Full wwPDB EM Validation Report (i)

Feb 26, 2024 – 06:16 AM EST

PDB ID	:	6WDD
EMDB ID	:	EMD-21632
Title	:	Cryo-EM of elongating ribosome with EF-Tu*GTP elucidates tRNA proof-reading (Cognate Structure V-A)
Authors	:	Loveland, A.B.; Demo, G.; Korostelev, A.A.
Deposited on	:	2020-03-31
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM Validation 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 (i) 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 (i)) were used in the production of this report:

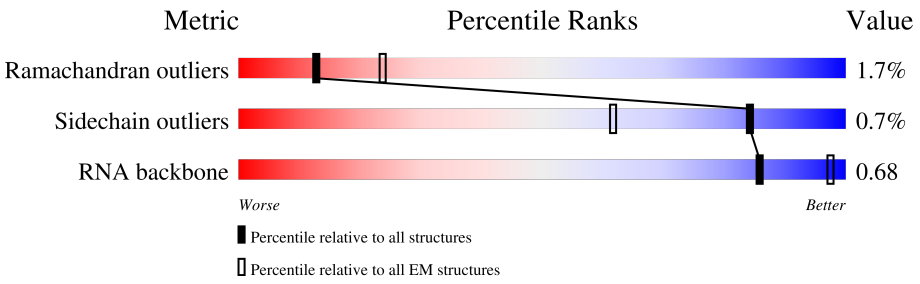
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	b	271	99%
2	c	209	99%
3	d	201	99%
4	e	177	98%
5	f	176	99%
6	g	149	13% 97%
7	h	131	23% 95%
8	i	141	31% 97%

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Mol	Chain	Length	Quality of chain
9	j	142	99%
10	k	122	96%
11	l	143	94% 6%
12	m	136	98%
13	n	120	98%
14	o	116	99%
15	p	114	100%
16	q	117	100%
17	r	103	97%
18	s	110	97%
19	t	93	99%
20	u	102	97%
21	v	94	99%
22	w	75	100%
23	x	77	100%
24	y	63	98%
25	z	58	98%
26	B	56	100%
27	C	50	100%
28	D	46	100%
29	E	64	98%
30	F	38	97%
31	G	225	99%
32	H	206	100%
33	I	205	97%

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Mol	Chain	Length	Quality of chain
34	J	157	96%
35	K	100	95% 5%
36	L	151	98%
37	M	129	98%
38	N	127	96%
39	O	98	93% 6%
40	P	116	97%
41	Q	123	95% 5%
42	R	114	96%
43	S	100	100%
44	T	88	98%
45	U	82	99%
46	V	80	98%
47	W	65	97%
48	X	79	96%
49	Y	85	100%
50	Z	65	89% 11%
51	a	223	60% 40%
52	3	1539	91% 9%
53	1	2903	88% 12%
54	2	120	90% 10%
55	5	77	87% 13%
55	6	77	91% 9%
56	4	18	6% 89% 11%
57	7	76	87% 13%

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 150222 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 protein called 50S ribosomal protein L2.

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

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

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

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L9.

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

- Molecule 7 is a protein called 50S ribosomal protein L10.

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

- Molecule 8 is a protein called 50S ribosomal protein L11.

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

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

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L32.

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

- Molecule 27 is a protein called 50S ribosomal protein L33.

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

- Molecule 28 is a protein called 50S ribosomal protein L34.

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

- Molecule 29 is a protein called 50S ribosomal protein L35.

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

- Molecule 30 is a protein called 50S ribosomal protein L36.

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

- Molecule 31 is a protein called 30S ribosomal protein S2.

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

- Molecule 32 is a protein called 30S ribosomal protein S3.

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

- Molecule 33 is a protein called 30S ribosomal protein S4.

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

- Molecule 34 is a protein called 30S ribosomal protein S5.

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

- Molecule 35 is a protein called 30S ribosomal protein S6.

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

- Molecule 36 is a protein called 30S ribosomal protein S7.

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

- Molecule 37 is a protein called 30S ribosomal protein S8.

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

- Molecule 38 is a protein called 30S ribosomal protein S9.

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

- Molecule 39 is a protein called 30S ribosomal protein S10.

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

- Molecule 40 is a protein called 30S ribosomal protein S11.

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

- Molecule 41 is a protein called 30S ribosomal protein S12.

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

- Molecule 42 is a protein called 30S ribosomal protein S13.

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

- Molecule 43 is a protein called 30S ribosomal protein S14.

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

- Molecule 44 is a protein called 30S ribosomal protein S15.

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

- Molecule 45 is a protein called 30S ribosomal protein S16.

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

- Molecule 46 is a protein called 30S ribosomal protein S17.

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

- Molecule 47 is a protein called 30S ribosomal protein S18.

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

- Molecule 48 is a protein called 30S ribosomal protein S19.

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

- Molecule 49 is a protein called 30S ribosomal protein S20.

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

- Molecule 50 is a protein called 30S ribosomal protein S21.

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

- Molecule 51 is a protein called 50S ribosomal protein L1.

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

- Molecule 52 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
52	3	1539	33012	14725	6052	10697	1538	0	0

- Molecule 53 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	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 54 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
54	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 55 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	5	77	1640	732	297	535	76	0	0
55	6	77	1640	732	297	535	76	0	0

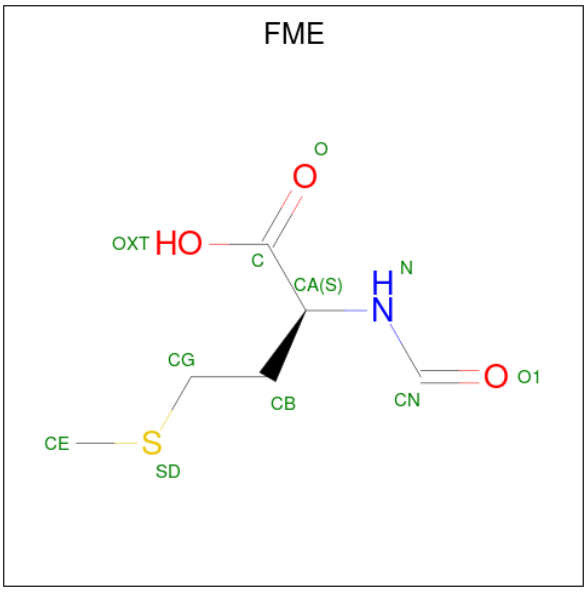
- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	4	18	388	175	76	120	17	0	0

- Molecule 57 is a RNA chain called tRNAPhe.

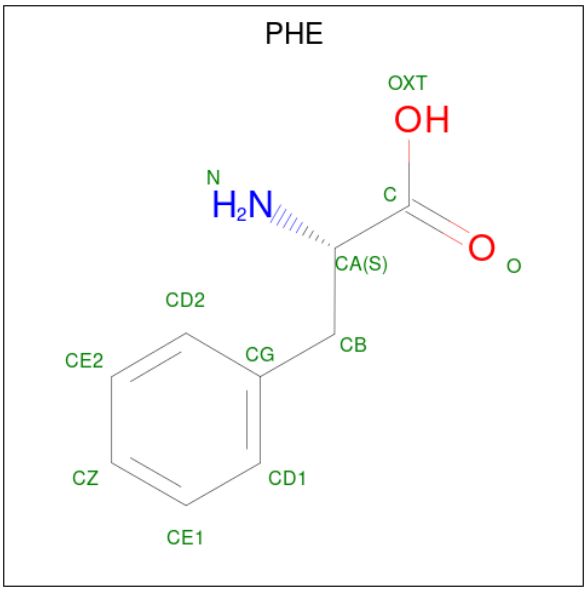
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
57	7	76	1619	723	290	531	75	0	0

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
58	5	1	10	6	1	2	1	0

- Molecule 59 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



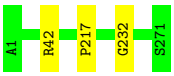
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
59	7	1	11	9	1	1	0

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.

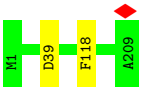
• Molecule 1: 50S ribosomal protein L2

Chain b: 99%



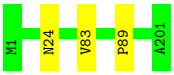
• Molecule 2: 50S ribosomal protein L3

Chain c: 99%



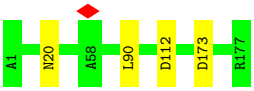
• Molecule 3: 50S ribosomal protein L4

Chain d: 99%



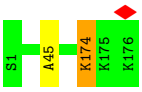
• Molecule 4: 50S ribosomal protein L5

Chain e: 98%



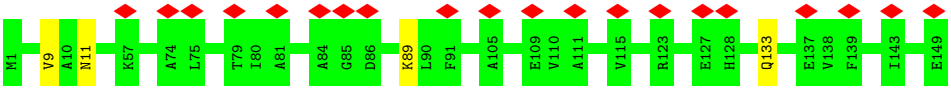
• Molecule 5: 50S ribosomal protein L6

Chain f: 99%



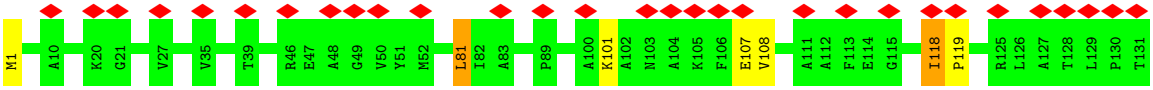
• Molecule 6: 50S ribosomal protein L9

Chain g: 13% 97%



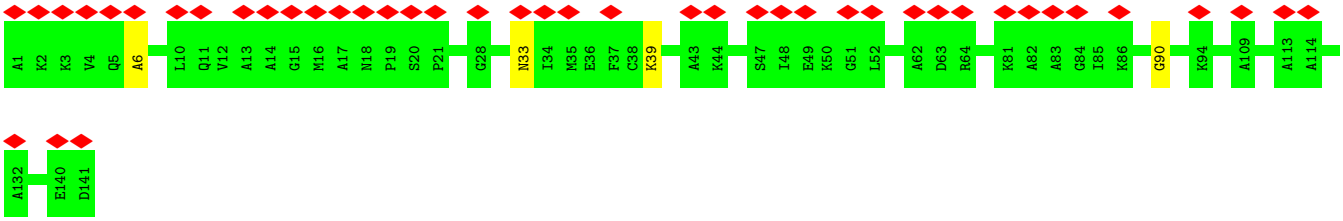
• Molecule 7: 50S ribosomal protein L10

Chain h: 23% 95%



• Molecule 8: 50S ribosomal protein L11

Chain i: 31% 97%



• Molecule 9: 50S ribosomal protein L13

Chain j: 99%

• Molecule 10: 50S ribosomal protein L14

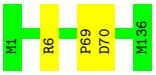
Chain k: 96%

• Molecule 11: 50S ribosomal protein L15

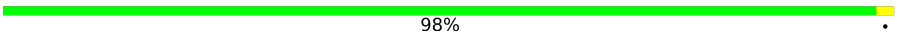
Chain l: 94% 6%

• Molecule 12: 50S ribosomal protein L16

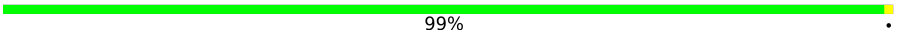
Chain m: 98%



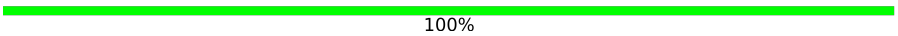
• Molecule 13: 50S ribosomal protein L17

Chain n: 

• Molecule 14: 50S ribosomal protein L18

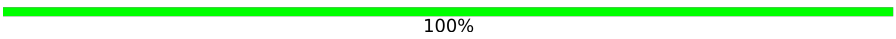
Chain o: 

• Molecule 15: 50S ribosomal protein L19

Chain p: 

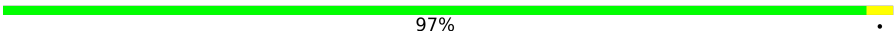
There are no outlier residues recorded for this chain.

