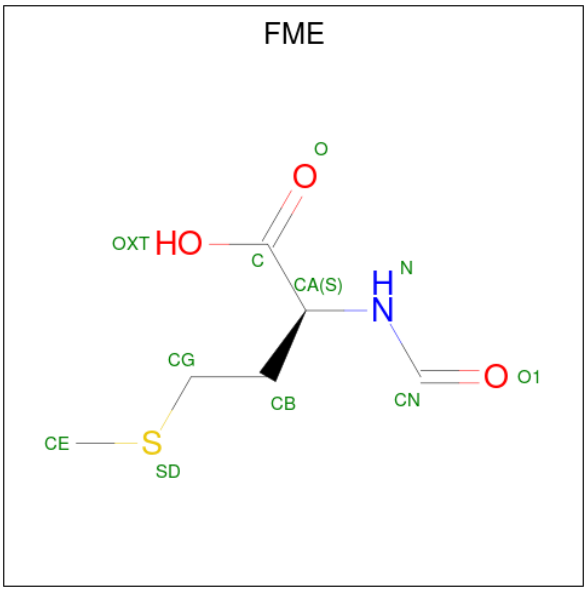
- Molecule 58 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	393	Total	C	N	O	S	0	0
			3031	1915	522	581	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	47	ASN	ASP	conflict	UNP P0CE48
z	84	ALA	HIS	engineered mutation	UNP P0CE48

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
59	A	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	A	965	Total	Mg	0
			965	965	
60	B	27	Total	Mg	0
			27	27	
60	C	2	Total	Mg	0
			2	2	
60	D	3	Total	Mg	0
			3	3	
60	E	3	Total	Mg	0
			3	3	
60	H	1	Total	Mg	0
			1	1	
60	L	3	Total	Mg	0
			3	3	
60	N	1	Total	Mg	0
			1	1	
60	Q	1	Total	Mg	0
			1	1	
60	S	1	Total	Mg	0
			1	1	
60	U	1	Total	Mg	0
			1	1	

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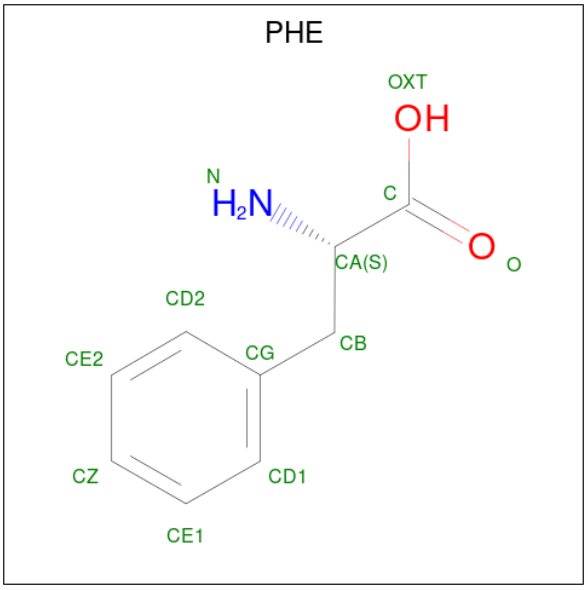
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Mol	Chain	Residues	Atoms	AltConf
60	X	1	Total Mg 1 1	0
60	Y	1	Total Mg 1 1	0
60	Z	1	Total Mg 1 1	0
60	0	1	Total Mg 1 1	0
60	2	1	Total Mg 1 1	0
60	4	1	Total Mg 1 1	0
60	a	375	Total Mg 375 375	0
60	c	1	Total Mg 1 1	0
60	d	1	Total Mg 1 1	0
60	e	1	Total Mg 1 1	0
60	f	1	Total Mg 1 1	0
60	g	1	Total Mg 1 1	0
60	i	2	Total Mg 2 2	0
60	k	1	Total Mg 1 1	0
60	l	1	Total Mg 1 1	0
60	m	1	Total Mg 1 1	0
60	q	1	Total Mg 1 1	0
60	v	9	Total Mg 9 9	0
60	w	3	Total Mg 3 3	0
60	x	1	Total Mg 1 1	0

- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

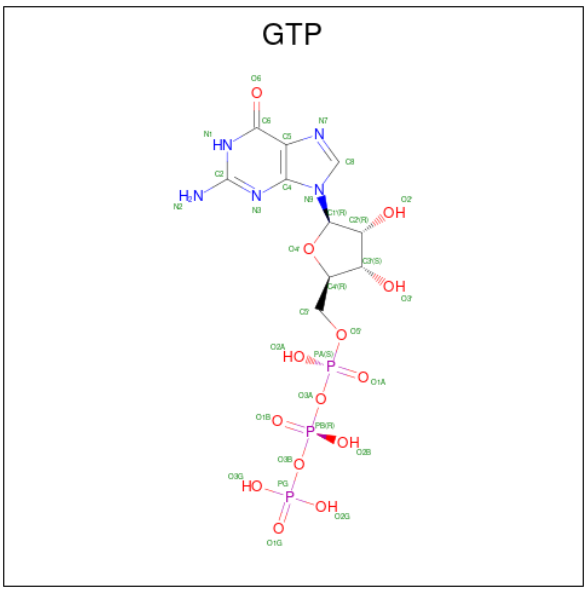
Mol	Chain	Residues	Atoms	AltConf
61	A	1	Total K 1 1	0

- Molecule 62 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms	AltConf
62	z	1	Total C N O 11 9 1 1	0

- Molecule 63 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
63	z	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
64	A	293	Total	O	0
			293	293	
64	B	8	Total	O	0
			8	8	
64	C	3	Total	O	0
			3	3	
64	D	3	Total	O	0
			3	3	
64	L	1	Total	O	0
			1	1	
64	N	1	Total	O	0
			1	1	
64	O	1	Total	O	0
			1	1	
64	Q	1	Total	O	0
			1	1	
64	V	1	Total	O	0
			1	1	
64	W	1	Total	O	0
			1	1	
64	0	1	Total	O	0
			1	1	
64	2	1	Total	O	0
			1	1	
64	3	1	Total	O	0
			1	1	
64	a	93	Total	O	0
			93	93	
64	l	1	Total	O	0
			1	1	
64	m	1	Total	O	0
			1	1	
64	o	1	Total	O	0
			1	1	
64	s	3	Total	O	0
			3	3	
64	t	1	Total	O	0
			1	1	

Continued on next page...

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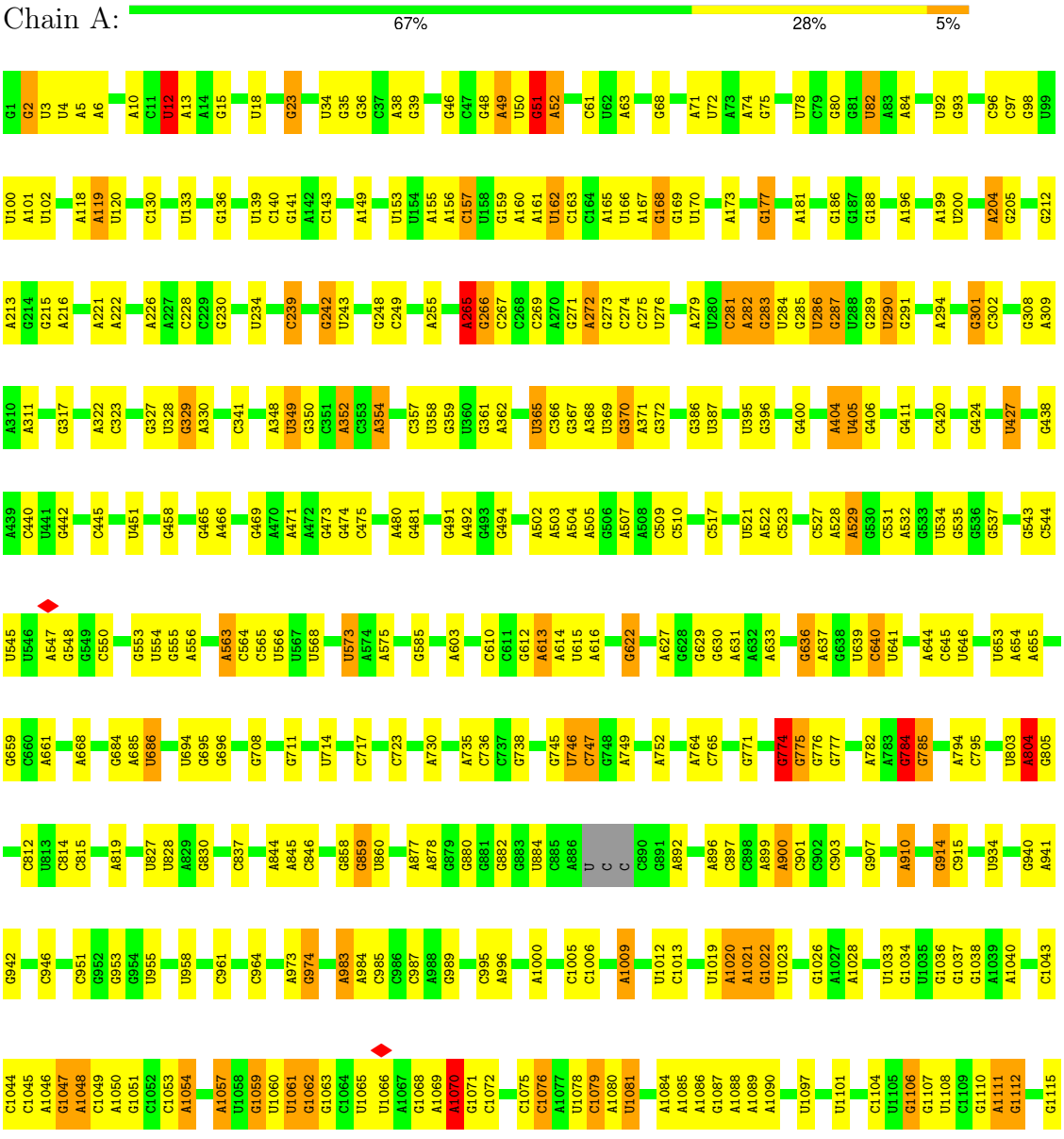
Mol	Chain	Residues	Atoms	AltConf
64	u	1	Total O 1 1	0
64	v	1	Total O 1 1	0
64	w	1	Total O 1 1	0

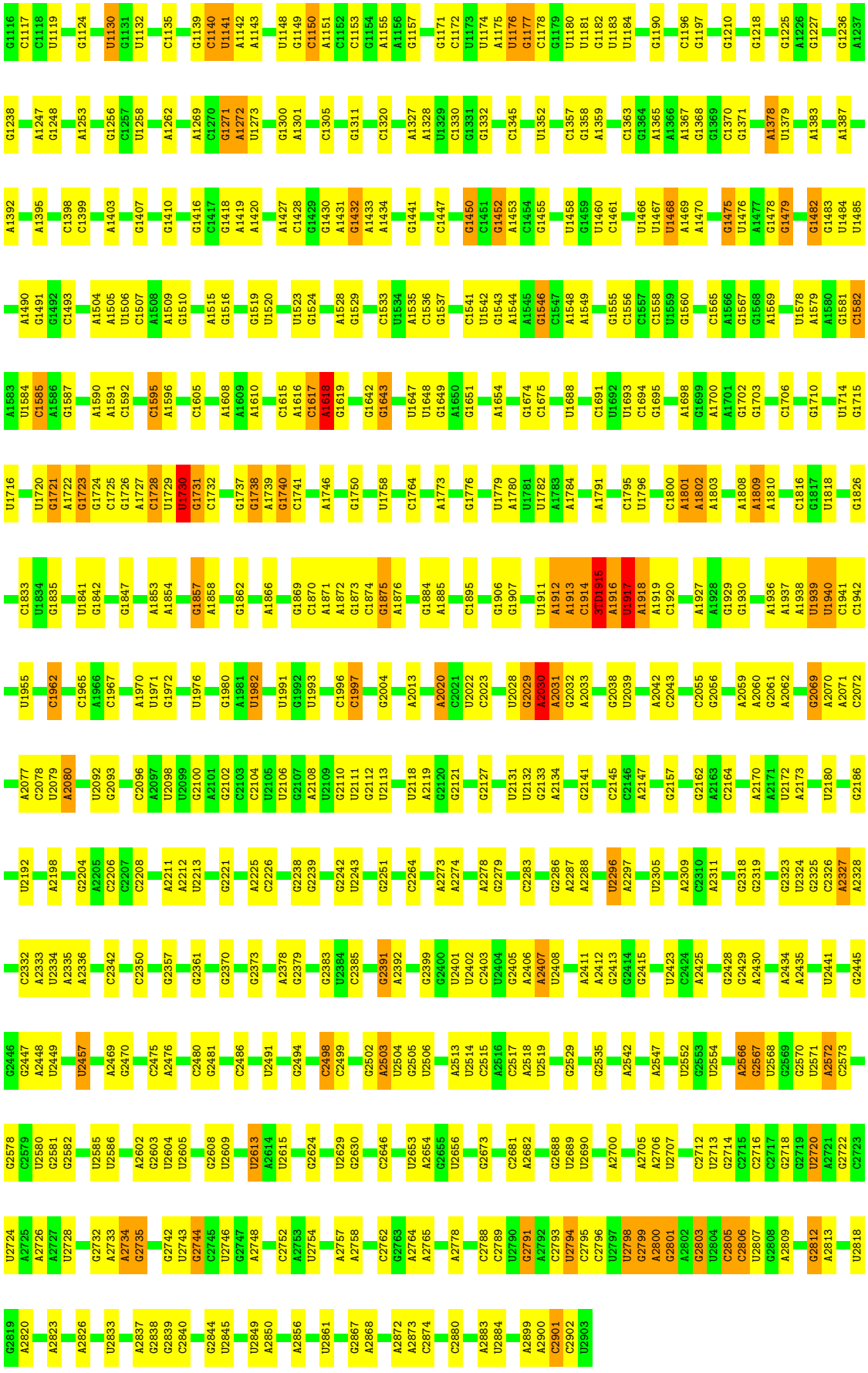
3 Residue-property plots (i)

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: 23S rRNA

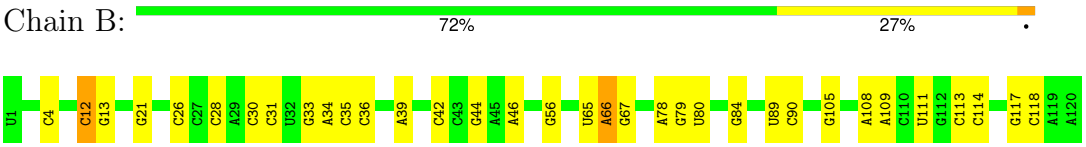
Chain A:




G1116 C1117 C1118 U1119 G1124 U1130 G1131 U1132 C1135 G1139 C1140 U1141 A1142 A1143 U1148 G1149 C1150 A1151 C1152 C1153 G1154 A1155 A1156 G1157 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1184 G1190 C1196 G1197 G1210 G1218 G1225 A1226 G1227 G1236 A1237
G1238 A1247 G1248 A1253 G1256 C1257 U1258 A1262 A1269 C1270 G1271 A1272 U1273 G1300 A1301 C1305 G1311 C1320 A1327 A1328 U1329 C1330 G1331 G1332 C1345 U1352 C1357 G1358 A1359 C1363 G1364 A1365 A1366 A1367 G1368 G1369 C1370 G1371 A1378 U1379 A1383 A1387
A1392 A1395 C1398 C1399 A1403 G1407 G1410 G1416 G1417 G1418 A1419 A1420 A1427 C1428 G1429 G1430 A1431 G1432 A1433 A1434 G1441 C1447 G1450 C1451 G1452 A1453 C1454 G1455 U1458 G1459 U1460 C1461 U1466 U1467 U1468 A1469 A1470 G1475 U1476 A1477 G1478 G1479 G1482 G1483 U1484 U1485
A1490 G1491 G1492 C1493 A1504 A1505 U1506 C1507 A1508 A1509 G1510 A1515 G1516 G1519 U1520 U1523 G1524 A1528 G1529 C1533 U1534 A1535 C1536 G1537 C1541 U1542 G1543 A1544 A1545 G1546 C1547 A1548 A1549 G1555 C1556 C1557 C1558 U1559 G1560 C1565 A1566 G1567 G1568 A1569 U1578 A1579 A1580 G1581 C1582
A1583 U1584 C1585 A1586 G1587 A1590 A1591 C1592 C1595 A1596 C1605 A1608 A1609 A1610 C1615 A1616 C1617 A1618 G1619 G1642 G1643 U1647 U1648 G1649 A1650 G1651 A1654 G1674 C1675 U1688 C1691 U1692 U1693 C1694 G1695 A1698 G1699 A1700 A1701 G1702 G1703 C1706 G1710 U1714 G1715
U1716 U1720 G1721 A1722 G1723 G1724 C1725 G1726 A1727 C1728 U1729 U1730 G1731 C1732 G1737 G1738 A1739 G1740 C1741 A1746 G1750 U1758 C1764 A1773 G1776 U1779 A1780 U1781 U1782 A1783 A1784 A1791 C1795 U1796 C1800 A1801 A1802 A1803 A1808 A1809 A1810 C1816 G1817 U1818 G1826
C1833 U1834 G1835 U1841 G1842 G1847 A1853 A1854 G1857 A1858 G1862 A1866 G1869 C1870 A1871 A1872 G1873 C1874 G1875 A1876 G1884 A1885 C1895 G1906 G1907 U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 A1918 A1919 C1920 A1927 A1928 G1929 G1930 A1936 A1937 A1938 U1939 U1940 C1941 C1942
U1955 C1962 C1965 A1966 C1967 A1970 U1971 G1972 U1976 G1980 A1981 U1982 U1991 G1992 U1993 C1996 C1997 G2004 A2013 A2020 C2021 U2022 C2023 U2028 G2029 A2030 A2031 G2032 A2033 G2038 U2039 A2042 C2043 C2055 G2056 A2059 A2060 G2061 A2062 G2069 A2070 A2071 C2072
A2077 C2078 U2079 A2080 U2092 G2093 C2096 A2097 U2098 U2099 G2100 A2101 G2102 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 U2118 A2119 G2120 G2121 G2127 U2131 U2132 G2133 A2134 G2141 C2145 C2146 A2147 G2157 G2162 A2163 C2164 A2170 A2171 U2172 A2173 U2180 G2186
U2192 A2198 G2204 A2205 C2206 C2207 C2208 A2211 A2212 U2213 G2221 A2225 C2226 G2238 G2239 G2242 U2243 G2251 C2264 A2273 A2274 A2278 G2279 C2283 G2286 A2287 A2288 U2296 A2297 U2305 A2309 C2310 A2311 G2318 G2319 G2323 U2324 G2325 C2326 A2327 A2328
C2332 A2333 U2334 A2335 A2336 C2342 C2350 G2357 G2361 G2370 G2373 A2378 G2379 G2383 U2384 C2385 G2391 A2392 G2399 G2400 U2401 U2402 C2403 U2404 G2405 A2406 A2407 U2408 A2411 A2412 G2413 G2414 G2415 U2423 C2424 A2425 G2428 G2429 A2430 A2434 A2435 U2441 G2445
G2446 G2447 A2448 U2449 U2457 A2469 C2470 C2475 A2476 C2480 G2481 C2486 U2491 G2494 C2498 C2499 G2502 A2503 U2504 G2505 U2506 A2513 U2514 C2515 A2516 C2517 A2518 U2519 G2529 G2535 A2542 A2547 U2552 G2553 U2554 A2566 G2567 U2568 G2569 G2570 U2571 A2572 C2573
G2578 C2579 U2580 G2581 G2582 U2585 U2586 A2602 G2603 U2604 U2605 G2608 U2609 U2613 A2614 U2615 G2624 U2629 G2630 C2646 U2653 A2654 G2655 U2656 G2673 C2681 A2682 G2688 U2689 U2690 A2700 A2705 A2706 U2707 C2712 U2713 G2714 C2715 C2716 C2717 G2718 G2719 U2720 A2721 G2722 C2723
U2724 A2725 A2726 A2727 U2728 G2732 A2733 A2734 G2735 G2742 U2743 G2744 C2745 U2746 G2747 A2748 C2752 A2753 U2754 A2757 A2758 C2762 G2763 A2764 A2765 A2778 C2788 C2789 U2790 G2791 A2792 C2793 U2794 C2795 C2796 U2797 U2798 G2799 A2800 G2801 A2802 G2803 U2804 C2805 C2806 U2807 G2808 A2809 G2812 A2813 U2818
G2819 A2820 A2823 A2826 U2833 A2837 G2838 G2839 C2840 G2844 U2845 U2849 A2850 A2856 U2861 G2867 A2868 A2872 A2873 C2874 C2880 A2883 U2884 A2899 A2900 C2901 C2902 U2903

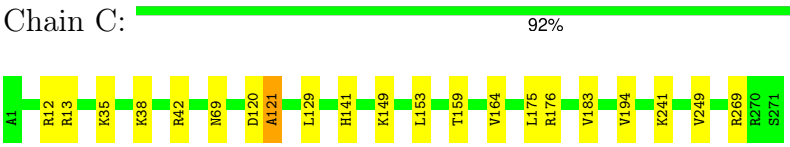
• Molecule 2: 5S rRNA

Chain B:



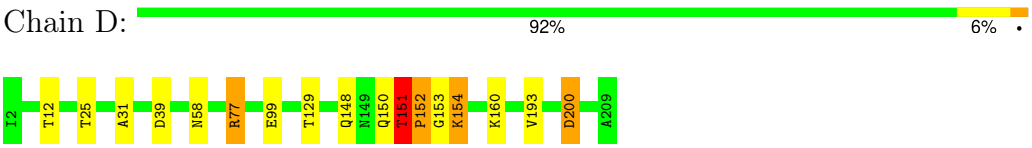
• Molecule 3: 50S ribosomal protein L2

Chain C:



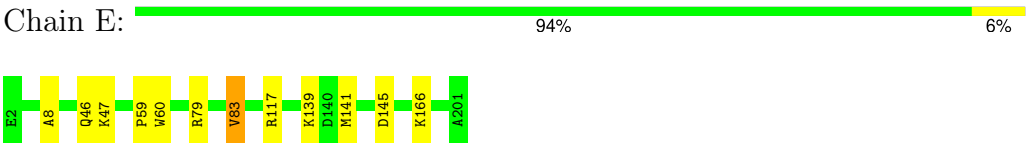
• Molecule 4: 50S ribosomal protein L3

Chain D:



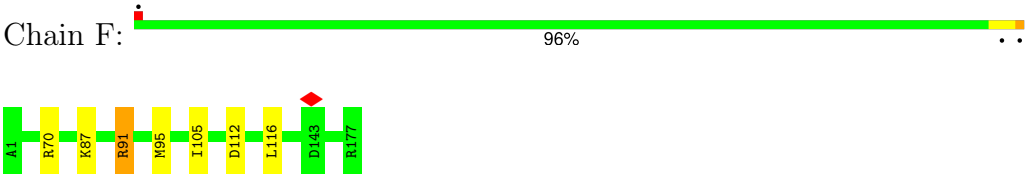
• Molecule 5: 50S ribosomal protein L4

Chain E:



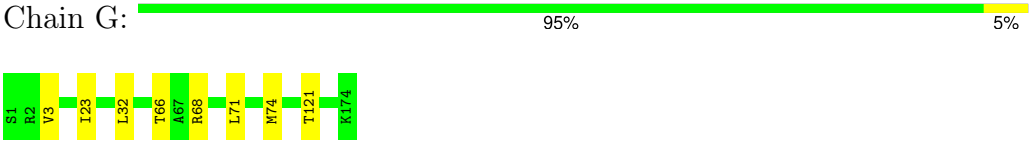
• Molecule 6: 50S ribosomal protein L5

Chain F:



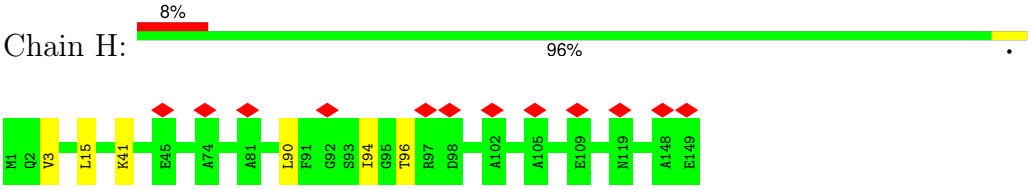
• Molecule 7: 50S ribosomal protein L6

Chain G:



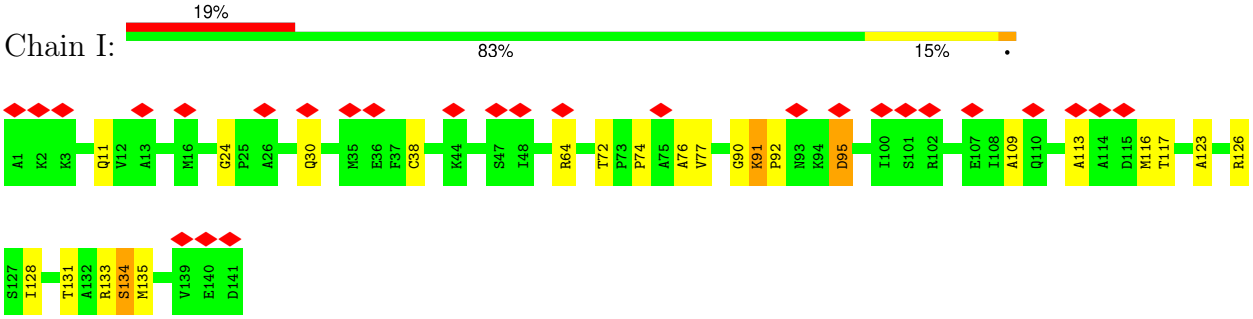
• Molecule 8: 50S ribosomal protein L9

Chain H:



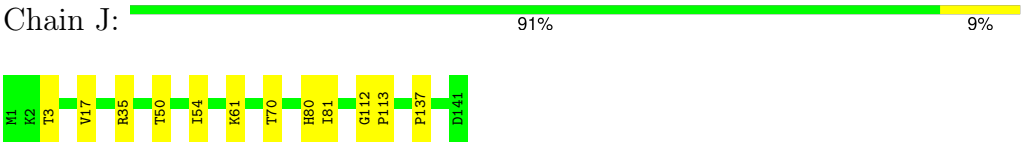
• Molecule 9: 50S ribosomal protein L11

Chain I:



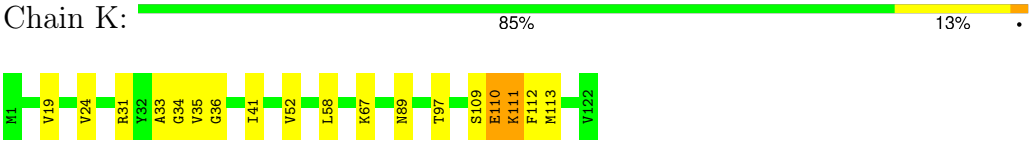
• Molecule 10: 50S ribosomal protein L13

Chain J:



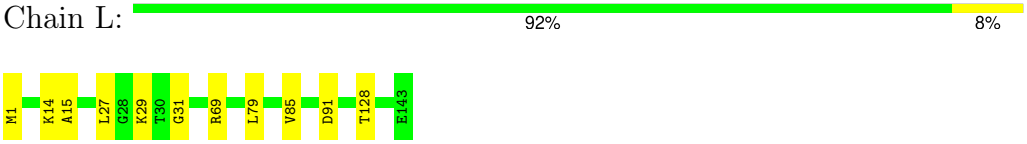
• Molecule 11: 50S ribosomal protein L14

Chain K:



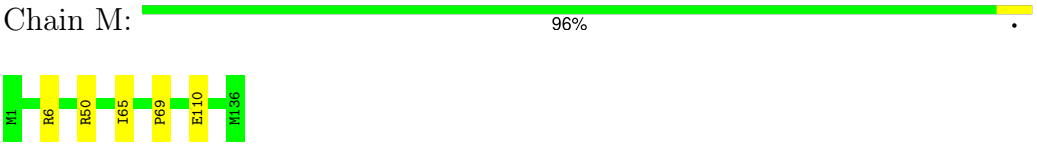
• Molecule 12: 50S ribosomal protein L15

Chain L:



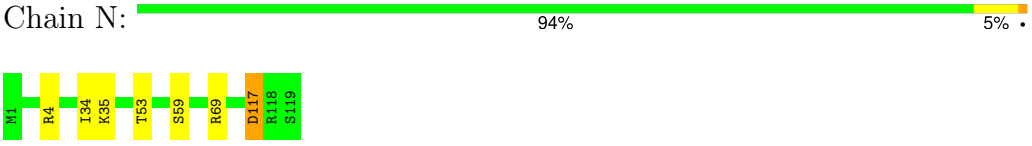
• Molecule 13: 50S ribosomal protein L16

Chain M:



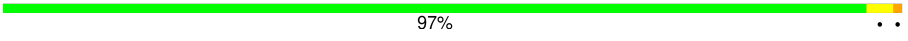
• Molecule 14: 50S ribosomal protein L17

Chain N:



• Molecule 15: 50S ribosomal protein L18

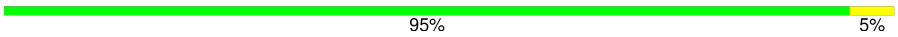
Chain O:





• Molecule 16: 50S ribosomal protein L19

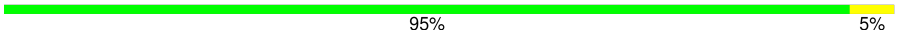
Chain P:

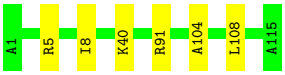




• Molecule 17: 50S ribosomal protein L20

Chain Q:





• Molecule 18: 50S ribosomal protein L21

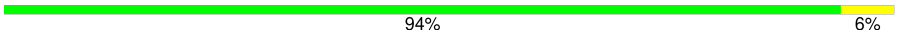
Chain R:

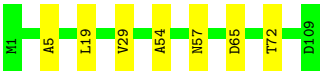




• Molecule 19: 50S ribosomal protein L22

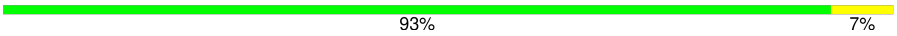
Chain S:

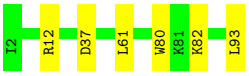




• Molecule 20: 50S ribosomal protein L23

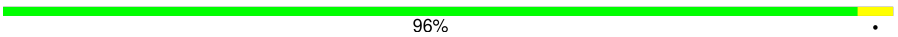
Chain T:





• Molecule 21: 50S ribosomal protein L24

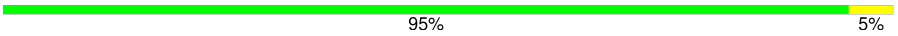
Chain U:





• Molecule 22: 50S ribosomal protein L25

Chain V:

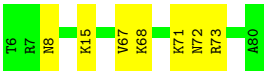




• Molecule 23: 50S ribosomal protein L27

Chain W:





• Molecule 24: 50S ribosomal protein L28

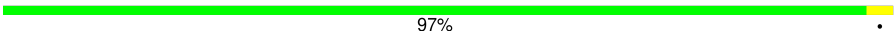
Chain X:



There are no outlier residues recorded for this chain.

• Molecule 25: 50S ribosomal protein L29

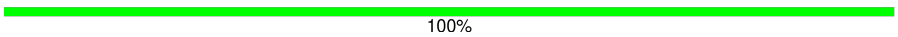
Chain Y:





• Molecule 26: 50S ribosomal protein L30

Chain Z:

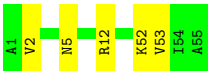


There are no outlier residues recorded for this chain.