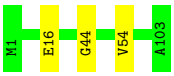
• Molecule 16: 50S ribosomal protein L20

Chain q: 

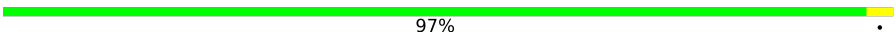
There are no outlier residues recorded for this chain.

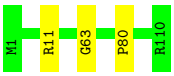
• Molecule 17: 50S ribosomal protein L21

Chain r: 

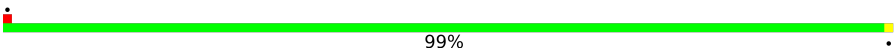


• Molecule 18: 50S ribosomal protein L22

Chain s: 



• Molecule 19: 50S ribosomal protein L23

Chain t: 

• Molecule 20: 50S ribosomal protein L24

Chain u: 97%

• Molecule 21: 50S ribosomal protein L25

Chain v: 99%

• Molecule 22: 50S ribosomal protein L27

Chain w: 100%

There are no outlier residues recorded for this chain.

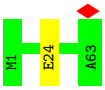
• Molecule 23: 50S ribosomal protein L28

Chain x: 100%

There are no outlier residues recorded for this chain.

• Molecule 24: 50S ribosomal protein L29

Chain y: 98%



• Molecule 25: 50S ribosomal protein L30

Chain z: 98%

• Molecule 26: 50S ribosomal protein L32

Chain B: 100%

• Molecule 27: 50S ribosomal protein L33

Chain C: 100%

There are no outlier residues recorded for this chain.

• Molecule 28: 50S ribosomal protein L34

Chain D: 100%

M1 K46

• Molecule 29: 50S ribosomal protein L35

Chain E: 98%

P1 I31 A64

• Molecule 30: 50S ribosomal protein L36

Chain F: 97%

M1 Q37 G38

• Molecule 31: 30S ribosomal protein S2

Chain G: 99%

A1 R94 P192 S225

• Molecule 32: 30S ribosomal protein S3

Chain H: 100%

There are no outlier residues recorded for this chain.

• Molecule 33: 30S ribosomal protein S4

Chain I: 97%

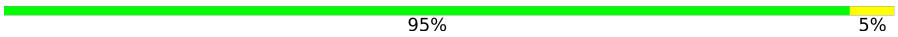
A1 L4 V24 R25 A26 I27 D28 G31 E34 L47 K147 S152 R183 K205

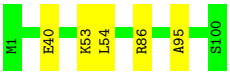
• Molecule 34: 30S ribosomal protein S5

Chain J: 96%

• Molecule 35: 30S ribosomal protein S6

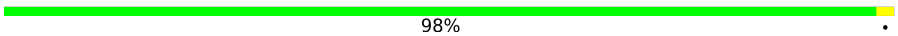
Chain K:

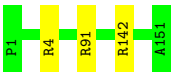




• Molecule 36: 30S ribosomal protein S7

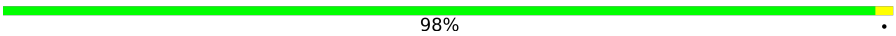
Chain L:





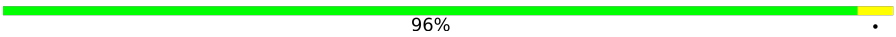
• Molecule 37: 30S ribosomal protein S8

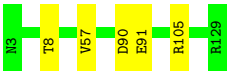
Chain M:



• Molecule 38: 30S ribosomal protein S9

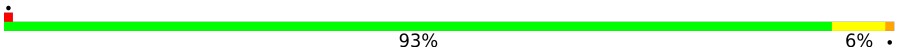
Chain N:

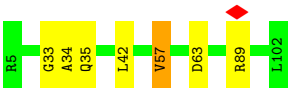




• Molecule 39: 30S ribosomal protein S10

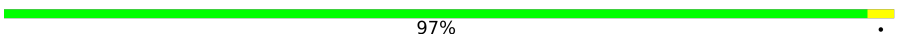
Chain O:





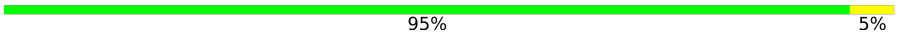
• Molecule 40: 30S ribosomal protein S11

Chain P:

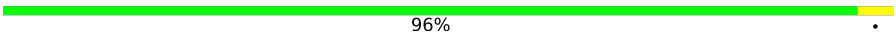


• Molecule 41: 30S ribosomal protein S12

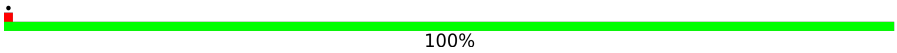
Chain Q:

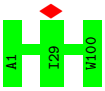


• Molecule 42: 30S ribosomal protein S13

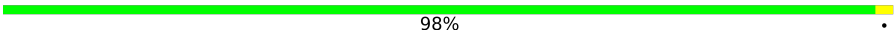
Chain R: 

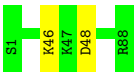
• Molecule 43: 30S ribosomal protein S14

Chain S: 

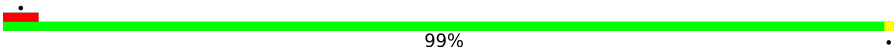


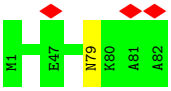
• Molecule 44: 30S ribosomal protein S15

Chain T: 

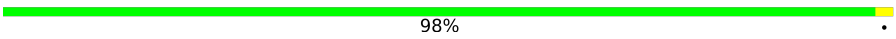


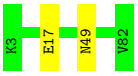
• Molecule 45: 30S ribosomal protein S16

Chain U: 

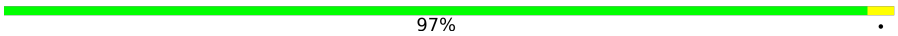


• Molecule 46: 30S ribosomal protein S17

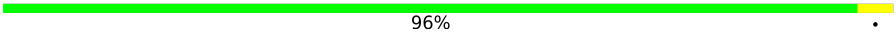
Chain V: 

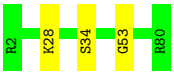


• Molecule 47: 30S ribosomal protein S18

Chain W: 

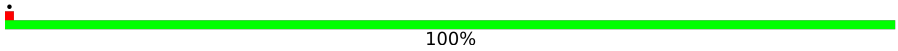
• Molecule 48: 30S ribosomal protein S19

Chain X: 



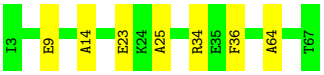
• Molecule 49: 30S ribosomal protein S20

Chain Y:



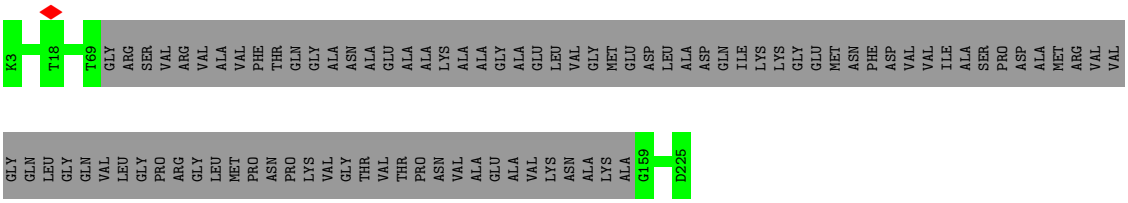
• Molecule 50: 30S ribosomal protein S21

Chain Z:



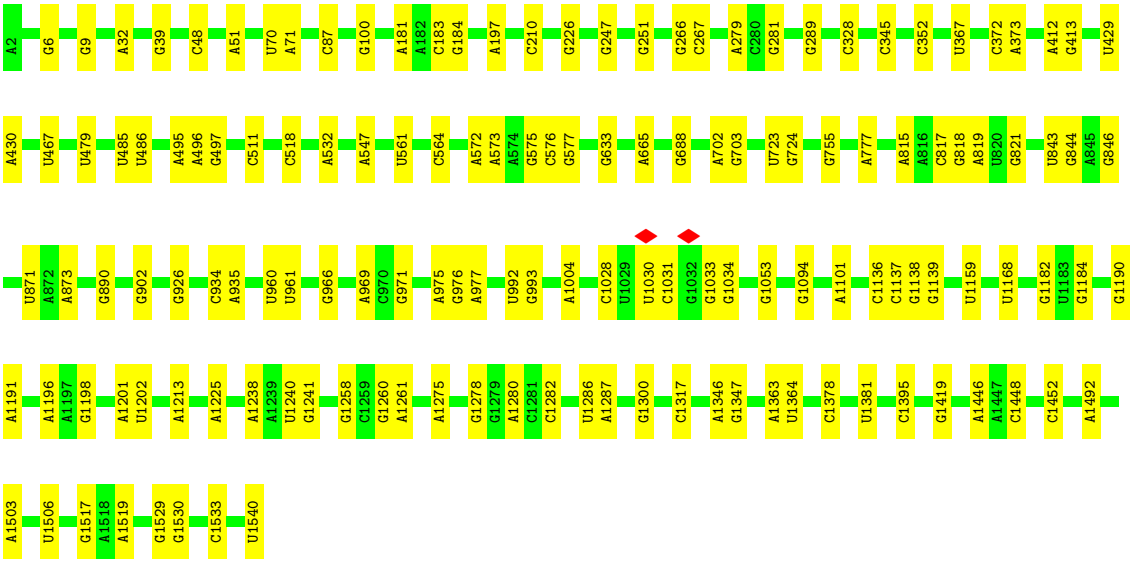
• Molecule 51: 50S ribosomal protein L1

Chain a:



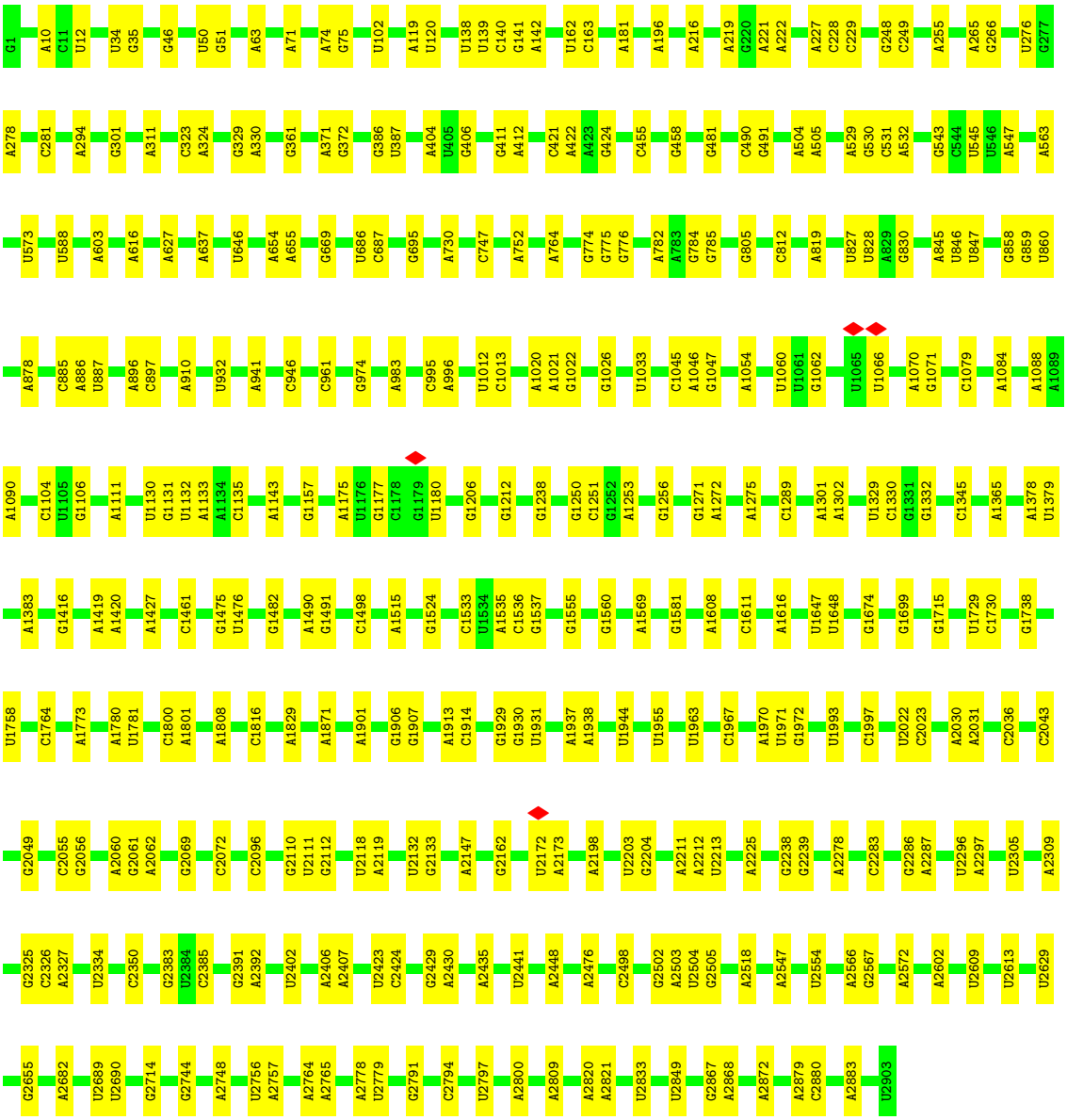
• Molecule 52: 16S ribosomal RNA

Chain 3:



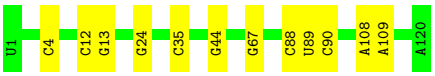
• Molecule 53: 23S ribosomal RNA

Chain 1: 88% 12%



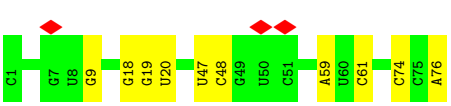
- Molecule 54: 5S ribosomal RNA

Chain 2: 90% 10%



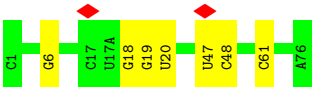
- Molecule 55: tRNAfMet

Chain 5: 87% 13%



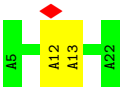
• Molecule 55: tRNAfMet

Chain 6:



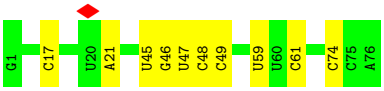
• Molecule 56: mRNA

Chain 4:



• Molecule 57: tRNAPhe

Chain 7:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32253	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 ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	28.501	Depositor
Minimum map value	-14.672	Depositor
Average map value	0.119	Depositor
Map value standard deviation	1.117	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	383.904, 383.904, 383.904	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.333, 1.333, 1.333	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: 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	b	0.26	0/2122	0.57	0/2852
2	c	0.28	0/1586	0.53	0/2134
3	d	0.27	0/1571	0.50	0/2113
4	e	0.32	0/1435	0.51	0/1926
5	f	0.27	0/1343	0.52	0/1816
6	g	0.30	0/1122	0.57	0/1515
7	h	0.33	0/1002	0.61	0/1350
8	i	0.30	0/1046	0.56	0/1410
9	j	0.26	0/1152	0.54	0/1551
10	k	0.27	0/948	0.60	0/1268
11	l	0.28	0/1054	0.60	0/1403
12	m	0.30	0/1093	0.55	0/1460
13	n	0.29	0/974	0.56	0/1301
14	o	0.28	0/902	0.53	0/1209
15	p	0.28	0/929	0.54	0/1242
16	q	0.30	0/960	0.49	0/1278
17	r	0.30	0/829	0.56	0/1107
18	s	0.25	0/864	0.56	0/1156
19	t	0.27	0/745	0.52	0/994
20	u	0.30	0/788	0.57	0/1051
21	v	0.29	0/766	0.57	0/1025
22	w	0.31	0/582	0.50	0/769
23	x	0.28	0/635	0.55	0/848
24	y	0.27	0/510	0.48	0/677
25	z	0.26	0/453	0.49	0/605
26	B	0.25	0/450	0.51	0/599
27	C	0.33	0/417	0.53	0/554
28	D	0.30	0/380	0.55	0/498
29	E	0.30	0/513	0.60	0/676
30	F	0.26	0/303	0.59	0/397
31	G	0.29	0/1788	0.52	0/2408
32	H	0.28	0/1652	0.50	0/2225

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	I	0.28	0/1665	0.53	0/2227
34	J	0.29	0/1170	0.57	0/1573
35	K	0.29	0/836	0.59	0/1128
36	L	0.28	0/1196	0.51	0/1602
37	M	0.28	0/989	0.57	0/1326
38	N	0.29	0/1034	0.58	0/1375
39	O	0.27	0/797	0.60	0/1077
40	P	0.29	0/886	0.59	0/1195
41	Q	0.28	0/969	0.65	0/1300
42	R	0.26	0/893	0.57	0/1193
43	S	0.29	0/817	0.51	0/1088
44	T	0.28	0/722	0.55	0/964
45	U	0.34	0/659	0.57	0/884
46	V	0.28	0/658	0.58	0/881
47	W	0.31	0/545	0.55	0/731
48	X	0.31	0/653	0.53	0/877
49	Y	0.28	0/671	0.51	0/888
50	Z	0.31	0/551	0.59	0/728
51	a	0.27	0/1034	0.53	0/1387
52	3	0.32	0/36963	0.66	0/57662
53	1	0.29	0/69796	0.65	0/108888
54	2	0.29	0/2872	0.65	0/4479
55	5	0.33	0/1832	0.65	0/2855
55	6	0.31	0/1832	0.66	0/2855
56	4	0.29	0/436	0.63	0/679
57	7	0.30	0/1809	0.65	0/2819
All	All	0.30	0/163199	0.63	0/244078

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	269/271 (99%)	235 (87%)	33 (12%)	1 (0%)	34	69
2	c	207/209 (99%)	189 (91%)	17 (8%)	1 (0%)	29	67
3	d	199/201 (99%)	180 (90%)	17 (8%)	2 (1%)	15	54
4	e	175/177 (99%)	156 (89%)	17 (10%)	2 (1%)	14	51
5	f	174/176 (99%)	160 (92%)	12 (7%)	2 (1%)	14	51
6	g	147/149 (99%)	126 (86%)	18 (12%)	3 (2%)	7	38
7	h	129/131 (98%)	95 (74%)	30 (23%)	4 (3%)	4	26
8	i	139/141 (99%)	124 (89%)	13 (9%)	2 (1%)	11	46
9	j	140/142 (99%)	133 (95%)	6 (4%)	1 (1%)	22	61
10	k	120/122 (98%)	98 (82%)	17 (14%)	5 (4%)	3	20
11	l	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	2	16
12	m	134/136 (98%)	113 (84%)	19 (14%)	2 (2%)	10	44
13	n	118/120 (98%)	106 (90%)	10 (8%)	2 (2%)	9	42
14	o	114/116 (98%)	106 (93%)	7 (6%)	1 (1%)	17	56
15	p	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
16	q	115/117 (98%)	107 (93%)	8 (7%)	0	100	100
17	r	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	4	28
18	s	108/110 (98%)	95 (88%)	10 (9%)	3 (3%)	5	29
19	t	91/93 (98%)	83 (91%)	8 (9%)	0	100	100
20	u	100/102 (98%)	84 (84%)	13 (13%)	3 (3%)	4	28
21	v	92/94 (98%)	85 (92%)	6 (6%)	1 (1%)	14	51
22	w	73/75 (97%)	64 (88%)	9 (12%)	0	100	100
23	x	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
24	y	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	9	43
25	z	56/58 (97%)	51 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	B	54/56 (96%)	49 (91%)	5 (9%)	0	100	100
27	C	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
28	D	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
29	E	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	9	43
30	F	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	5	29
31	G	223/225 (99%)	202 (91%)	20 (9%)	1 (0%)	34	69
32	H	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
33	I	203/205 (99%)	184 (91%)	15 (7%)	4 (2%)	7	38
34	J	155/157 (99%)	124 (80%)	27 (17%)	4 (3%)	5	31
35	K	98/100 (98%)	81 (83%)	12 (12%)	5 (5%)	2	15
36	L	149/151 (99%)	131 (88%)	17 (11%)	1 (1%)	22	61
37	M	127/129 (98%)	112 (88%)	13 (10%)	2 (2%)	9	43
38	N	125/127 (98%)	103 (82%)	18 (14%)	4 (3%)	4	26
39	O	96/98 (98%)	80 (83%)	11 (12%)	5 (5%)	2	15
40	P	114/116 (98%)	94 (82%)	17 (15%)	3 (3%)	5	31
41	Q	121/123 (98%)	94 (78%)	21 (17%)	6 (5%)	2	16
42	R	112/114 (98%)	98 (88%)	10 (9%)	4 (4%)	3	23
43	S	98/100 (98%)	76 (78%)	22 (22%)	0	100	100
44	T	86/88 (98%)	78 (91%)	6 (7%)	2 (2%)	6	34
45	U	80/82 (98%)	71 (89%)	8 (10%)	1 (1%)	12	47
46	V	78/80 (98%)	64 (82%)	12 (15%)	2 (3%)	5	31
47	W	63/65 (97%)	57 (90%)	5 (8%)	1 (2%)	9	43
48	X	77/79 (98%)	65 (84%)	10 (13%)	2 (3%)	5	31
49	Y	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
50	Z	63/65 (97%)	47 (75%)	9 (14%)	7 (11%)	0	2
51	a	130/223 (58%)	124 (95%)	6 (5%)	0	100	100
All	All	5919/6112 (97%)	5192 (88%)	625 (11%)	102 (2%)	13	42

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	b	232	GLY
5	f	45	ALA

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Mol	Chain	Res	Type
5	f	174	LYS
6	g	9	VAL
7	h	81	LEU
7	h	118	ILE
10	k	92	GLU
13	n	118	ARG
14	o	34	HIS
17	r	54	VAL
24	y	24	GLU
29	E	31	ILE
30	F	37	GLN
33	I	34	GLU
34	J	93	VAL
34	J	122	VAL
35	K	53	LYS
35	K	54	LEU
37	M	47	ASP
38	N	57	VAL
38	N	90	ASP
40	P	92	ARG
40	P	125	LYS
42	R	4	ALA
44	T	46	LYS
50	Z	14	ALA
7	h	108	VAL
8	i	90	GLY
10	k	89	ASN
11	l	28	GLY
11	l	31	GLY
11	l	115	GLU
18	s	63	GLY
20	u	56	GLY
20	u	98	ASN
35	K	40	GLU
38	N	91	GLU
41	Q	24	GLU
41	Q	77	SER
42	R	14	ALA
44	T	48	ASP
46	V	17	GLU
46	V	49	ASN
48	X	34	SER

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Mol	Chain	Res	Type
50	Z	25	ALA
4	e	20	ASN
11	l	15	ALA
11	l	29	LYS
12	m	69	PRO
18	s	11	ARG
33	I	152	SER
34	J	98	ALA
35	K	86	ARG
35	K	95	ALA
36	L	4	ARG
38	N	8	THR
39	O	33	GLY
39	O	35	GLN
40	P	13	LYS
41	Q	43	LYS
45	U	79	ASN
50	Z	23	GLU
50	Z	34	ARG
50	Z	36	PHE
2	c	118	PHE
7	h	107	GLU
33	I	28	ASP
39	O	34	ALA
39	O	42	LEU
41	Q	101	LEU
42	R	65	GLU
48	X	53	GLY
50	Z	9	GLU
4	e	173	ASP
6	g	11	ASN
8	i	6	ALA
10	k	26	GLY
11	l	85	VAL
12	m	6	ARG
13	n	14	SER
17	r	16	GLU
33	I	47	LEU
34	J	11	GLN
41	Q	35	ARG
41	Q	75	GLU
42	R	6	ILE

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Mol	Chain	Res	Type
50	Z	64	ALA
6	g	89	LYS
10	k	93	GLN
20	u	54	PRO
21	v	81	PRO
47	W	24	ASP
3	d	89	PRO
10	k	68	GLY
3	d	83	VAL
11	l	56	PRO
39	O	57	VAL
17	r	44	GLY
9	j	81	ILE
18	s	80	PRO
31	G	192	PRO
37	M	102	VAL

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	
1	b	216/216 (100%)	214 (99%)	2 (1%)	78	91
2	c	164/164 (100%)	163 (99%)	1 (1%)	86	94
3	d	165/165 (100%)	164 (99%)	1 (1%)	86	94
4	e	148/148 (100%)	146 (99%)	2 (1%)	67	86
5	f	137/137 (100%)	136 (99%)	1 (1%)	84	94
6	g	114/114 (100%)	113 (99%)	1 (1%)	78	91
7	h	100/100 (100%)	95 (95%)	5 (5%)	24	60
8	i	109/109 (100%)	107 (98%)	2 (2%)	59	82
9	j	116/116 (100%)	116 (100%)	0	100	100
10	k	103/103 (100%)	102 (99%)	1 (1%)	76	90
11	l	102/102 (100%)	101 (99%)	1 (1%)	76	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	m	109/109 (100%)	108 (99%)	1 (1%)	78	91
13	n	100/100 (100%)	100 (100%)	0	100	100
14	o	86/86 (100%)	86 (100%)	0	100	100
15	p	99/99 (100%)	99 (100%)	0	100	100
16	q	89/89 (100%)	89 (100%)	0	100	100
17	r	84/84 (100%)	84 (100%)	0	100	100
18	s	93/93 (100%)	93 (100%)	0	100	100
19	t	80/80 (100%)	79 (99%)	1 (1%)	69	87
20	u	83/83 (100%)	83 (100%)	0	100	100
21	v	78/78 (100%)	78 (100%)	0	100	100
22	w	57/57 (100%)	57 (100%)	0	100	100
23	x	67/67 (100%)	67 (100%)	0	100	100
24	y	55/55 (100%)	55 (100%)	0	100	100
25	z	48/48 (100%)	47 (98%)	1 (2%)	53	79
26	B	47/47 (100%)	47 (100%)	0	100	100
27	C	45/45 (100%)	45 (100%)	0	100	100
28	D	38/38 (100%)	38 (100%)	0	100	100
29	E	51/51 (100%)	51 (100%)	0	100	100
30	F	34/34 (100%)	34 (100%)	0	100	100
31	G	186/186 (100%)	185 (100%)	1 (0%)	88	95
32	H	170/170 (100%)	170 (100%)	0	100	100
33	I	172/172 (100%)	169 (98%)	3 (2%)	60	83
34	J	119/119 (100%)	117 (98%)	2 (2%)	60	83
35	K	87/87 (100%)	87 (100%)	0	100	100
36	L	124/124 (100%)	122 (98%)	2 (2%)	62	84
37	M	104/104 (100%)	104 (100%)	0	100	100
38	N	105/105 (100%)	104 (99%)	1 (1%)	76	90
39	O	86/86 (100%)	83 (96%)	3 (4%)	36	69
40	P	89/89 (100%)	88 (99%)	1 (1%)	73	88
41	Q	103/103 (100%)	103 (100%)	0	100	100
42	R	92/92 (100%)	91 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	S	83/83 (100%)	83 (100%)	0	100	100
44	T	76/76 (100%)	76 (100%)	0	100	100
45	U	65/65 (100%)	65 (100%)	0	100	100
46	V	74/74 (100%)	74 (100%)	0	100	100
47	W	56/56 (100%)	55 (98%)	1 (2%)	59	82
48	X	70/70 (100%)	69 (99%)	1 (1%)	67	86
49	Y	65/65 (100%)	65 (100%)	0	100	100
50	Z	55/55 (100%)	55 (100%)	0	100	100
51	a	110/174 (63%)	110 (100%)	0	100	100
All	All	4908/4972 (99%)	4872 (99%)	36 (1%)	84	94

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	42	ARG
1	b	217	PRO
2	c	39	ASP
3	d	24	ASN
4	e	90	LEU
4	e	112	ASP
5	f	174	LYS
6	g	133	GLN
7	h	1	MET
7	h	81	LEU
7	h	101	LYS
7	h	118	ILE
7	h	119	PRO
8	i	33	ASN
8	i	39	LYS
10	k	89	ASN
11	l	94	THR
12	m	70	ASP
19	t	2	ILE
25	z	30	ARG
31	G	94	ARG
33	I	31	CYS
33	I	147	LYS
33	I	183	ARG
34	J	55	VAL

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Mol	Chain	Res	Type
34	J	68	ARG
36	L	91	ARG
36	L	142	ARG
38	N	105	ARG
39	O	57	VAL
39	O	63	ASP
39	O	89	ARG
40	P	100	ASN
42	R	99	GLN
47	W	11	ARG
48	X	28	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	36	ASN
1	b	45	ASN
1	b	52	HIS
1	b	69	ASN
1	b	89	ASN
1	b	116	GLN
1	b	127	ASN
1	b	225	ASN
1	b	238	ASN
2	c	58	ASN
2	c	130	GLN
2	c	173	GLN
3	d	24	ASN
3	d	41	GLN
3	d	97	ASN
4	e	20	ASN
5	f	19	ASN
5	f	110	HIS
5	f	138	GLN
6	g	11	ASN
6	g	18	GLN
6	g	43	ASN
6	g	119	ASN
6	g	133	GLN
6	g	135	HIS
6	g	145	ASN
7	h	4	ASN