• Molecule 27: 50S ribosomal protein L32

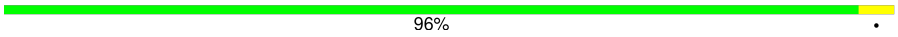
Chain 0:





• Molecule 28: 50S ribosomal protein L33

Chain 1:





• Molecule 29: 50S ribosomal protein L34

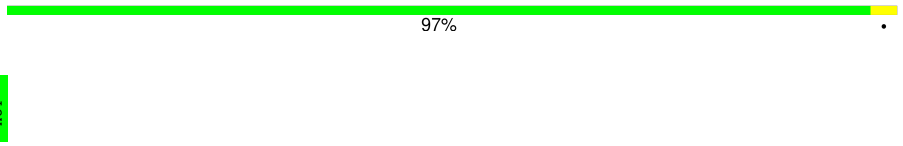
Chain 2:





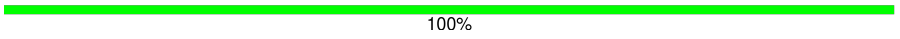
• Molecule 30: 50S ribosomal protein L35

Chain 3:



• Molecule 31: 50S ribosomal protein L36

Chain 4:

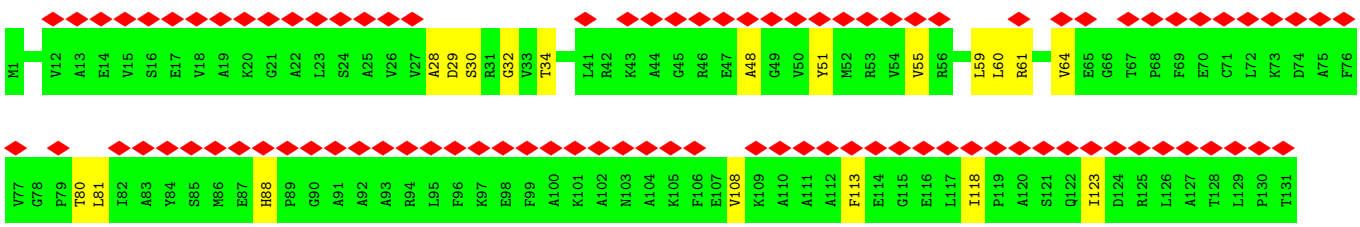


There are no outlier residues recorded for this chain.

• Molecule 32: 50S ribosomal protein L10

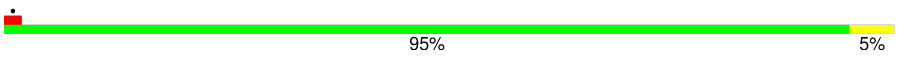
Chain 5:

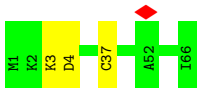




• Molecule 33: 50S ribosomal protein L31

Chain 6:

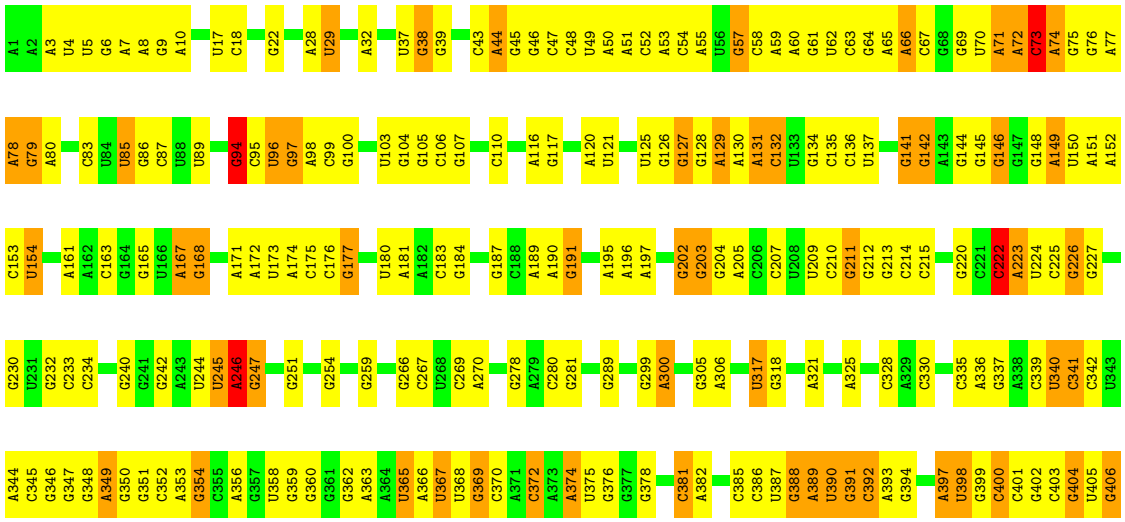


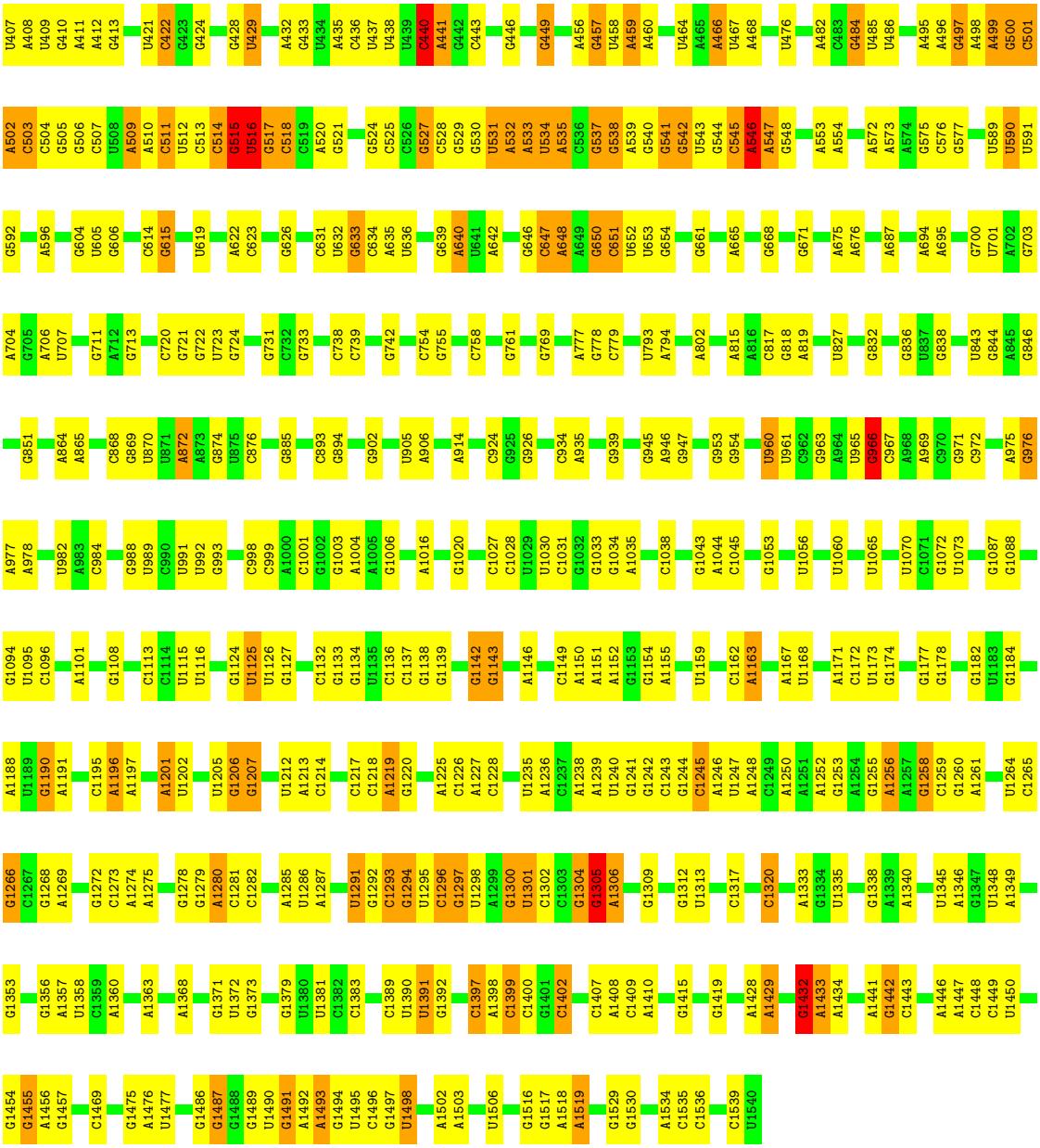


• Molecule 34: 16S rRNA

Chain a:

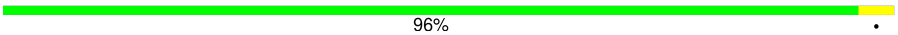






• Molecule 35: 30S ribosomal protein S2

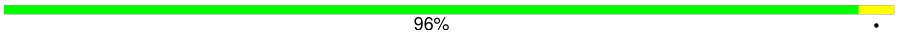
Chain b:

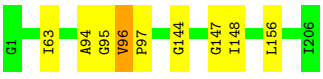




• Molecule 36: 30S ribosomal protein S3

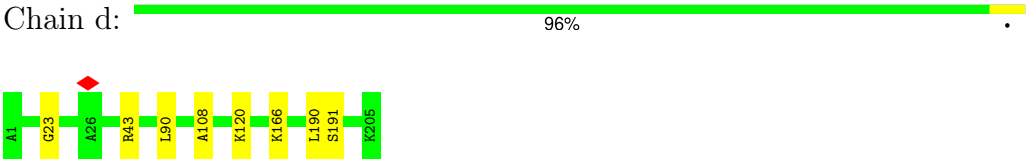
Chain c:





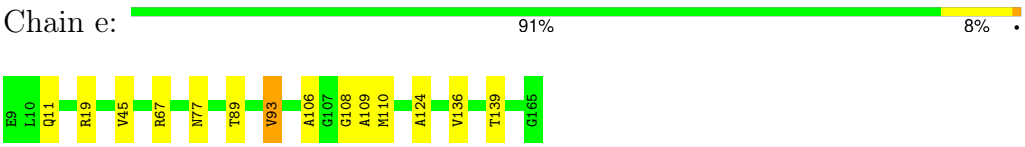
• Molecule 37: 30S ribosomal protein S4

Chain d:



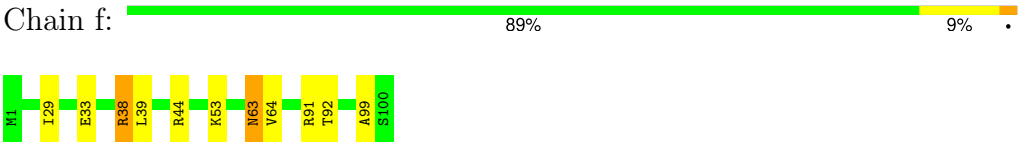
• Molecule 38: 30S ribosomal protein S5

Chain e:



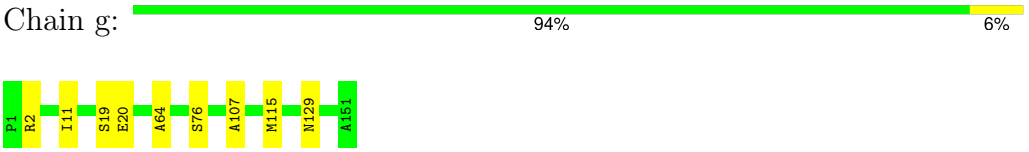
• Molecule 39: 30S ribosomal protein S6

Chain f:



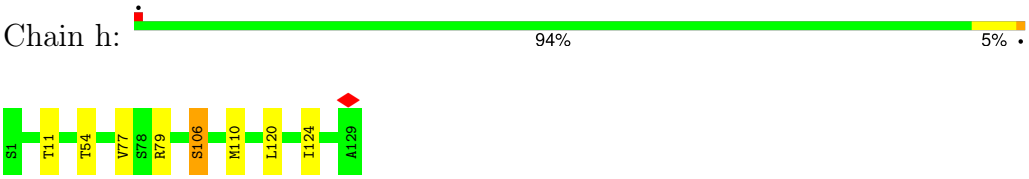
• Molecule 40: 30S ribosomal protein S7

Chain g:



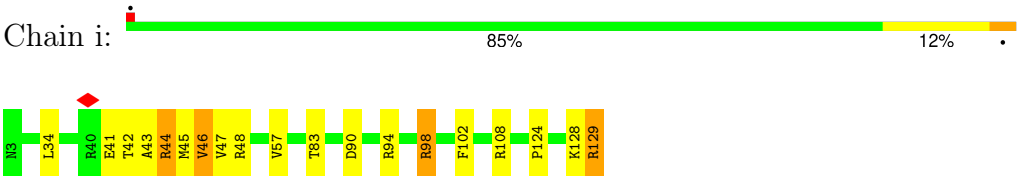
• Molecule 41: 30S ribosomal protein S8

Chain h:



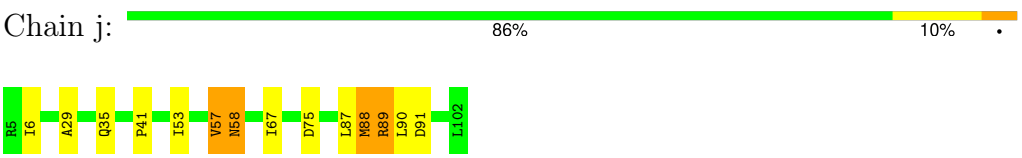
• Molecule 42: 30S ribosomal protein S9

Chain i:



• Molecule 43: 30S ribosomal protein S10

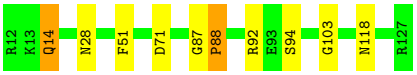
Chain j:



• Molecule 44: 30S ribosomal protein S11

Chain k:





• Molecule 45: 30S ribosomal protein S12

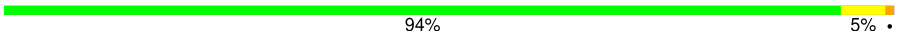
Chain l:





• Molecule 46: 30S ribosomal protein S13

Chain m:

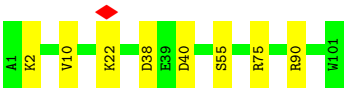




• Molecule 47: 30S ribosomal protein S14

Chain n:





• Molecule 48: 30S ribosomal protein S15

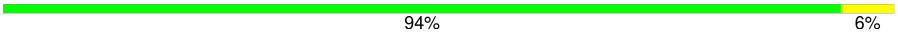
Chain o:





• Molecule 49: 30S ribosomal protein S16

Chain p:





• Molecule 50: 30S ribosomal protein S17

Chain q:





• Molecule 51: 30S ribosomal protein S18

Chain r:

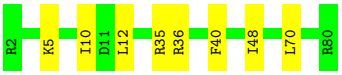




• Molecule 52: 30S ribosomal protein S19

Chain s:

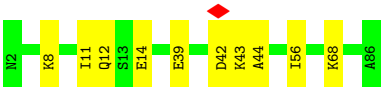




• Molecule 53: 30S ribosomal protein S20

Chain t:

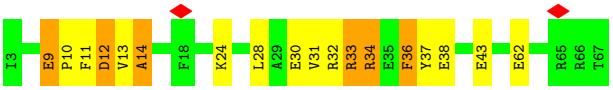




• Molecule 54: 30S ribosomal protein S21

Chain u:

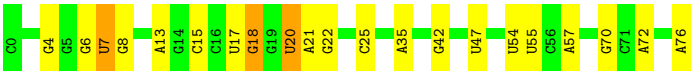




• Molecule 55: tRNA-fMet

Chain v:

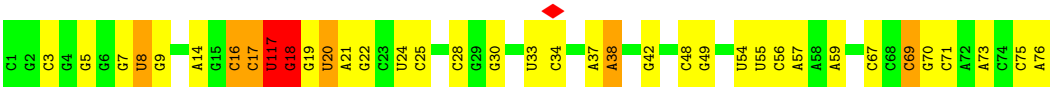




• Molecule 55: tRNA-fMet

Chain w:





• Molecule 56: mRNA

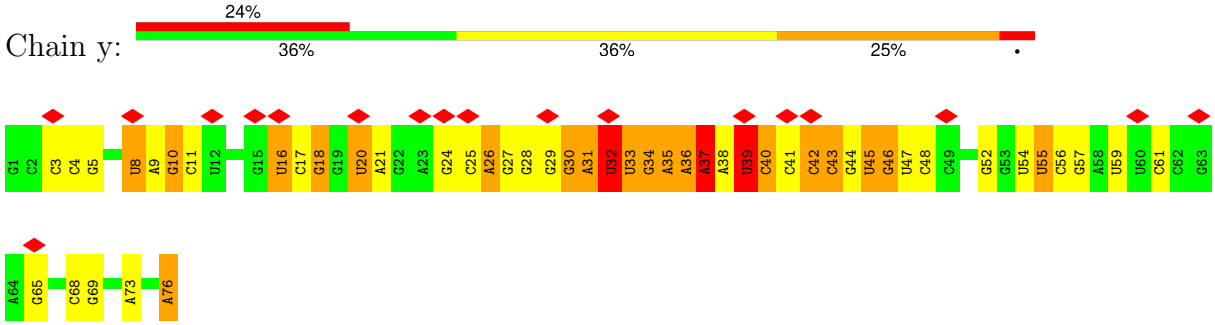
Chain x:





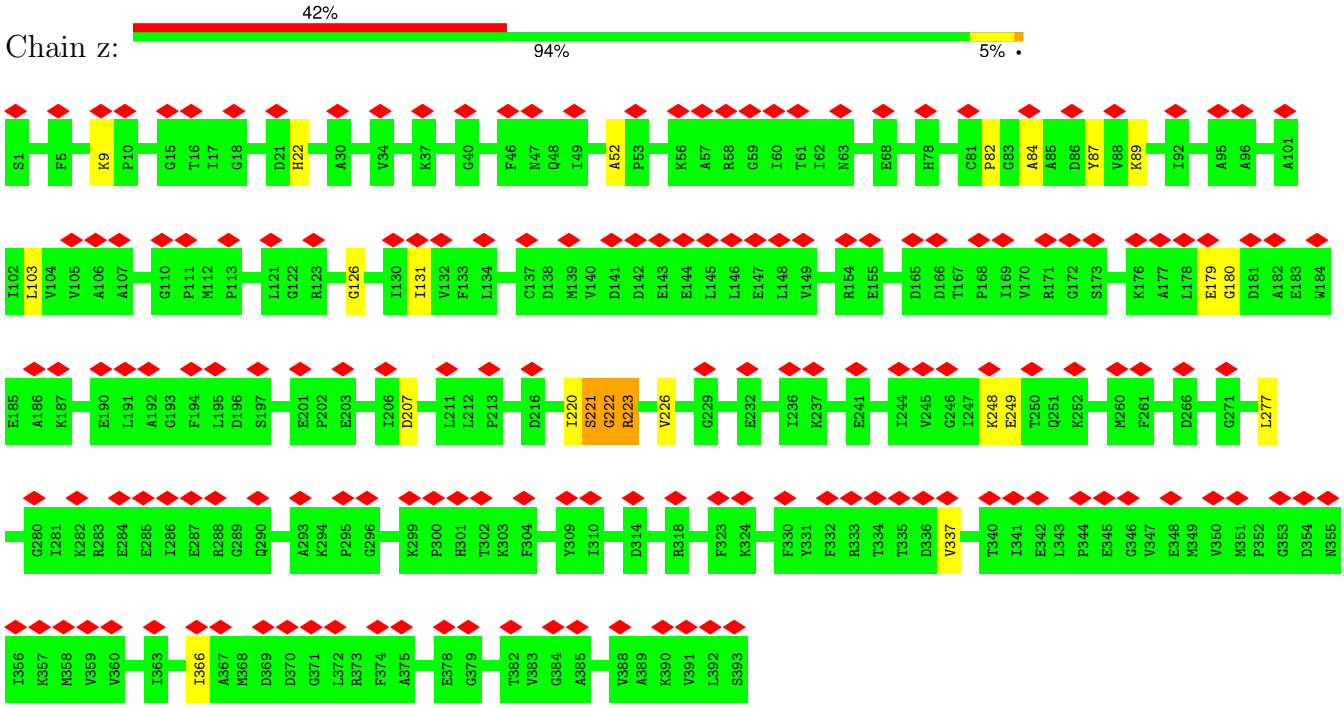
• Molecule 57: Phe-tRNA-Phe

Chain y:



• Molecule 58: Elongation factor Tu 2

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17523	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	67	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	51020	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.178	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.00651	Depositor
Map size (Å)	390.04, 390.04, 390.04	wwPDB
Map dimensions	398, 398, 398	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 5MC, 7MG, 6MZ, FME, GTP, H2U, OMG, MA6, MIA, 5MU, 1MG, UR3, OMU, PSU, 2MA, MG, K, 3TD, 2MG, 4OC, 4SU

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	A	0.37	0/69174	0.71	32/107907 (0.0%)
2	B	0.37	0/2876	0.69	2/4483 (0.0%)
3	C	0.53	0/2121	0.74	0/2852
4	D	0.53	0/1578	0.78	2/2124 (0.1%)
5	E	0.51	0/1563	0.82	0/2103
6	F	0.55	0/1434	0.81	1/1926 (0.1%)
7	G	0.54	0/1324	0.75	0/1794
8	H	0.56	0/1122	0.76	0/1515
9	I	0.68	0/1046	0.91	2/1410 (0.1%)
10	J	0.52	0/1143	0.81	2/1540 (0.1%)
11	K	0.53	0/947	0.73	0/1268
12	L	0.55	0/1052	0.85	0/1401
13	M	0.50	0/1093	0.78	0/1460
14	N	0.57	0/964	0.87	0/1289
15	O	0.54	0/902	0.86	0/1209
16	P	0.50	0/929	0.73	0/1242
17	Q	0.54	0/946	0.91	0/1260
18	R	0.52	0/823	0.74	2/1100 (0.2%)
19	S	0.51	0/852	0.83	0/1142
20	T	0.53	0/736	0.76	0/984
21	U	0.51	0/787	0.75	0/1051
22	V	0.50	0/752	0.75	0/1008
23	W	0.49	0/579	0.68	0/767
24	X	0.51	0/635	0.74	0/848
25	Y	0.55	0/495	0.87	0/658
26	Z	0.57	0/438	0.82	0/586
27	0	0.50	0/440	0.81	0/588
28	1	0.47	0/424	0.66	0/565
29	2	0.58	0/370	1.00	0/487
30	3	0.50	0/513	0.87	0/676
31	4	0.48	0/303	0.71	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	5	0.65	0/1001	0.86	0/1350
33	6	0.57	0/531	0.81	0/709
34	a	0.38	0/36776	0.74	32/57365 (0.1%)
35	b	0.57	0/1735	0.80	0/2338
36	c	0.55	0/1651	0.80	0/2225
37	d	0.55	0/1665	0.82	0/2227
38	e	0.55	0/1180	0.83	0/1587
39	f	0.58	0/835	0.82	0/1128
40	g	0.54	0/1195	0.82	0/1602
41	h	0.53	0/989	0.83	0/1326
42	i	0.56	0/1034	0.77	0/1375
43	j	0.56	0/796	0.74	0/1077
44	k	0.54	0/885	0.79	0/1195
45	l	0.57	0/954	0.77	1/1282 (0.1%)
46	m	0.58	0/900	0.87	0/1204
47	n	0.55	0/822	0.81	0/1095
48	o	0.52	0/722	0.85	0/964
49	p	0.55	0/659	0.79	0/884
50	q	0.56	0/657	0.72	0/881
51	r	0.57	0/544	0.82	0/731
52	s	0.57	0/652	0.77	0/877
53	t	0.56	0/671	0.88	0/888
54	u	0.66	0/550	0.98	0/728
55	v	0.40	1/1747 (0.1%)	0.71	0/2721
55	w	0.84	1/1747 (0.1%)	0.86	5/2721 (0.2%)
56	x	0.37	0/280	0.74	1/433 (0.2%)
57	y	0.39	0/1607	0.70	0/2501
58	z	0.56	0/3086	0.76	0/4175
All	All	0.44	2/164232 (0.0%)	0.74	82/245229 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	117	U	O3'-P	-31.02	1.14	1.61
55	v	7	4SU	O3'-P	5.11	1.61	1.56

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	w	117	U	P-O3'-C3'	18.64	148.16	120.20
55	w	117	U	O3'-P-O5'	10.76	120.13	104.00
1	A	51	G	C2'-C3'-O3'	9.48	123.73	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	1305	G	C2'-C3'-O3'	9.24	123.36	109.50
1	A	242	G	C2'-C3'-O3'	9.18	123.27	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62277	0	31339	268	0
2	B	2572	0	1302	4	0
3	C	2082	0	2157	5	0
4	D	1557	0	1604	6	0
5	E	1544	0	1607	4	0
6	F	1410	0	1447	1	0
7	G	1304	0	1348	5	0
8	H	1111	0	1148	1	0
9	I	1032	0	1088	11	0
10	J	1120	0	1151	3	0
11	K	938	0	1012	12	0
12	L	1043	0	1123	1	0
13	M	1074	0	1157	1	0
14	N	951	0	994	2	0
15	O	892	0	923	1	0
16	P	917	0	965	2	0
17	Q	933	0	1006	3	0
18	R	810	0	834	6	0
19	S	845	0	909	1	0
20	T	730	0	795	2	0
21	U	779	0	834	0	0
22	V	739	0	763	2	0
23	W	572	0	593	1	0
24	X	625	0	655	0	0
25	Y	494	0	530	1	0
26	Z	434	0	477	0	0
27	0	434	0	448	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	1	417	0	451	2	0
29	2	367	0	405	3	0
30	3	504	0	574	0	0
31	4	302	0	343	0	0
32	5	988	0	1025	7	0
33	6	522	0	524	0	0
34	a	33095	0	16676	386	0
35	b	1704	0	1732	0	0
36	c	1624	0	1699	3	0
37	d	1643	0	1710	2	0
38	e	1164	0	1212	7	0
39	f	817	0	808	4	0
40	g	1181	0	1240	2	0
41	h	979	0	1034	3	0
42	i	1022	0	1070	16	0
43	j	786	0	828	7	0
44	k	869	0	878	2	0
45	l	940	0	1001	5	0
46	m	891	0	955	2	0
47	n	810	0	852	0	0
48	o	714	0	736	8	0
49	p	649	0	666	1	0
50	q	648	0	691	2	0
51	r	535	0	552	3	0
52	s	637	0	665	4	0
53	t	665	0	714	6	0
54	u	544	0	579	7	0
55	v	1644	0	840	4	0
55	w	1644	0	841	16	0
56	x	252	0	130	38	0
57	y	1632	0	843	127	0
58	z	3031	0	3052	13	0
59	A	10	0	10	0	0
60	0	1	0	0	0	0
60	2	1	0	0	0	0
60	4	1	0	0	0	0
60	A	965	0	0	0	0
60	B	27	0	0	0	0
60	C	2	0	0	0	0
60	D	3	0	0	0	0
60	E	3	0	0	0	0
60	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	L	3	0	0	0	0
60	N	1	0	0	0	0
60	Q	1	0	0	0	0
60	S	1	0	0	0	0
60	U	1	0	0	0	0
60	X	1	0	0	0	0
60	Y	1	0	0	0	0
60	Z	1	0	0	0	0
60	a	375	0	0	0	0
60	c	1	0	0	0	0
60	d	1	0	0	0	0
60	e	1	0	0	0	0
60	f	1	0	0	0	0
60	g	1	0	0	0	0
60	i	2	0	0	0	0
60	k	1	0	0	0	0
60	l	1	0	0	0	0
60	m	1	0	0	0	0
60	q	1	0	0	0	0
60	v	9	0	0	0	0
60	w	3	0	0	0	0
60	x	1	0	0	0	0
61	A	1	0	0	0	0
62	z	11	0	8	0	0
63	z	32	0	12	0	0
64	0	1	0	0	0	0
64	2	1	0	0	0	0
64	3	1	0	0	0	0
64	A	293	0	0	0	0
64	B	8	0	0	0	0
64	C	3	0	0	0	0
64	D	3	0	0	0	0
64	L	1	0	0	0	0
64	N	1	0	0	0	0
64	O	1	0	0	0	0
64	Q	1	0	0	0	0
64	V	1	0	0	0	0
64	W	1	0	0	0	0
64	a	93	0	0	0	0
64	l	1	0	0	0	0
64	m	1	0	0	0	0
64	o	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	s	3	0	0	0	0
64	t	1	0	0	0	0
64	u	1	0	0	0	0
64	v	1	0	0	0	0
64	w	1	0	0	0	0
All	All	154325	0	103565	929	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 929 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:w:117:U:O3'	55:w:18:G:P	1.14	1.54
57:y:25:C:C2'	57:y:26:A:H5"	1.46	1.46
1:A:1913:A:H2'	34:a:1492[A]:A:N1	1.36	1.38
57:y:30:G:C2	57:y:31:A:N6	1.90	1.37
57:y:41:C:H2'	57:y:42:C:O4'	1.20	1.36

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	269/271 (99%)	240 (89%)	26 (10%)	3 (1%)	11 38
4	D	206/208 (99%)	187 (91%)	16 (8%)	3 (2%)	8 30
5	E	198/200 (99%)	181 (91%)	15 (8%)	2 (1%)	12 40
6	F	175/177 (99%)	157 (90%)	18 (10%)	0	100 100
7	G	172/174 (99%)	158 (92%)	14 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	H	147/149 (99%)	127 (86%)	17 (12%)	3 (2%)	6 25
9	I	139/141 (99%)	109 (78%)	26 (19%)	4 (3%)	3 19
10	J	139/141 (99%)	132 (95%)	7 (5%)	0	100 100
11	K	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	4 21
12	L	141/143 (99%)	116 (82%)	20 (14%)	5 (4%)	3 16
13	M	134/136 (98%)	126 (94%)	6 (4%)	2 (2%)	8 30
14	N	117/119 (98%)	104 (89%)	11 (9%)	2 (2%)	7 28
15	O	114/116 (98%)	106 (93%)	8 (7%)	0	100 100
16	P	112/114 (98%)	98 (88%)	14 (12%)	0	100 100
17	Q	113/115 (98%)	112 (99%)	1 (1%)	0	100 100
18	R	100/102 (98%)	80 (80%)	16 (16%)	4 (4%)	2 15
19	S	107/109 (98%)	96 (90%)	10 (9%)	1 (1%)	14 42
20	T	90/92 (98%)	81 (90%)	8 (9%)	1 (1%)	11 38
21	U	100/102 (98%)	86 (86%)	11 (11%)	3 (3%)	3 18
22	V	90/92 (98%)	83 (92%)	6 (7%)	1 (1%)	11 38
23	W	73/75 (97%)	66 (90%)	6 (8%)	1 (1%)	9 31
24	X	75/77 (97%)	69 (92%)	6 (8%)	0	100 100
25	Y	58/60 (97%)	54 (93%)	4 (7%)	0	100 100
26	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100 100
27	0	53/55 (96%)	49 (92%)	3 (6%)	1 (2%)	6 26
28	1	49/51 (96%)	42 (86%)	6 (12%)	1 (2%)	6 25
29	2	43/45 (96%)	42 (98%)	1 (2%)	0	100 100
30	3	62/64 (97%)	57 (92%)	5 (8%)	0	100 100
31	4	36/38 (95%)	32 (89%)	4 (11%)	0	100 100
32	5	129/131 (98%)	98 (76%)	21 (16%)	10 (8%)	1 4
33	6	64/66 (97%)	55 (86%)	8 (12%)	1 (2%)	7 29
35	b	216/218 (99%)	187 (87%)	23 (11%)	6 (3%)	4 19
36	c	204/206 (99%)	187 (92%)	12 (6%)	5 (2%)	4 21
37	d	203/205 (99%)	181 (89%)	20 (10%)	2 (1%)	12 40
38	e	156/157 (99%)	133 (85%)	20 (13%)	3 (2%)	6 26
39	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	2 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
40	g	149/151 (99%)	132 (89%)	13 (9%)	4 (3%)	4 20
41	h	127/129 (98%)	118 (93%)	9 (7%)	0	100 100
42	i	125/127 (98%)	94 (75%)	26 (21%)	5 (4%)	2 15
43	j	96/98 (98%)	73 (76%)	15 (16%)	8 (8%)	0 4
44	k	114/116 (98%)	100 (88%)	9 (8%)	5 (4%)	2 13
45	l	119/121 (98%)	96 (81%)	15 (13%)	8 (7%)	1 6
46	m	113/115 (98%)	102 (90%)	9 (8%)	2 (2%)	6 26
47	n	99/101 (98%)	85 (86%)	9 (9%)	5 (5%)	1 10
48	o	86/88 (98%)	79 (92%)	2 (2%)	5 (6%)	1 8
49	p	80/82 (98%)	69 (86%)	8 (10%)	3 (4%)	2 15
50	q	78/80 (98%)	68 (87%)	9 (12%)	1 (1%)	9 33
51	r	63/65 (97%)	52 (82%)	7 (11%)	4 (6%)	1 7
52	s	77/79 (98%)	67 (87%)	9 (12%)	1 (1%)	9 33
53	t	83/85 (98%)	75 (90%)	6 (7%)	2 (2%)	4 22
54	u	63/65 (97%)	40 (64%)	14 (22%)	9 (14%)	0 0
58	z	391/393 (100%)	349 (89%)	32 (8%)	10 (3%)	4 21
All	All	6219/6322 (98%)	5471 (88%)	605 (10%)	143 (2%)	7 23