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Mol	Chain	Res	Type
7	h	122	GLN
8	i	5	GLN
8	i	93	ASN
9	j	58	ASN
9	j	80	HIS
9	j	135	GLN
10	k	5	GLN
10	k	13	ASN
10	k	89	ASN
12	m	22	GLN
13	n	31	HIS
13	n	62	ASN
15	p	2	ASN
16	q	71	ASN
17	r	82	HIS
19	t	59	ASN
20	u	73	ASN
21	v	24	ASN
24	y	20	ASN
27	C	18	HIS
27	C	44	GLN
28	D	13	ASN
30	F	37	GLN
31	G	17	HIS
31	G	38	HIS
31	G	176	ASN
31	G	202	ASN
32	H	18	ASN
32	H	99	GLN
32	H	184	ASN
33	I	39	GLN
33	I	115	GLN
33	I	130	ASN
33	I	195	ASN
34	J	77	ASN
34	J	131	ASN
34	J	134	ASN
35	K	11	HIS
35	K	14	GLN
36	L	67	ASN
36	L	129	ASN
37	M	17	GLN

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Mol	Chain	Res	Type
37	M	66	GLN
38	N	31	GLN
40	P	108	ASN
41	Q	4	ASN
41	Q	58	ASN
41	Q	111	GLN
42	R	99	GLN
43	S	59	GLN
43	S	70	HIS
45	U	26	ASN
46	V	44	HIS
46	V	50	ASN
48	X	55	GLN
48	X	56	HIS
49	Y	12	GLN
49	Y	20	ASN
51	a	188	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	3	1538/1539 (99%)	141 (9%)	4 (0%)
53	1	2902/2903 (99%)	332 (11%)	14 (0%)
54	2	119/120 (99%)	11 (9%)	1 (0%)
55	5	76/77 (98%)	10 (13%)	0
55	6	76/77 (98%)	7 (9%)	0
56	4	17/18 (94%)	2 (11%)	0
57	7	75/76 (98%)	10 (13%)	0
All	All	4803/4810 (99%)	513 (10%)	19 (0%)

All (513) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	3	6	G
52	3	9	G
52	3	32	A
52	3	39	G
52	3	48	C
52	3	51	A
52	3	71	A
52	3	87	C

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Mol	Chain	Res	Type
52	3	100	G
52	3	181	A
52	3	183	C
52	3	184	G
52	3	197	A
52	3	210	C
52	3	226	G
52	3	247	G
52	3	251	G
52	3	266	G
52	3	267	C
52	3	279	A
52	3	281	G
52	3	289	G
52	3	328	C
52	3	345	C
52	3	352	C
52	3	367	U
52	3	372	C
52	3	373	A
52	3	412	A
52	3	413	G
52	3	429	U
52	3	430	A
52	3	467	U
52	3	479	U
52	3	485	U
52	3	486	U
52	3	496	A
52	3	497	G
52	3	511	C
52	3	518	C
52	3	532	A
52	3	547	A
52	3	561	U
52	3	564	C
52	3	572	A
52	3	573	A
52	3	575	G
52	3	576	C
52	3	577	G
52	3	633	G

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Mol	Chain	Res	Type
52	3	665	A
52	3	688	G
52	3	702	A
52	3	703	G
52	3	723	U
52	3	724	G
52	3	755	G
52	3	777	A
52	3	815	A
52	3	817	C
52	3	818	G
52	3	819	A
52	3	821	G
52	3	843	U
52	3	844	G
52	3	846	G
52	3	871	U
52	3	873	A
52	3	890	G
52	3	902	G
52	3	926	G
52	3	934	C
52	3	935	A
52	3	960	U
52	3	961	U
52	3	966	G
52	3	969	A
52	3	971	G
52	3	975	A
52	3	976	G
52	3	977	A
52	3	992	U
52	3	993	G
52	3	1004	A
52	3	1028	C
52	3	1030	U
52	3	1031	C
52	3	1033	G
52	3	1034	G
52	3	1053	G
52	3	1094	G
52	3	1101	A

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Mol	Chain	Res	Type
52	3	1136	C
52	3	1137	C
52	3	1138	G
52	3	1139	G
52	3	1159	U
52	3	1168	U
52	3	1182	G
52	3	1184	G
52	3	1191	A
52	3	1196	A
52	3	1198	G
52	3	1201	A
52	3	1202	U
52	3	1213	A
52	3	1225	A
52	3	1238	A
52	3	1240	U
52	3	1241	G
52	3	1258	G
52	3	1260	G
52	3	1261	A
52	3	1275	A
52	3	1278	G
52	3	1280	A
52	3	1282	C
52	3	1286	U
52	3	1287	A
52	3	1300	G
52	3	1317	C
52	3	1346	A
52	3	1347	G
52	3	1363	A
52	3	1364	U
52	3	1378	C
52	3	1381	U
52	3	1395	C
52	3	1419	G
52	3	1446	A
52	3	1448	C
52	3	1452	C
52	3	1492	A
52	3	1503	A

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Mol	Chain	Res	Type
52	3	1506	U
52	3	1517	G
52	3	1519	A
52	3	1529	G
52	3	1530	G
52	3	1533	C
52	3	1540	U
53	1	10	A
53	1	12	U
53	1	34	U
53	1	35	G
53	1	46	G
53	1	50	U
53	1	51	G
53	1	63	A
53	1	71	A
53	1	74	A
53	1	75	G
53	1	102	U
53	1	119	A
53	1	120	U
53	1	138	U
53	1	139	U
53	1	140	C
53	1	141	G
53	1	142	A
53	1	162	U
53	1	163	C
53	1	181	A
53	1	196	A
53	1	216	A
53	1	219	A
53	1	221	A
53	1	222	A
53	1	228	C
53	1	229	C
53	1	248	G
53	1	249	C
53	1	255	A
53	1	265	A
53	1	266	G
53	1	276	U

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Mol	Chain	Res	Type
53	1	278	A
53	1	281	C
53	1	294	A
53	1	301	G
53	1	311	A
53	1	323	C
53	1	324	A
53	1	329	G
53	1	330	A
53	1	361	G
53	1	371	A
53	1	372	G
53	1	386	G
53	1	387	U
53	1	404	A
53	1	406	G
53	1	411	G
53	1	412	A
53	1	422	A
53	1	424	G
53	1	455	C
53	1	458	G
53	1	481	G
53	1	491	G
53	1	504	A
53	1	505	A
53	1	529	A
53	1	530	G
53	1	531	C
53	1	532	A
53	1	543	G
53	1	545	U
53	1	547	A
53	1	563	A
53	1	573	U
53	1	588	U
53	1	603	A
53	1	616	A
53	1	627	A
53	1	637	A
53	1	646	U
53	1	654	A

Continued on next page...

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Mol	Chain	Res	Type
53	1	655	A
53	1	669	G
53	1	686	U
53	1	687	C
53	1	695	G
53	1	730	A
53	1	747	C
53	1	752	A
53	1	764	A
53	1	775	G
53	1	776	G
53	1	782	A
53	1	784	G
53	1	785	G
53	1	805	G
53	1	812	C
53	1	819	A
53	1	827	U
53	1	828	U
53	1	830	G
53	1	845	A
53	1	846	U
53	1	847	U
53	1	858	G
53	1	859	G
53	1	860	U
53	1	878	A
53	1	885	C
53	1	886	A
53	1	887	U
53	1	896	A
53	1	897	C
53	1	910	A
53	1	932	U
53	1	941	A
53	1	946	C
53	1	961	C
53	1	974	G
53	1	983	A
53	1	995	C
53	1	996	A
53	1	1012	U

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Mol	Chain	Res	Type
53	1	1013	C
53	1	1021	A
53	1	1022	G
53	1	1026	G
53	1	1033	U
53	1	1045	C
53	1	1046	A
53	1	1047	G
53	1	1054	A
53	1	1060	U
53	1	1062	G
53	1	1066	U
53	1	1070	A
53	1	1071	G
53	1	1079	C
53	1	1084	A
53	1	1088	A
53	1	1090	A
53	1	1104	C
53	1	1106	G
53	1	1111	A
53	1	1131	G
53	1	1132	U
53	1	1133	A
53	1	1135	C
53	1	1143	A
53	1	1157	G
53	1	1175	A
53	1	1177	G
53	1	1180	U
53	1	1206	G
53	1	1212	G
53	1	1238	G
53	1	1250	G
53	1	1251	C
53	1	1253	A
53	1	1256	G
53	1	1271	G
53	1	1272	A
53	1	1275	A
53	1	1289	C
53	1	1301	A

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Mol	Chain	Res	Type
53	1	1302	A
53	1	1329	U
53	1	1330	C
53	1	1332	G
53	1	1345	C
53	1	1365	A
53	1	1378	A
53	1	1379	U
53	1	1383	A
53	1	1416	G
53	1	1419	A
53	1	1420	A
53	1	1427	A
53	1	1461	C
53	1	1476	U
53	1	1482	G
53	1	1490	A
53	1	1491	G
53	1	1498	C
53	1	1515	A
53	1	1524	G
53	1	1533	C
53	1	1535	A
53	1	1536	C
53	1	1537	G
53	1	1555	G
53	1	1560	G
53	1	1569	A
53	1	1581	G
53	1	1608	A
53	1	1611	C
53	1	1616	A
53	1	1647	U
53	1	1648	U
53	1	1674	G
53	1	1699	G
53	1	1715	G
53	1	1729	U
53	1	1730	C
53	1	1738	G
53	1	1758	U
53	1	1764	C

Continued on next page...

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Mol	Chain	Res	Type
53	1	1773	A
53	1	1780	A
53	1	1781	U
53	1	1800	C
53	1	1801	A
53	1	1808	A
53	1	1816	C
53	1	1829	A
53	1	1871	A
53	1	1901	A
53	1	1906	G
53	1	1907	G
53	1	1913	A
53	1	1914	C
53	1	1929	G
53	1	1930	G
53	1	1931	U
53	1	1937	A
53	1	1938	A
53	1	1944	U
53	1	1955	U
53	1	1963	U
53	1	1967	C
53	1	1970	A
53	1	1971	U
53	1	1972	G
53	1	1993	U
53	1	1997	C
53	1	2022	U
53	1	2023	C
53	1	2030	A
53	1	2031	A
53	1	2036	C
53	1	2043	C
53	1	2049	G
53	1	2055	C
53	1	2056	G
53	1	2060	A
53	1	2061	G
53	1	2062	A
53	1	2069	G
53	1	2072	C

Continued on next page...