5 of 143 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	89	ASN
11	K	111	LYS
12	L	31	GLY
18	R	51	VAL
21	U	6	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	216/216 (100%)	206 (95%)	10 (5%)	24 50
4	D	163/163 (100%)	154 (94%)	9 (6%)	19 46
5	E	164/164 (100%)	160 (98%)	4 (2%)	43 62
6	F	148/148 (100%)	143 (97%)	5 (3%)	32 57
7	G	135/135 (100%)	134 (99%)	1 (1%)	76 78
8	H	114/114 (100%)	113 (99%)	1 (1%)	70 76
9	I	109/109 (100%)	101 (93%)	8 (7%)	13 39
10	J	115/115 (100%)	109 (95%)	6 (5%)	21 48
11	K	103/103 (100%)	97 (94%)	6 (6%)	18 45
12	L	102/102 (100%)	97 (95%)	5 (5%)	22 49
13	M	109/109 (100%)	108 (99%)	1 (1%)	70 76
14	N	99/99 (100%)	95 (96%)	4 (4%)	28 53
15	O	86/86 (100%)	82 (95%)	4 (5%)	23 50
16	P	99/99 (100%)	96 (97%)	3 (3%)	36 59
17	Q	88/88 (100%)	85 (97%)	3 (3%)	32 57
18	R	84/84 (100%)	82 (98%)	2 (2%)	43 62
19	S	92/92 (100%)	88 (96%)	4 (4%)	26 51
20	T	79/79 (100%)	77 (98%)	2 (2%)	42 62
21	U	83/83 (100%)	82 (99%)	1 (1%)	63 72
22	V	77/77 (100%)	76 (99%)	1 (1%)	61 71
23	W	57/57 (100%)	53 (93%)	4 (7%)	14 40
24	X	67/67 (100%)	67 (100%)	0	100 100
25	Y	55/55 (100%)	54 (98%)	1 (2%)	51 67
26	Z	47/47 (100%)	47 (100%)	0	100 100
27	0	46/46 (100%)	44 (96%)	2 (4%)	26 51
28	1	46/46 (100%)	46 (100%)	0	100 100
29	2	37/37 (100%)	34 (92%)	3 (8%)	11 36
30	3	51/51 (100%)	49 (96%)	2 (4%)	28 53
31	4	34/34 (100%)	34 (100%)	0	100 100
32	5	100/100 (100%)	99 (99%)	1 (1%)	68 75
33	6	59/59 (100%)	57 (97%)	2 (3%)	32 57
35	b	180/180 (100%)	178 (99%)	2 (1%)	65 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	c	170/170 (100%)	170 (100%)	0	100 100
37	d	172/172 (100%)	169 (98%)	3 (2%)	53 67
38	e	120/119 (101%)	115 (96%)	5 (4%)	26 52
39	f	87/87 (100%)	83 (95%)	4 (5%)	24 50
40	g	124/124 (100%)	122 (98%)	2 (2%)	55 68
41	h	104/104 (100%)	99 (95%)	5 (5%)	23 50
42	i	105/105 (100%)	100 (95%)	5 (5%)	23 50
43	j	86/86 (100%)	82 (95%)	4 (5%)	23 50
44	k	89/89 (100%)	85 (96%)	4 (4%)	24 51
45	l	102/102 (100%)	99 (97%)	3 (3%)	37 60
46	m	93/93 (100%)	90 (97%)	3 (3%)	34 58
47	n	83/83 (100%)	80 (96%)	3 (4%)	31 56
48	o	76/76 (100%)	74 (97%)	2 (3%)	40 61
49	p	65/65 (100%)	64 (98%)	1 (2%)	57 69
50	q	74/74 (100%)	70 (95%)	4 (5%)	20 47
51	r	56/56 (100%)	52 (93%)	4 (7%)	13 39
52	s	70/70 (100%)	68 (97%)	2 (3%)	37 60
53	t	65/65 (100%)	61 (94%)	4 (6%)	16 43
54	u	55/55 (100%)	50 (91%)	5 (9%)	9 30
58	z	325/325 (100%)	321 (99%)	4 (1%)	63 72
All	All	5165/5164 (100%)	5001 (97%)	164 (3%)	35 58

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	h	120	LEU
50	q	63	CYS
42	i	98	ARG
45	l	77	SER
52	s	12	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
23	W	8	ASN
52	s	56	HIS
36	c	122	GLN
50	q	49	ASN
58	z	13	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2897/2903 (99%)	735 (25%)	73 (2%)
2	B	119/120 (99%)	27 (22%)	4 (3%)
34	a	1537/1540 (99%)	465 (30%)	0
55	v	76/77 (98%)	17 (22%)	0
55	w	76/77 (98%)	34 (44%)	0
56	x	11/12 (91%)	7 (63%)	0
57	y	75/76 (98%)	42 (56%)	0
All	All	4791/4805 (99%)	1327 (27%)	77 (1%)

5 of 1327 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	U
1	A	4	U
1	A	5	A
1	A	6	A

5 of 77 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2296	U
1	A	2849	U
1	A	2326	C
1	A	2517	C
2	B	66	A

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

52 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
34	MA6	a	1518	34	23,26,27	1.77	5 (21%)	33,38,41	2.40	11 (33%)
1	PSU	A	2605	1	18,21,22	1.41	2 (11%)	21,30,33	2.04	4 (19%)
1	PSU	A	746	60,1	18,21,22	1.42	2 (11%)	21,30,33	2.05	5 (23%)
34	MA6	a	1519	34	23,26,27	1.74	5 (21%)	33,38,41	2.47	15 (45%)
55	5MU	w	54	55	19,22,23	1.49	4 (21%)	27,32,35	2.07	10 (37%)
1	6MZ	A	2030	1	22,25,26	1.53	4 (18%)	29,36,39	2.30	10 (34%)
57	PSU	y	32	57	18,21,22	1.33	2 (11%)	21,30,33	2.27	5 (23%)
57	H2U	y	16	57	18,21,22	0.82	1 (5%)	19,30,33	1.40	4 (21%)
1	PSU	A	955	1	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
1	2MG	A	1835	1	23,26,27	1.32	4 (17%)	33,38,41	2.28	7 (21%)
1	PSU	A	2504	1	18,21,22	1.41	2 (11%)	21,30,33	2.01	4 (19%)
1	OMC	A	2498	60,1	19,22,23	0.86	0	25,31,34	1.25	3 (12%)
55	5MU	v	54	55	19,22,23	1.49	4 (21%)	27,32,35	1.96	9 (33%)
57	5MU	y	54	57	19,22,23	1.46	4 (21%)	27,32,35	2.07	8 (29%)
1	1MG	A	745	1	23,26,27	1.42	3 (13%)	33,39,42	2.05	8 (24%)
1	2MG	A	2445	1	23,26,27	1.25	3 (13%)	33,38,41	2.35	10 (30%)
1	OMG	A	2251	55,1	23,26,27	1.25	3 (13%)	32,38,41	2.01	6 (18%)
57	PSU	y	39	57	18,21,22	1.33	2 (11%)	21,30,33	2.28	5 (23%)
55	PSU	v	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.00	4 (19%)
55	4SU	w	8	55	18,21,22	1.83	5 (27%)	25,30,33	2.23	5 (20%)
57	PSU	y	55	57	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
34	5MC	a	1407	34	19,22,23	2.05	2 (10%)	26,32,35	1.65	6 (23%)
34	2MG	a	1207	34	23,26,27	1.26	3 (13%)	33,38,41	2.77	10 (30%)
1	PSU	A	1911	1	18,21,22	1.44	2 (11%)	21,30,33	2.18	5 (23%)
1	PSU	A	2604	1	18,21,22	1.43	2 (11%)	21,30,33	2.01	5 (23%)
1	5MC	A	747	1	19,22,23	1.96	2 (10%)	26,32,35	1.54	5 (19%)
55	H2U	v	20	55	18,21,22	0.83	1 (5%)	19,30,33	1.59	3 (15%)
1	H2U	A	2449	1	18,21,22	0.92	2 (11%)	19,30,33	1.56	3 (15%)
1	PSU	A	1917	1	18,21,22	1.43	2 (11%)	21,30,33	2.07	5 (23%)
34	PSU	a	516	34	18,21,22	1.36	2 (11%)	21,30,33	2.12	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
57	7MG	y	46	57	23,26,27	1.42	3 (13%)	27,39,42	2.47	7 (25%)
55	4SU	v	7	55	18,21,22	1.79	4 (22%)	25,30,33	2.33	6 (24%)
1	5MU	A	1939	1	19,22,23	1.49	4 (21%)	27,32,35	2.08	8 (29%)
55	PSU	w	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.08	5 (23%)
1	7MG	A	2069	60,1	23,26,27	1.46	4 (17%)	27,39,42	2.52	11 (40%)
1	OMU	A	2552	60,1	19,22,23	1.30	3 (15%)	25,31,34	2.03	8 (32%)
1	5MC	A	1962	1	19,22,23	2.01	2 (10%)	26,32,35	1.48	4 (15%)
57	4SU	y	8	57	18,21,22	1.83	5 (27%)	25,30,33	2.37	7 (28%)
57	H2U	y	20	57	18,21,22	0.86	1 (5%)	19,30,33	1.48	4 (21%)
57	MIA	y	37	57	28,31,32	2.35	6 (21%)	38,44,47	2.86	15 (39%)
34	2MG	a	966	34	23,26,27	1.29	4 (17%)	33,38,41	2.63	11 (33%)
1	2MA	A	2503	60,1	22,25,26	1.59	4 (18%)	32,37,40	2.27	9 (28%)
1	PSU	A	2457	1	18,21,22	1.44	2 (11%)	21,30,33	2.08	5 (23%)
55	H2U	w	20	55	18,21,22	0.81	1 (5%)	19,30,33	1.56	3 (15%)
34	UR3	a	1498	34	19,22,23	1.16	2 (10%)	26,32,35	1.98	5 (19%)
1	PSU	A	2580	1	18,21,22	1.48	2 (11%)	21,30,33	2.07	5 (23%)
34	2MG	a	1516	34	23,26,27	1.29	4 (17%)	33,38,41	2.30	8 (24%)
34	4OC	a	1402	34	20,23,24	0.85	1 (5%)	25,32,35	1.30	4 (16%)
1	3TD	A	1915	1	19,22,23	7.12	14 (73%)	23,32,35	1.86	4 (17%)
34	7MG	a	527	34	23,26,27	1.40	2 (8%)	27,39,42	2.58	7 (25%)
34	5MC	a	967	34	19,22,23	2.06	2 (10%)	26,32,35	1.52	4 (15%)
1	6MZ	A	1618	1	22,25,26	1.52	4 (18%)	29,36,39	2.28	10 (34%)

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
34	MA6	a	1518	34	-	4/11/29/30	0/3/3/3
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	A	746	60,1	-	1/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	3/11/29/30	0/3/3/3
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
1	6MZ	A	2030	1	-	3/9/27/28	0/3/3/3
57	PSU	y	32	57	-	0/7/25/26	0/2/2/2
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/9/27/28	0/3/3/3
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
1	OMC	A	2498	60,1	-	0/9/27/28	0/2/2/2
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/7/25/26	0/3/3/3
1	2MG	A	2445	1	-	2/9/27/28	0/3/3/3
1	OMG	A	2251	55,1	-	0/9/27/28	0/3/3/3
57	PSU	y	39	57	-	2/7/25/26	0/2/2/2
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
57	PSU	y	55	57	-	2/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	2/9/27/28	0/3/3/3
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
55	H2U	v	20	55	-	0/7/38/39	0/2/2/2
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
34	PSU	a	516	34	-	3/7/25/26	0/2/2/2
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	2/7/25/26	0/2/2/2
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
1	7MG	A	2069	60,1	-	2/7/37/38	0/3/3/3
1	OMU	A	2552	60,1	-	2/9/27/28	0/2/2/2
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
57	MIA	y	37	57	-	8/15/33/34	0/3/3/3
34	2MG	a	966	34	-	3/9/27/28	0/3/3/3
1	2MA	A	2503	60,1	-	2/7/25/26	0/3/3/3
1	PSU	A	2457	1	-	2/7/25/26	0/2/2/2
55	H2U	w	20	55	-	1/7/38/39	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	2580	1	-	1/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
1	3TD	A	1915	1	-	4/7/25/26	0/2/2/2
34	7MG	a	527	34	-	2/7/37/38	0/3/3/3
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
1	6MZ	A	1618	1	-	5/9/27/28	0/3/3/3

The worst 5 of 155 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.24	1.66	1.43
1	A	1915	3TD	C2'-C1'	-15.57	1.32	1.53
1	A	1915	3TD	C6-C5	15.33	1.52	1.35
1	A	1915	3TD	C2-N1	8.61	1.47	1.37
34	a	967	5MC	C5-C4	7.81	1.50	1.44

The worst 5 of 338 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	y	37	MIA	C12-C13-C14	-8.94	110.97	127.01
34	a	527	7MG	N9-C4-N3	8.47	137.88	125.46
34	a	966	2MG	C2-N3-C4	8.36	122.46	112.00
34	a	1207	2MG	C2-N3-C4	8.31	122.40	112.00
57	y	46	7MG	N9-C4-N3	8.12	137.35	125.46

There are no chirality outliers.

5 of 86 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	a	1402	4OC	O4'-C4'-C5'-O5'
34	a	1518	MA6	C5-C6-N6-C9
34	a	1519	MA6	C5-C6-N6-C10
55	v	55	PSU	O4'-C1'-C5-C4
55	v	55	PSU	O4'-C1'-C5-C6

There are no ring outliers.

10 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	2030	6MZ	9	0
57	y	32	PSU	2	0
57	y	39	PSU	6	0
1	A	1917	PSU	3	0
34	a	516	PSU	1	0
57	y	37	MIA	10	0
34	a	966	2MG	2	0
34	a	1498	UR3	1	0
1	A	1915	3TD	1	0
1	A	1618	6MZ	8	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1417 ligands modelled in this entry, 1414 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
63	GTP	z	402	-	33,34,34	1.20	3 (9%)	50,54,54	1.73	8 (16%)
59	FME	A	3001	-	8,9,10	0.50	0	8,9,11	0.95	0
62	PHE	z	401	-	10,11,12	0.48	0	8,13,15	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	GTP	z	402	-	-	2/22/38/38	0/3/3/3
59	FME	A	3001	-	-	1/7/9/11	-
62	PHE	z	401	-	-	0/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GTP	C5-C4	3.30	1.47	1.38
63	z	402	GTP	C5-N7	-2.18	1.34	1.39
63	z	402	GTP	C6-N1	-2.07	1.35	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	z	402	GTP	C5-C4-N3	-6.11	118.67	128.39
63	z	402	GTP	C2-N3-C4	5.13	121.13	112.30
63	z	402	GTP	N9-C4-N3	4.58	135.11	125.95
63	z	402	GTP	C6-C5-N7	3.29	136.28	130.29
63	z	402	GTP	C4-C5-N7	-2.57	106.60	110.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

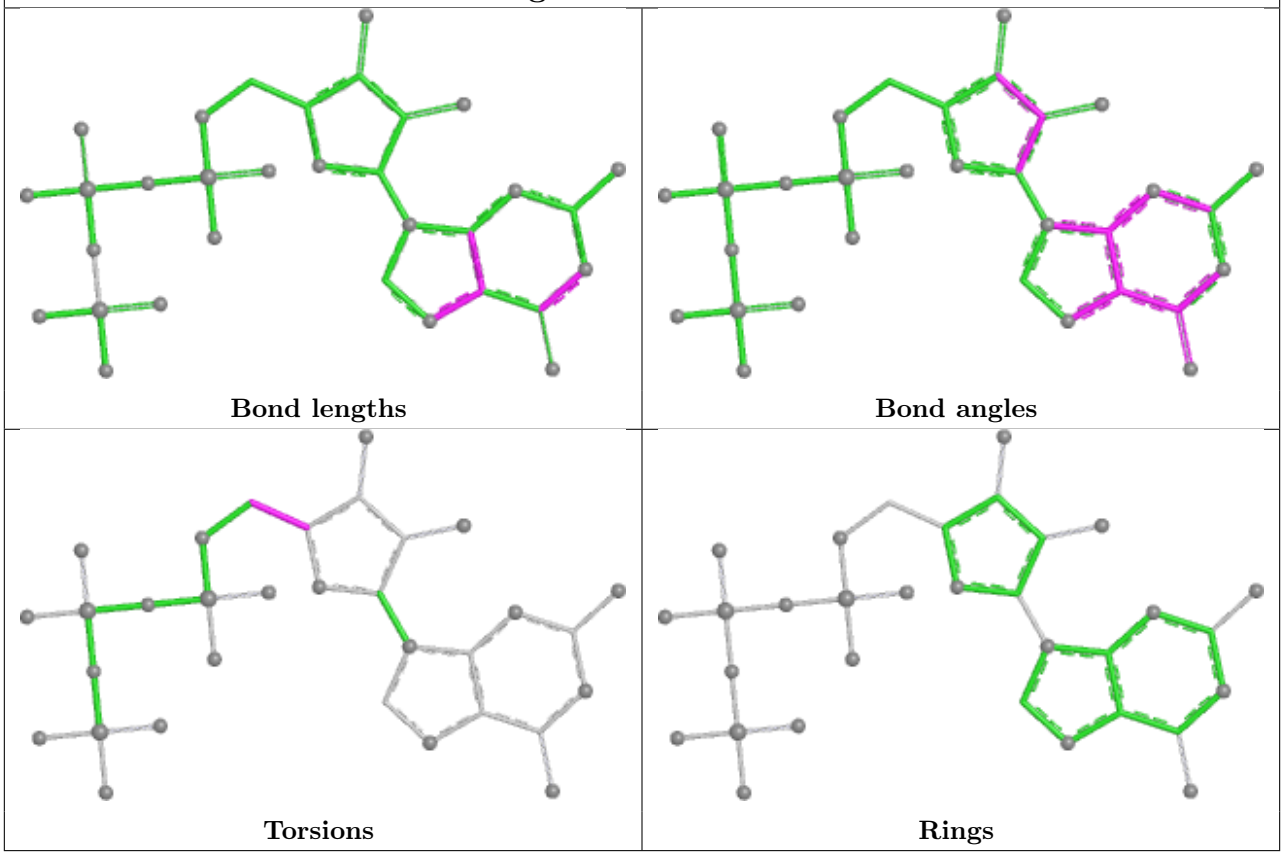
Mol	Chain	Res	Type	Atoms
59	A	3001	FME	O-C-CA-CB
63	z	402	GTP	C3'-C4'-C5'-O5'
63	z	402	GTP	O4'-C4'-C5'-O5'

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 GTP z 402



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	w	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	117:U	O3'	18:G	P	1.14

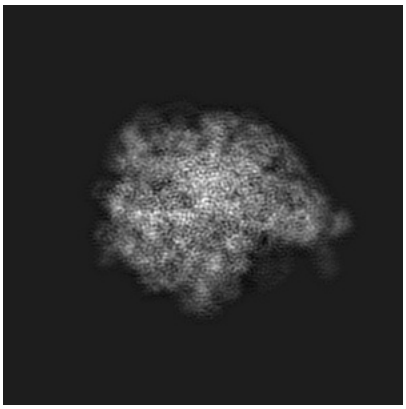
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8828. These allow visual inspection of the internal detail of the map and identification of artifacts.

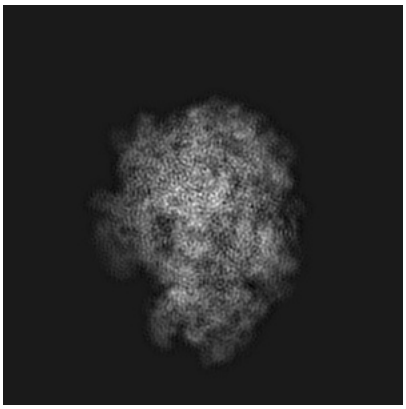
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

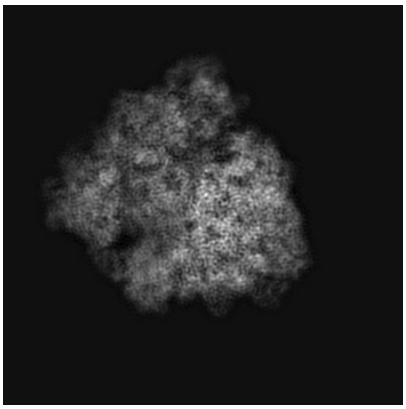
6.1.1 Primary map



X

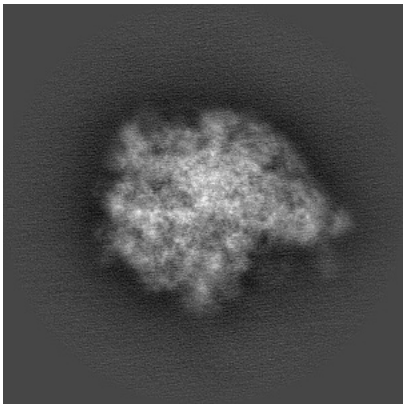


Y

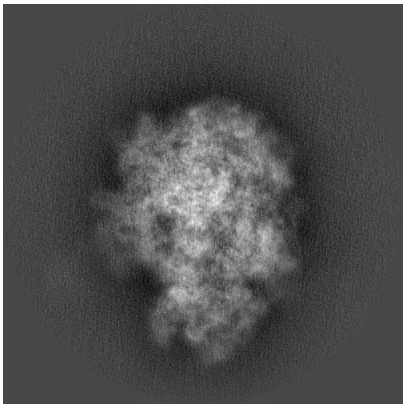


Z

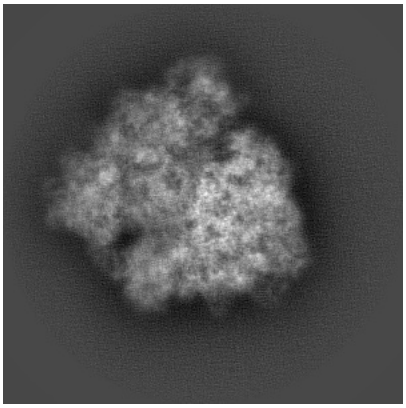
6.1.2 Raw map



X



Y

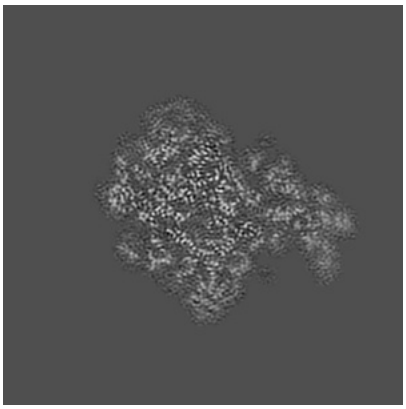


Z

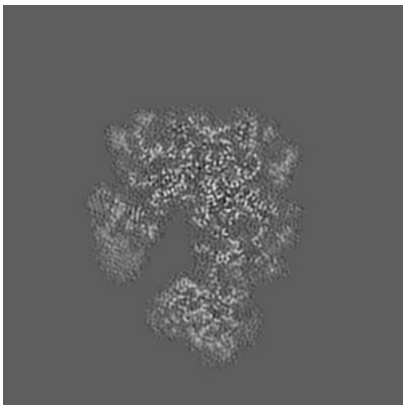
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

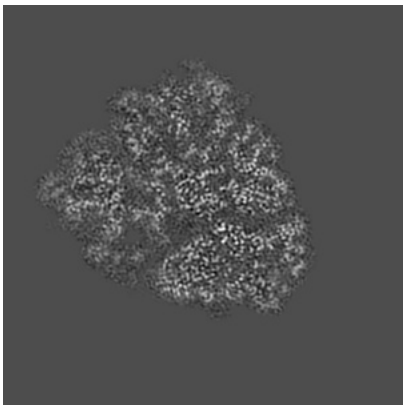
6.2.1 Primary map



X Index: 199

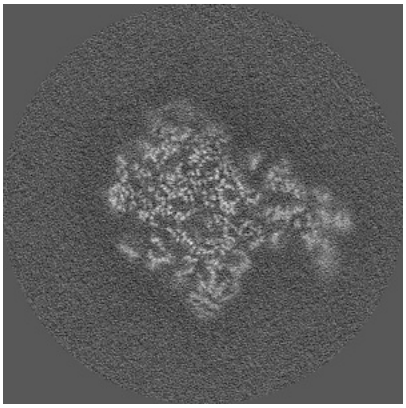


Y Index: 199

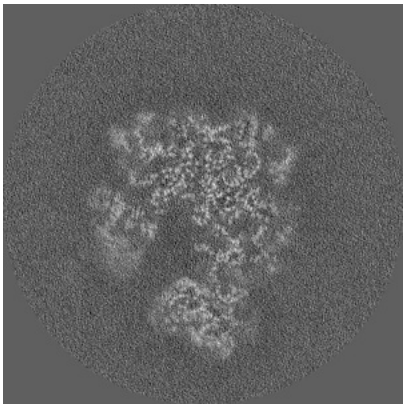


Z Index: 199

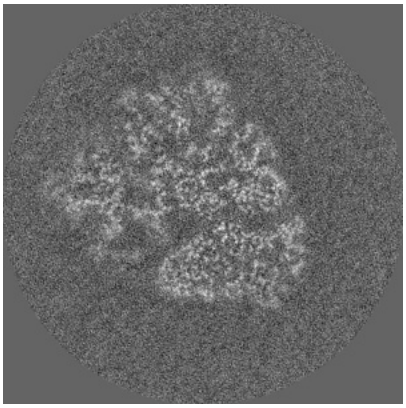
6.2.2 Raw map



X Index: 199



Y Index: 199

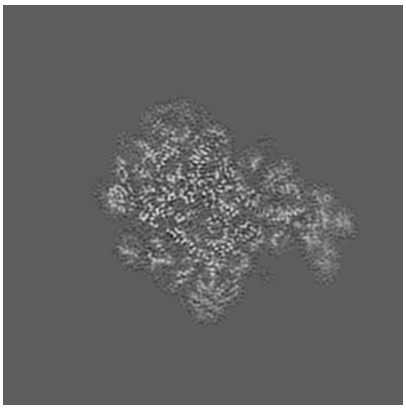


Z Index: 199

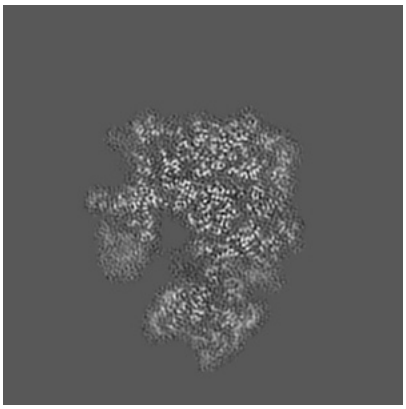
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

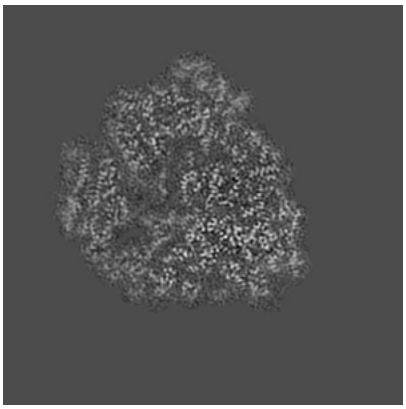
6.3.1 Primary map



X Index: 200

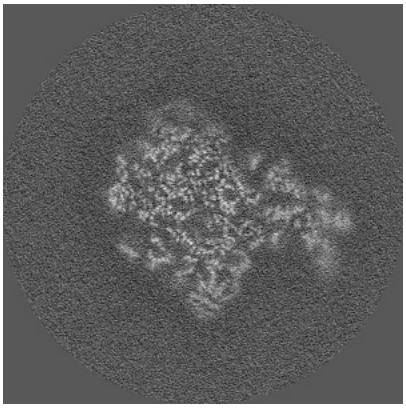


Y Index: 207

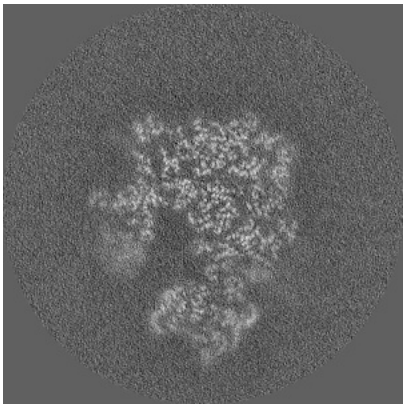


Z Index: 189

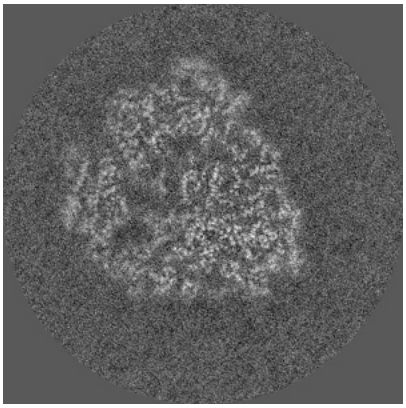
6.3.2 Raw map



X Index: 199



Y Index: 207

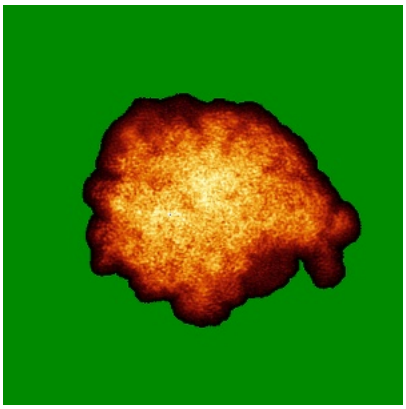


Z Index: 189

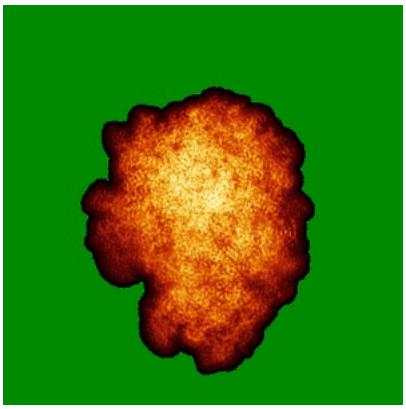
The images above show the largest variance slices of the map in three orthogonal directions.