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Mol	Chain	Res	Type
53	1	2096	C
53	1	2110	G
53	1	2111	U
53	1	2112	G
53	1	2118	U
53	1	2119	A
53	1	2132	U
53	1	2133	G
53	1	2147	A
53	1	2162	G
53	1	2172	U
53	1	2173	A
53	1	2198	A
53	1	2203	U
53	1	2204	G
53	1	2211	A
53	1	2212	A
53	1	2213	U
53	1	2225	A
53	1	2238	G
53	1	2239	G
53	1	2278	A
53	1	2283	C
53	1	2287	A
53	1	2297	A
53	1	2305	U
53	1	2309	A
53	1	2325	G
53	1	2327	A
53	1	2334	U
53	1	2350	C
53	1	2383	G
53	1	2385	C
53	1	2392	A
53	1	2402	U
53	1	2406	A
53	1	2407	A
53	1	2423	U
53	1	2424	C
53	1	2429	G
53	1	2430	A
53	1	2435	A

Continued on next page...

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Mol	Chain	Res	Type
53	1	2441	U
53	1	2448	A
53	1	2476	A
53	1	2498	C
53	1	2502	G
53	1	2503	A
53	1	2504	U
53	1	2505	G
53	1	2518	A
53	1	2547	A
53	1	2554	U
53	1	2566	A
53	1	2567	G
53	1	2572	A
53	1	2602	A
53	1	2609	U
53	1	2613	U
53	1	2629	U
53	1	2655	G
53	1	2682	A
53	1	2689	U
53	1	2690	U
53	1	2714	G
53	1	2744	G
53	1	2748	A
53	1	2757	A
53	1	2764	A
53	1	2765	A
53	1	2778	A
53	1	2779	U
53	1	2791	G
53	1	2794	C
53	1	2797	U
53	1	2800	A
53	1	2809	A
53	1	2820	A
53	1	2821	A
53	1	2833	U
53	1	2849	U
53	1	2867	G
53	1	2868	A
53	1	2872	A

Continued on next page...

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Mol	Chain	Res	Type
53	1	2879	A
53	1	2880	C
53	1	2883	A
54	2	4	C
54	2	12	C
54	2	13	G
54	2	24	G
54	2	35	C
54	2	44	G
54	2	67	G
54	2	89	U
54	2	90	C
54	2	108	A
54	2	109	A
55	5	9	G
55	5	18	G
55	5	19	G
55	5	20	U
55	5	47	U
55	5	48	C
55	5	59	A
55	5	61	C
55	5	74	C
55	5	76	A
55	6	6	G
55	6	18	G
55	6	19	G
55	6	20	U
55	6	47	U
55	6	48	C
55	6	61	C
56	4	12	A
56	4	13	A
57	7	17	C
57	7	21	A
57	7	45	U
57	7	46	G
57	7	47	U
57	7	48	C
57	7	49	C
57	7	59	U
57	7	61	C

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Mol	Chain	Res	Type
57	7	74	C

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	3	70	U
52	3	429	U
52	3	495	A
52	3	1190	G
53	1	227	A
53	1	421	C
53	1	490	C
53	1	774	G
53	1	859	G
53	1	1020	A
53	1	1130	U
53	1	1475	G
53	1	1930	G
53	1	2286	G
53	1	2296	U
53	1	2326	C
53	1	2391	G
53	1	2756	U
54	2	88	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	PHE	7	101	57	10,11,12	1.16	1 (10%)	10,13,15	1.09	1 (10%)
58	FME	5	101	55	8,9,10	0.75	0	7,9,11	1.02	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
59	PHE	7	101	57	-	0/5/6/8	0/1/1/1
58	FME	5	101	55	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	7	101	PHE	CB-CG	-2.76	1.44	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	7	101	PHE	CB-CA-C	-3.00	105.84	111.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	5	101	FME	O1-CN-N-CA
58	5	101	FME	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

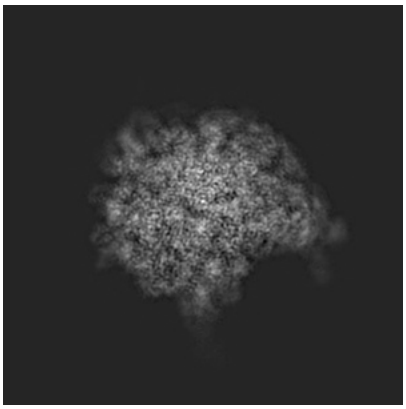
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21632. These allow visual inspection of the internal detail of the map and identification of artifacts.

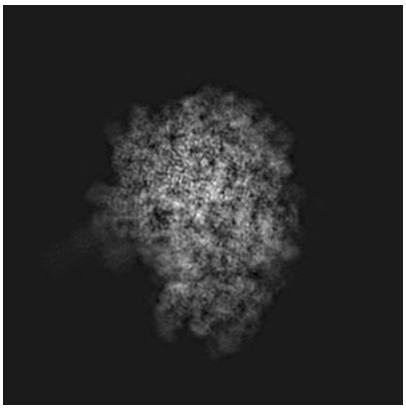
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

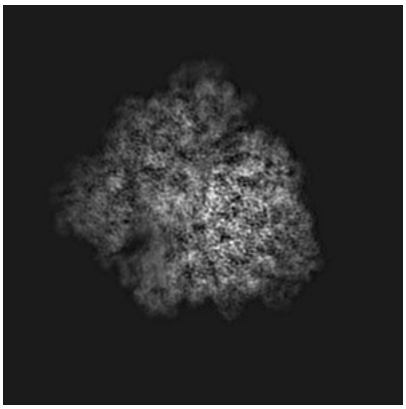
6.1.1 Primary map



X

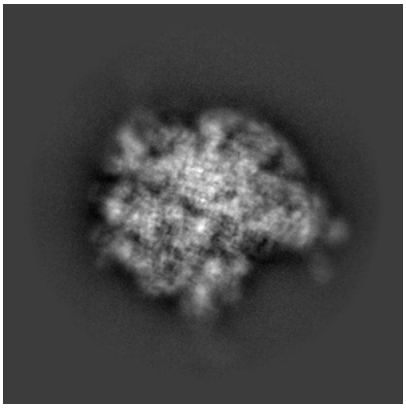


Y

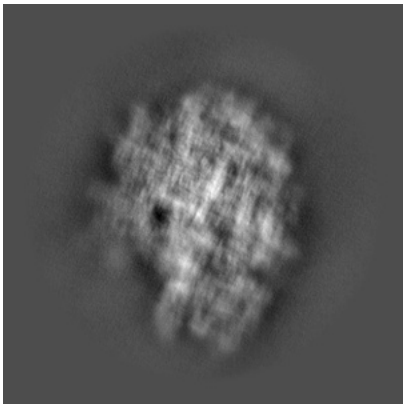


Z

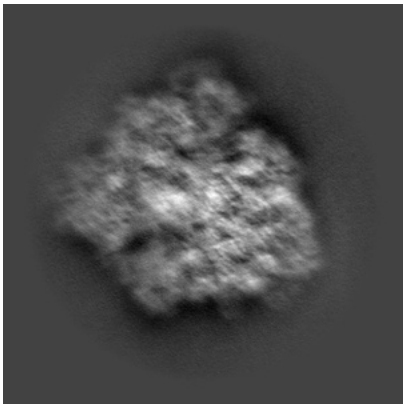
6.1.2 Raw map



X



Y

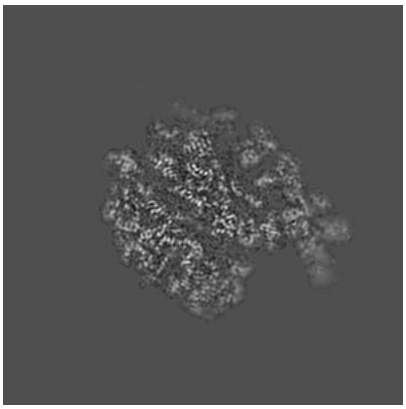


Z

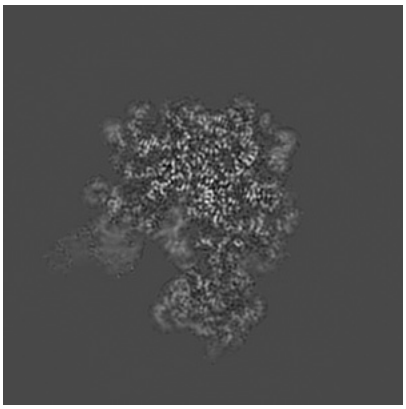
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