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

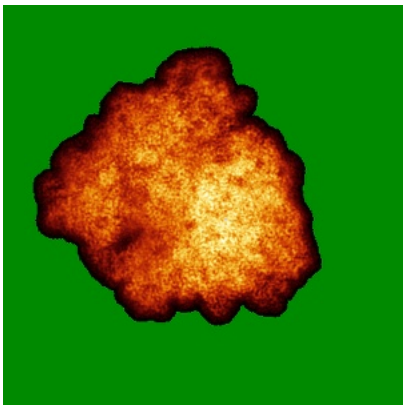
6.4.1 Primary map



X

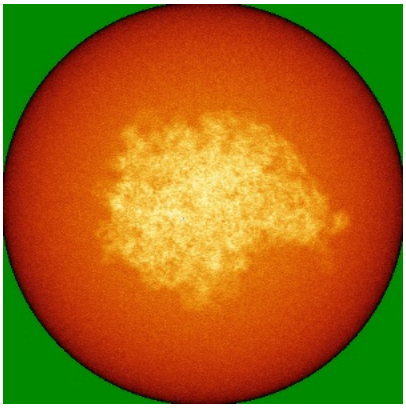


Y

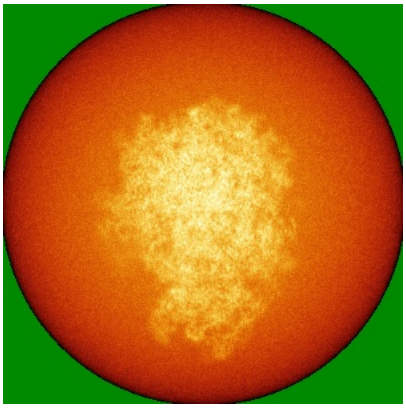


Z

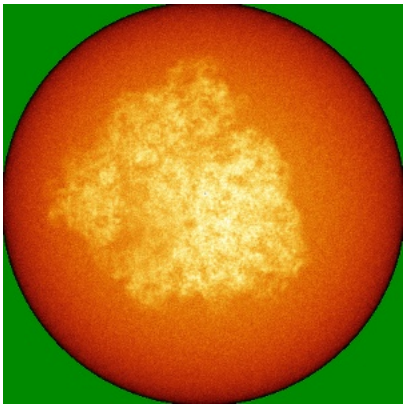
6.4.2 Raw map



X



Y

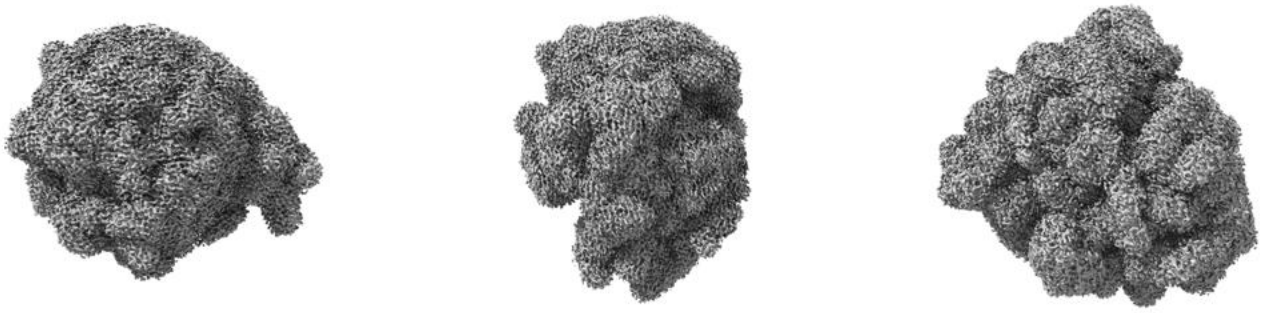


Z

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)

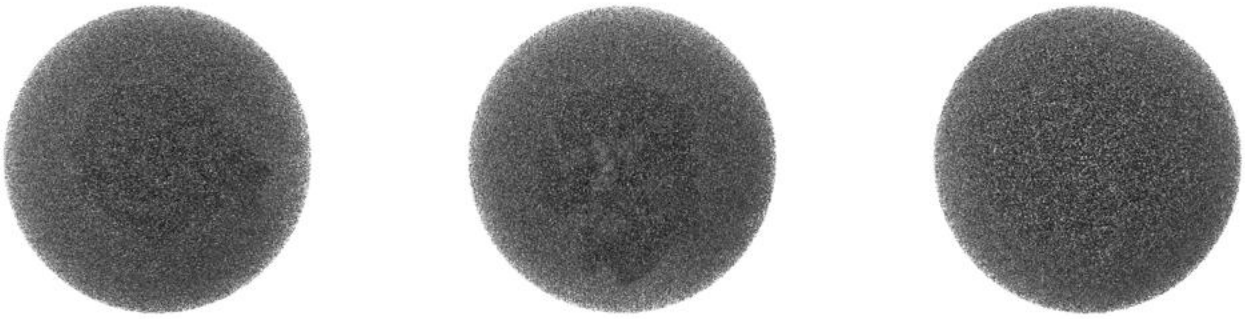
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00651. 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.

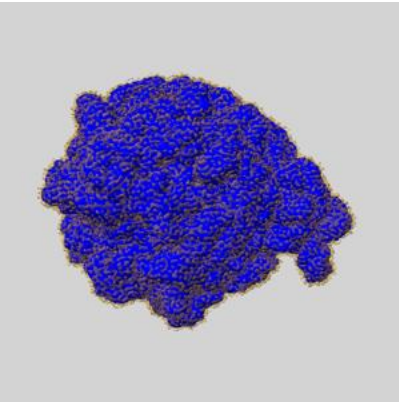
6.6 Mask visualisation (i)

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

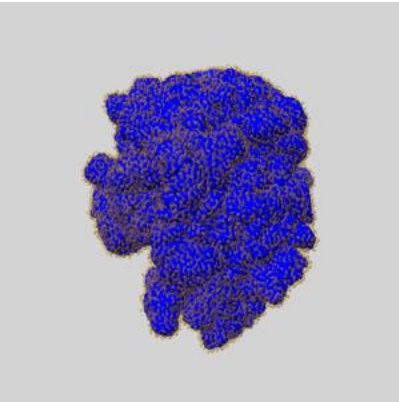
A mask typically either:

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

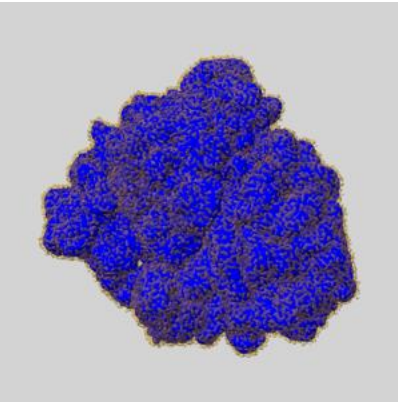
6.6.1 emd_8828_msk_1.map (i)



X



Y

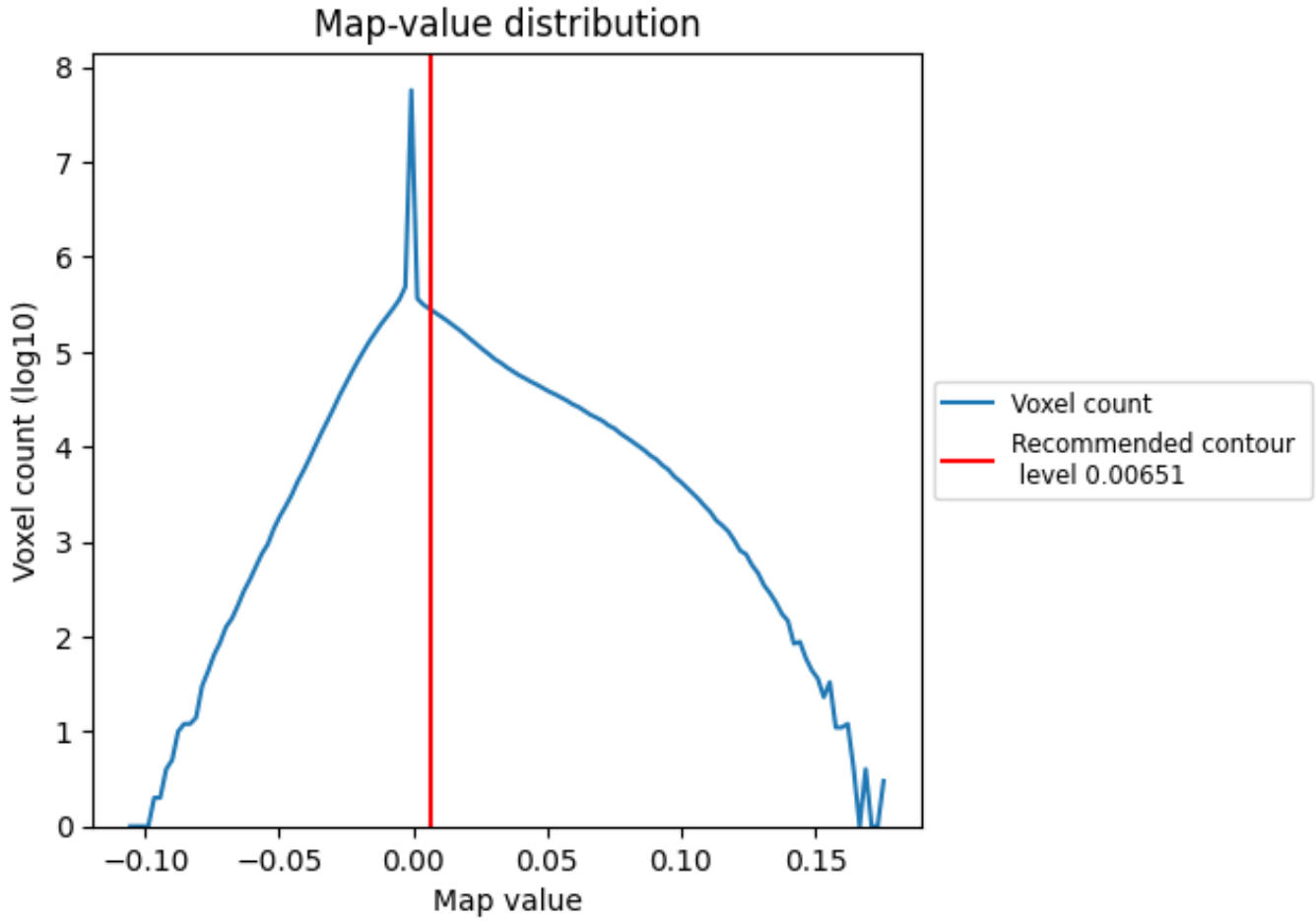


Z

7 Map analysis

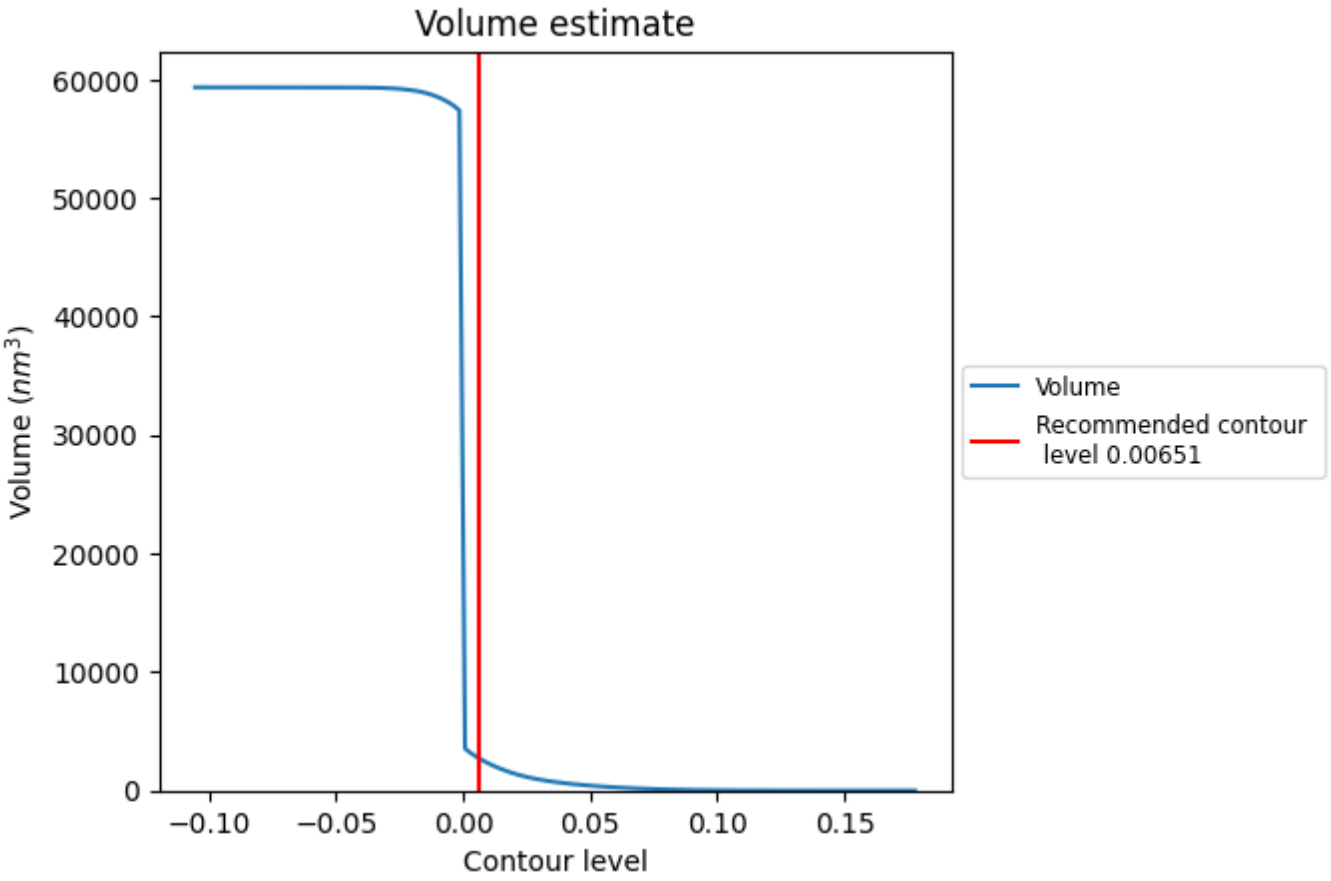
This section contains the results of statistical analysis of the map.

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.