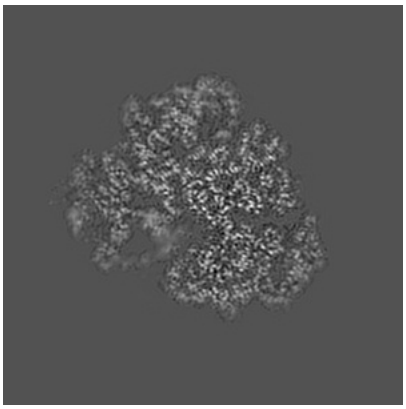
6.2.1 Primary map



X Index: 144

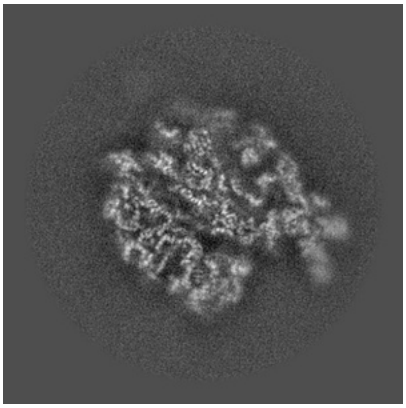


Y Index: 144

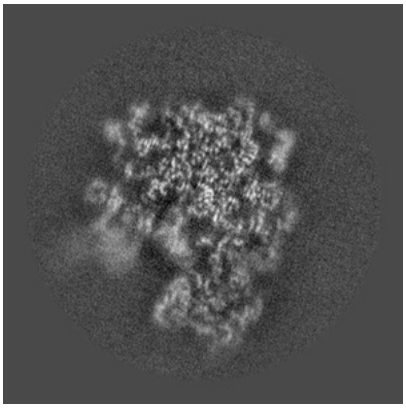


Z Index: 144

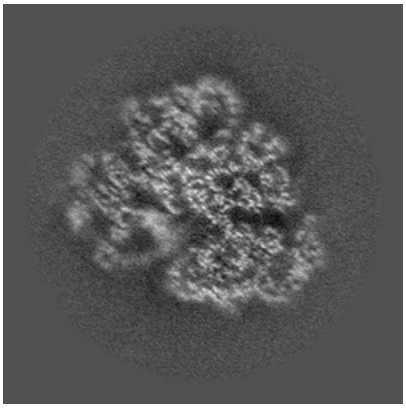
6.2.2 Raw map



X Index: 144



Y Index: 144

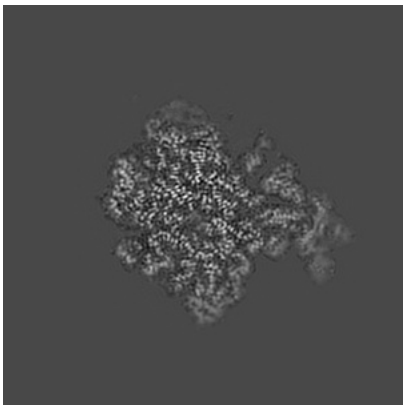


Z Index: 144

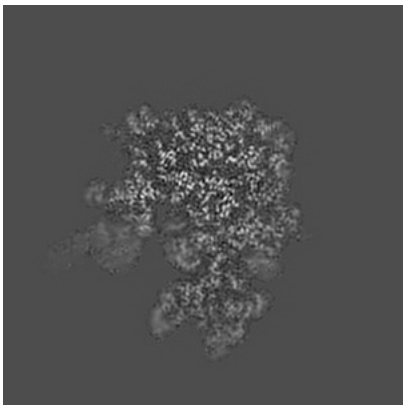
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

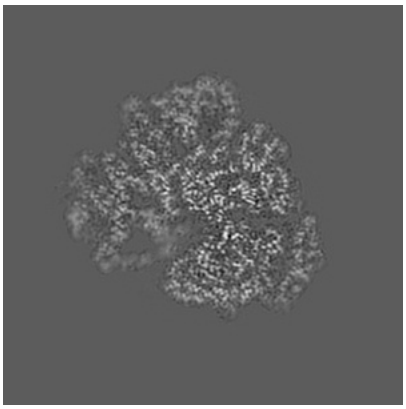
6.3.1 Primary map



X Index: 149

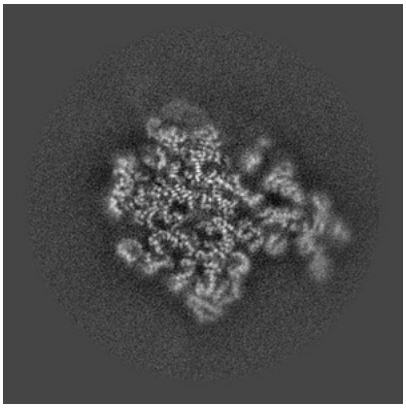


Y Index: 149

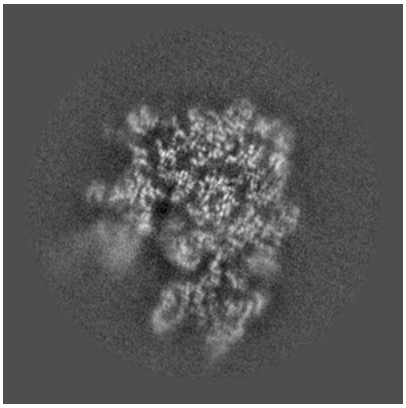


Z Index: 143

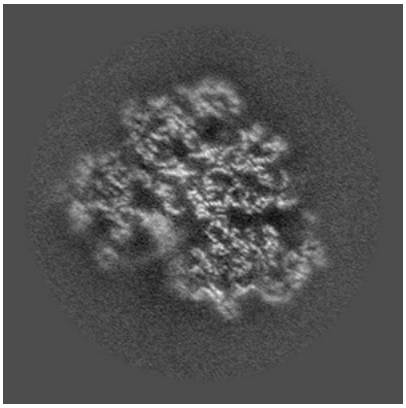
6.3.2 Raw map



X Index: 149



Y Index: 149

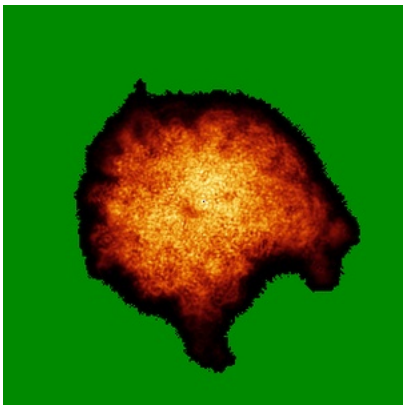


Z Index: 146

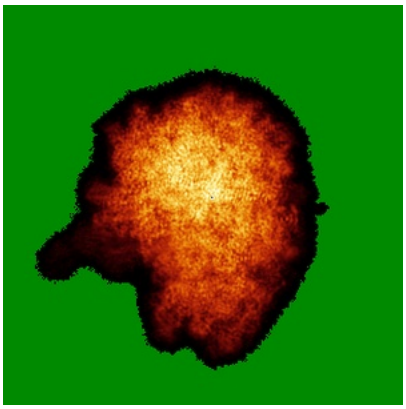
The images above show the largest variance slices of the map in three orthogonal directions.

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

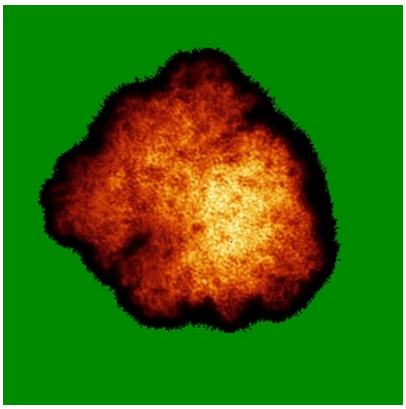
6.4.1 Primary map



X

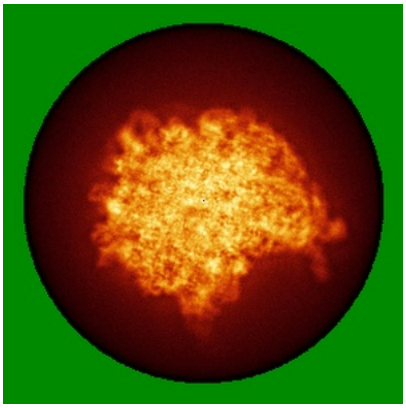


Y

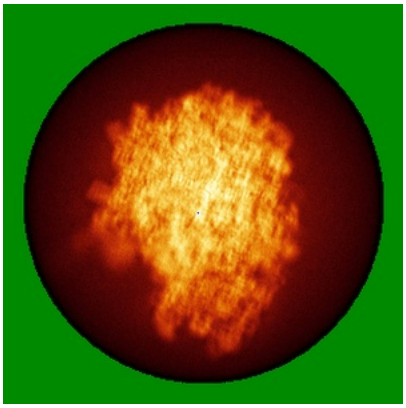


Z

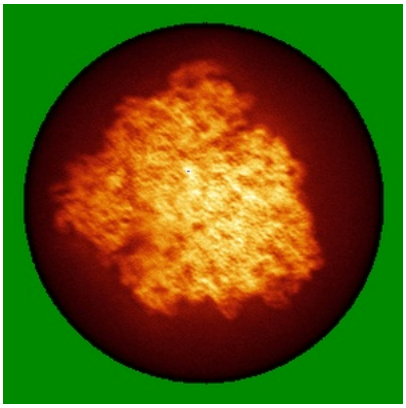
6.4.2 Raw map



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.

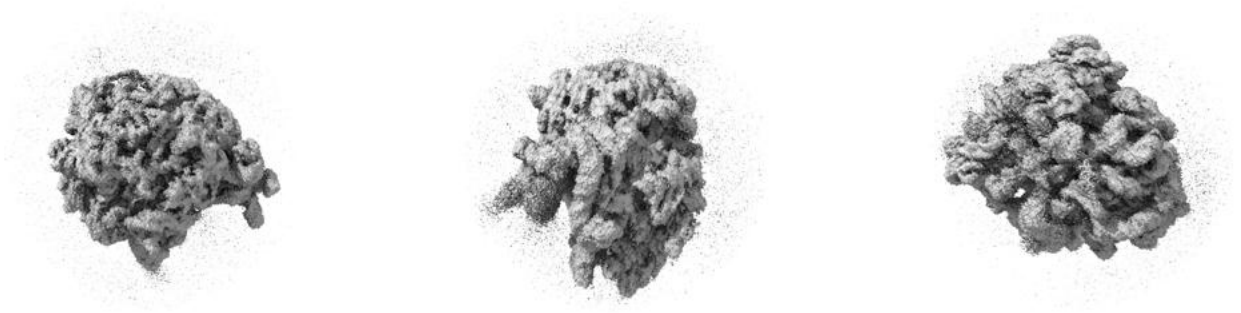
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. 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.