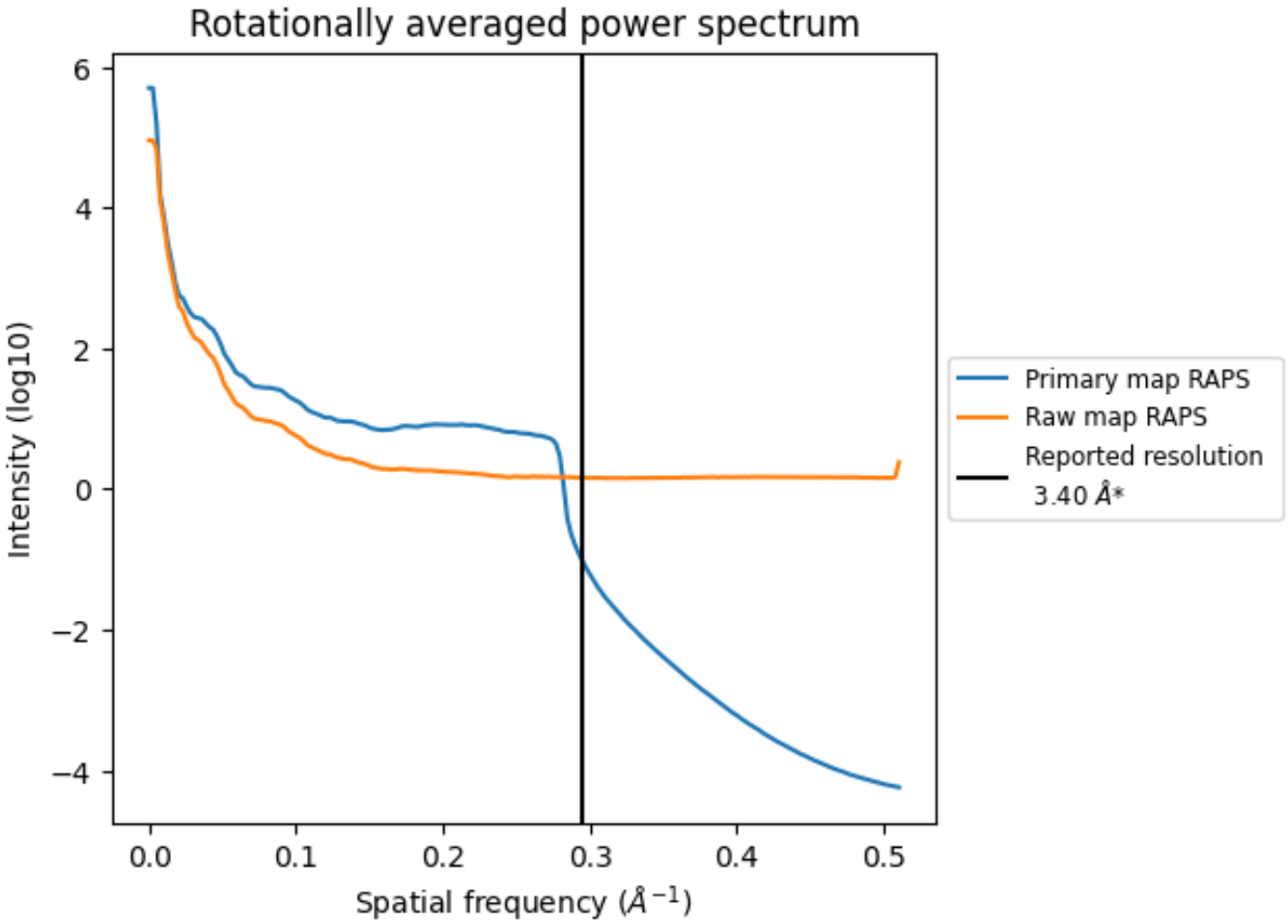
7.2 Volume estimate (i)



The volume at the recommended contour level is 2690 nm^3; this corresponds to an approximate mass of 2430 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)

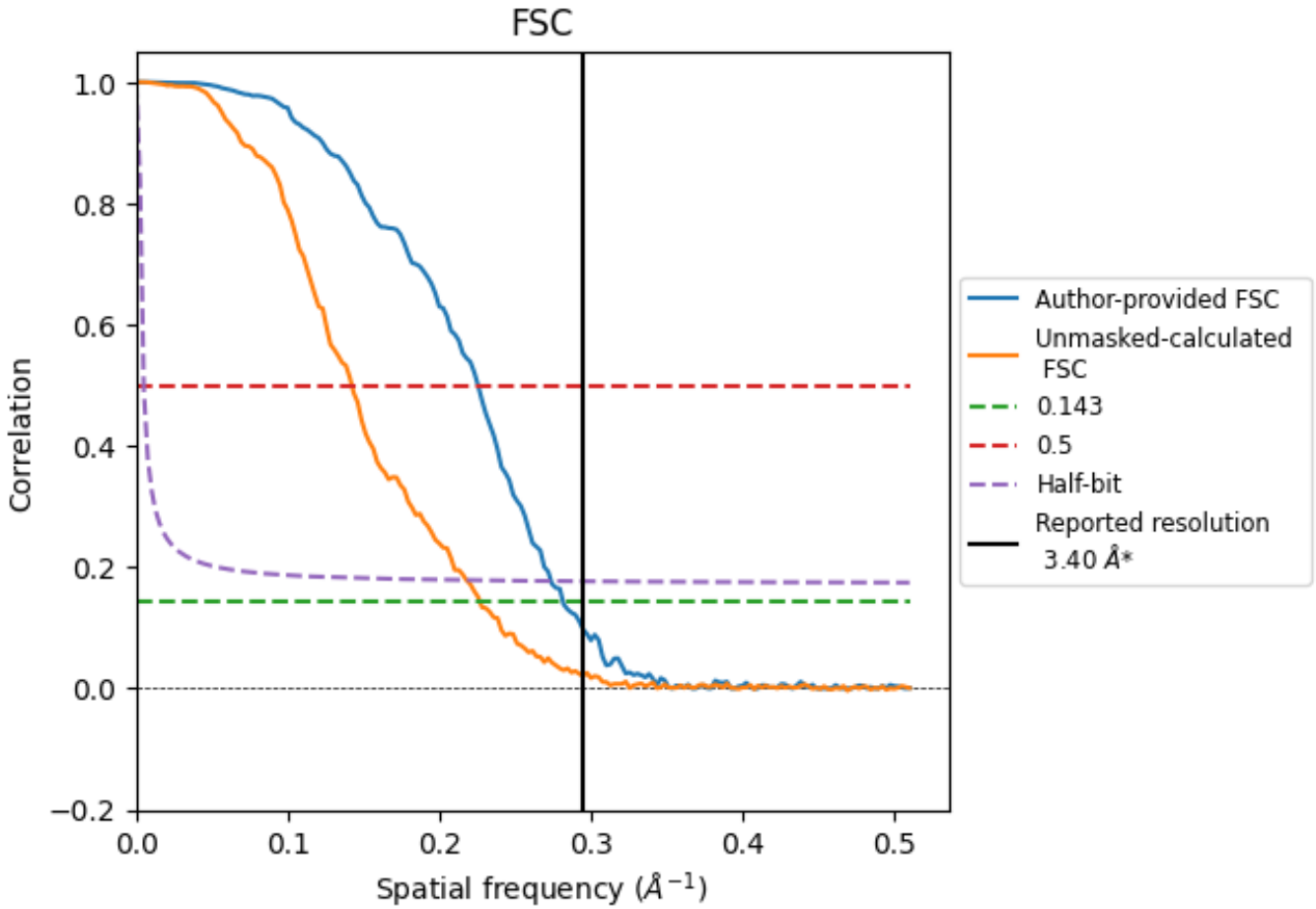


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

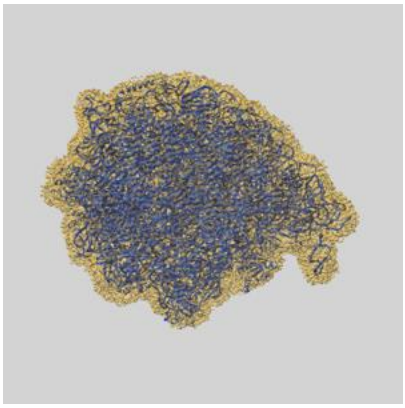
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.55	4.43	3.65
Unmasked-calculated*	4.41	7.03	4.59

*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 4.41 differs from the reported value 3.4 by more than 10 %

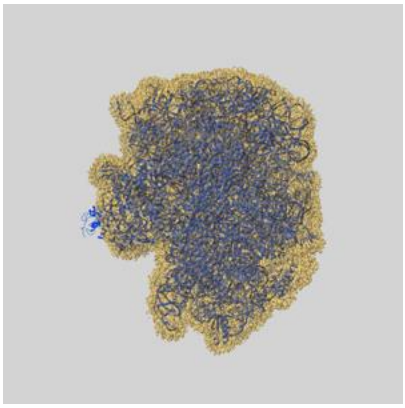
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8828 and PDB model 5WFK. Per-residue inclusion information can be found in section 3 on page 20.

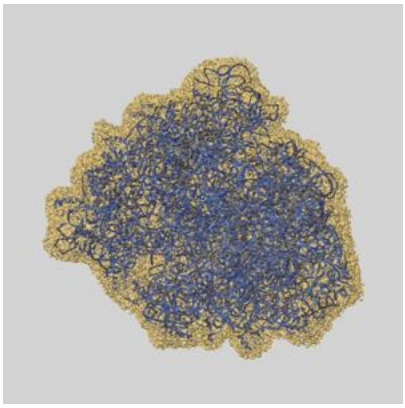
9.1 Map-model overlay



X



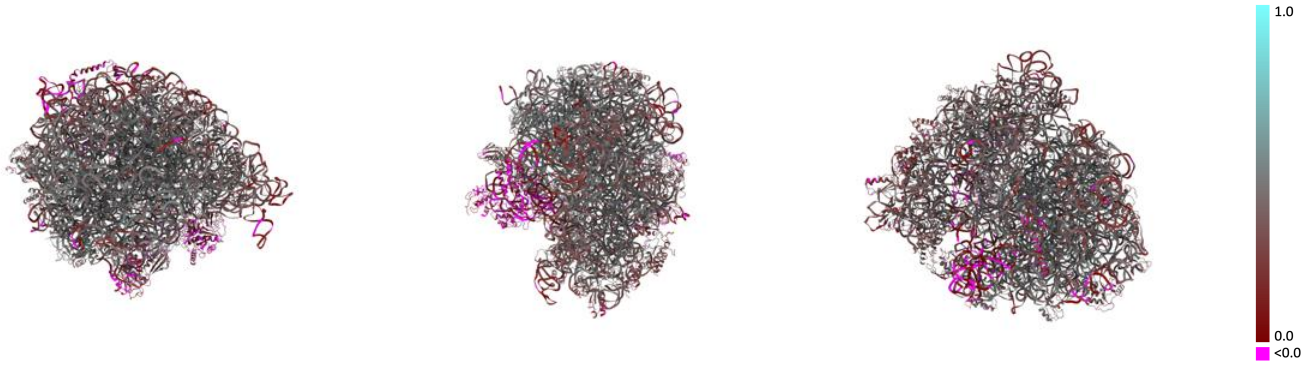
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00651 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.

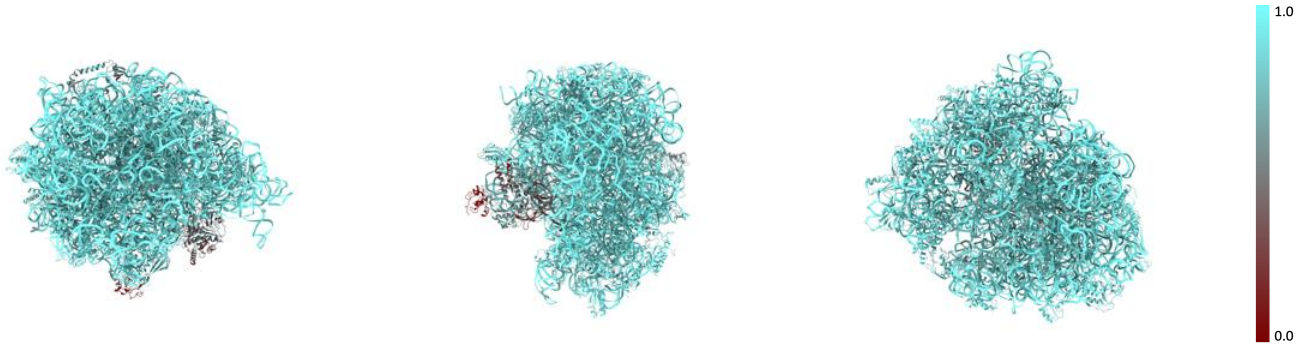
9.2 Q-score mapped to coordinate model (i)



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.

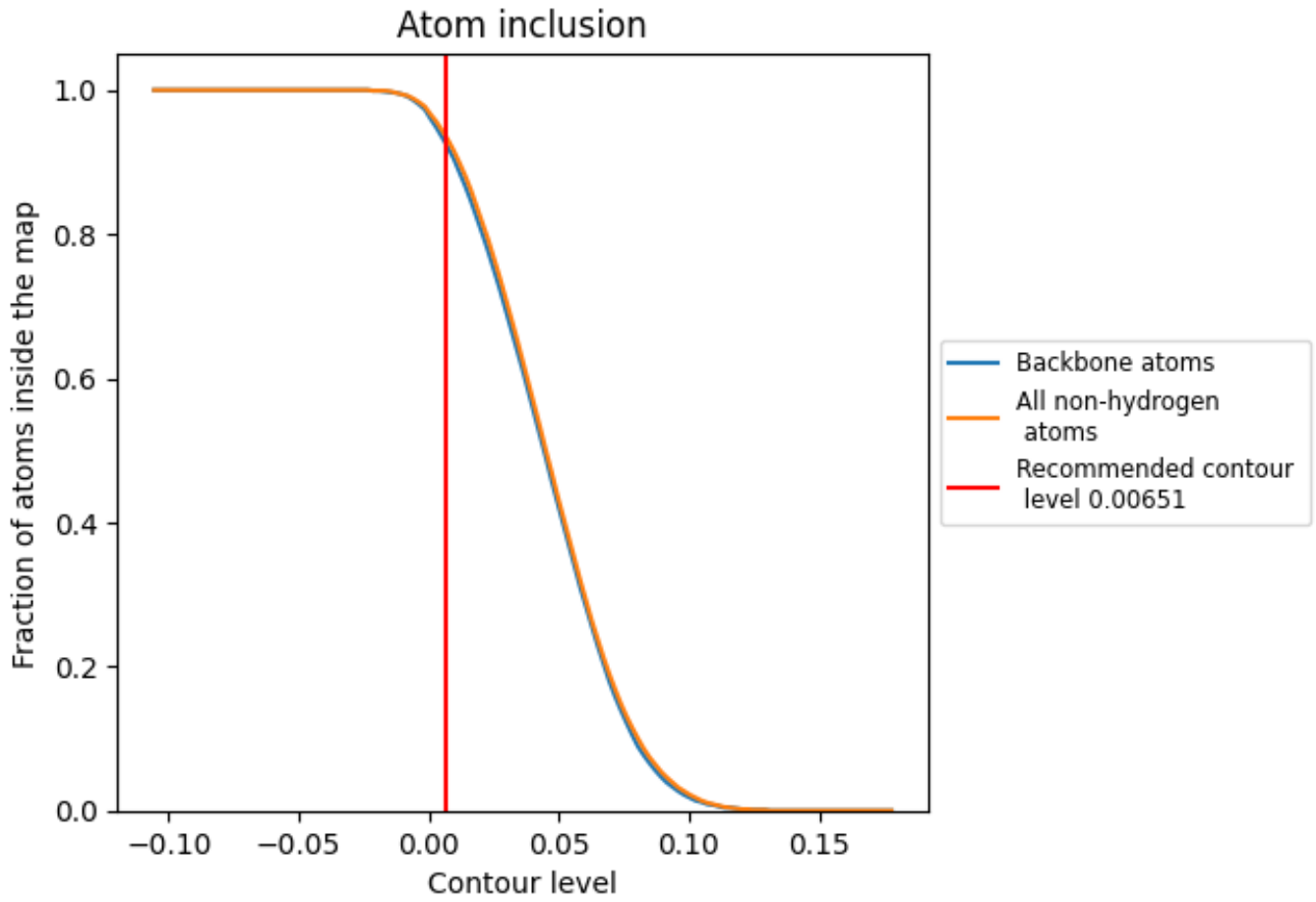
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.00651).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 94% 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 (0.00651) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9360	0.3850
0	0.9570	0.4610
1	0.9490	0.4460
2	0.9420	0.4890
3	0.9550	0.5060
4	0.9420	0.4720
5	0.2240	0.0090
6	0.8750	0.2840
A	0.9750	0.4110
B	0.9820	0.3850
C	0.9430	0.4790
D	0.9510	0.4630
E	0.9360	0.4350
F	0.9180	0.3570
G	0.9190	0.3330
H	0.6960	0.1660
I	0.6220	0.0280
J	0.9360	0.4550
K	0.9110	0.4420
L	0.9520	0.4600
M	0.9540	0.4540
N	0.9540	0.4660
O	0.9560	0.4010
P	0.9490	0.4570
Q	0.9650	0.4790
R	0.9460	0.4430
S	0.9470	0.4680
T	0.9220	0.4040
U	0.9480	0.4070
V	0.9350	0.4100
W	0.9530	0.4760
X	0.9390	0.4610
Y	0.9400	0.3860
Z	0.9650	0.4830
a	0.9790	0.3950



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Chain	Atom inclusion	Q-score
b	0.8980	0.3220
c	0.9120	0.3800
d	0.9210	0.3730
e	0.9290	0.4330
f	0.9100	0.3760
g	0.9140	0.3330
h	0.9170	0.4230
i	0.9010	0.3380
j	0.9030	0.3210
k	0.9470	0.4200
l	0.9160	0.4290
m	0.9220	0.3680
n	0.9180	0.3640
o	0.9360	0.4000
p	0.9360	0.4140
q	0.9370	0.3840
r	0.9030	0.3720
s	0.9450	0.3970
t	0.9140	0.3650
u	0.8180	0.2530
v	0.9550	0.3780
w	0.7960	0.0760
x	0.9330	0.3390
y	0.5280	0.0470
z	0.4550	0.0680