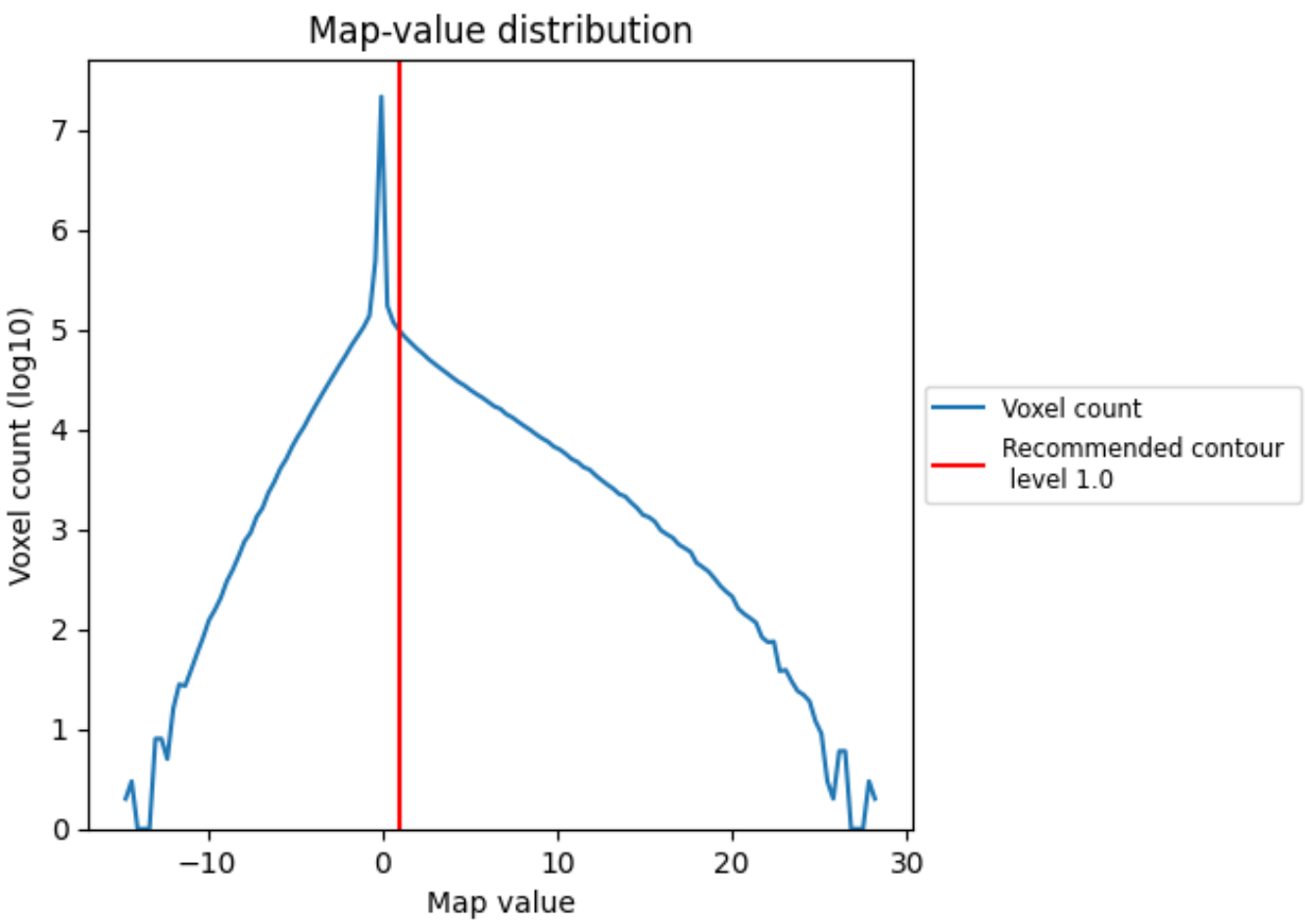
6.6 Mask visualisation (i)

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

7 Map analysis (i)

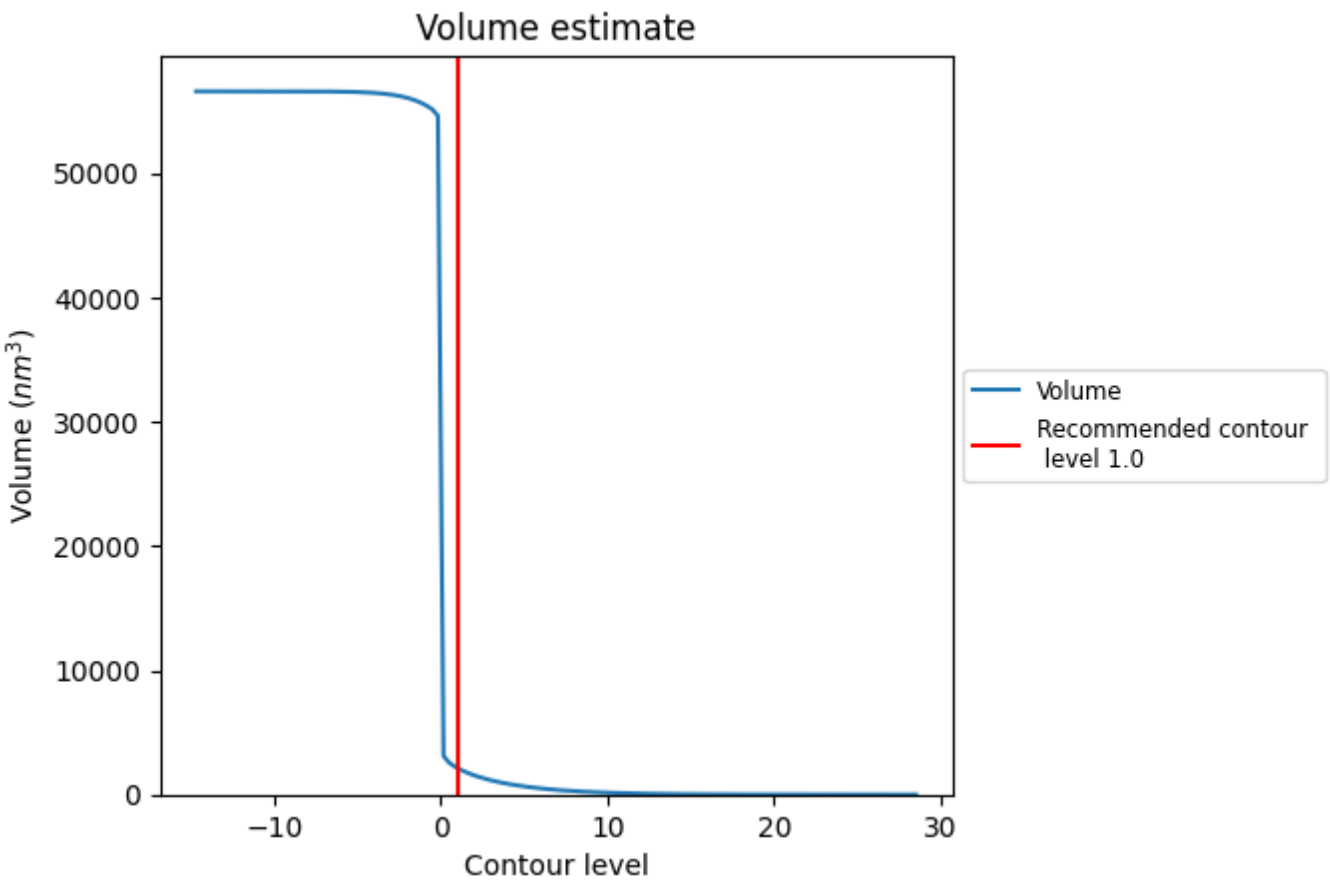
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

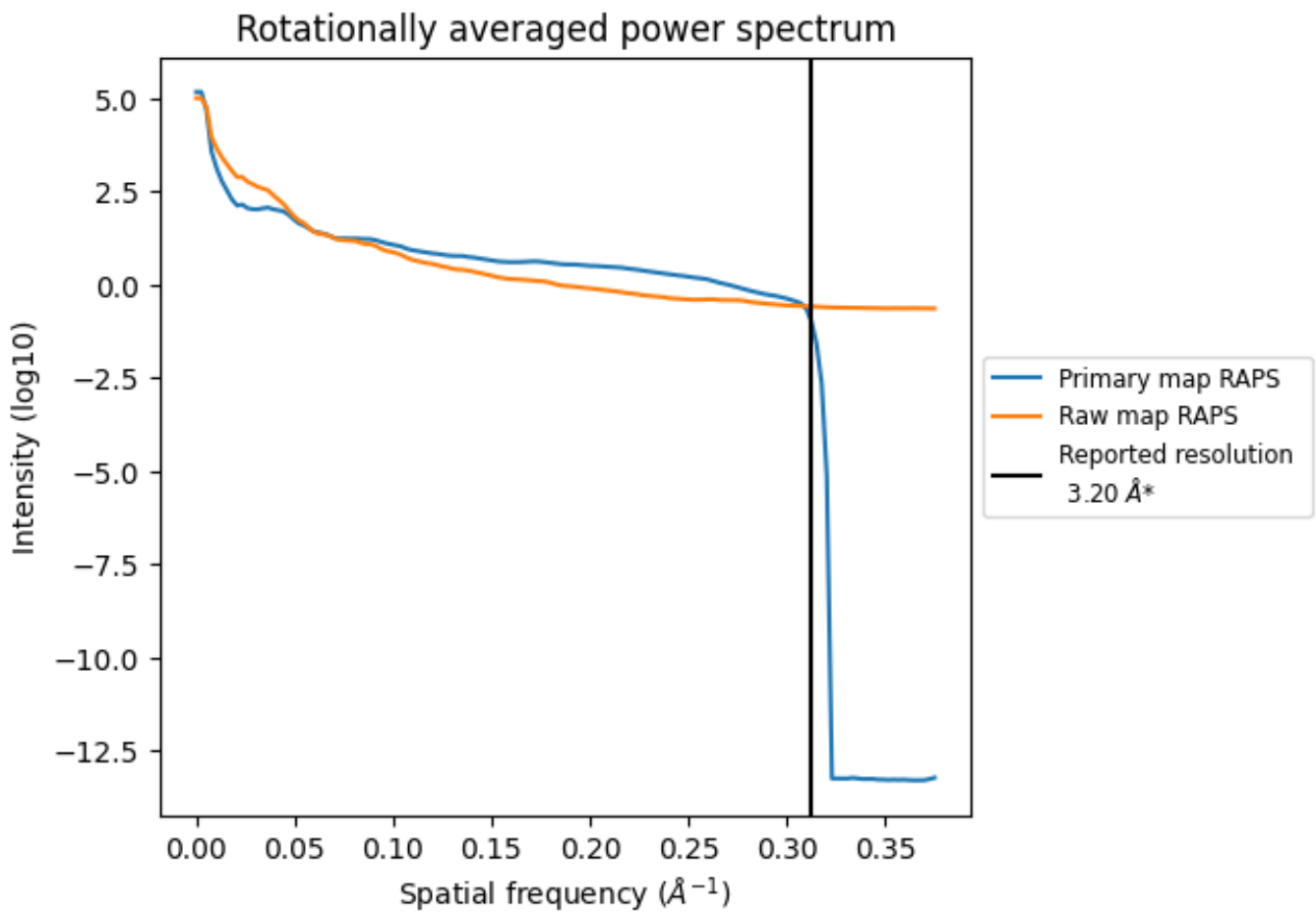
7.2 Volume estimate (i)



The volume at the recommended contour level is 2140 nm^3; this corresponds to an approximate mass of 1933 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)

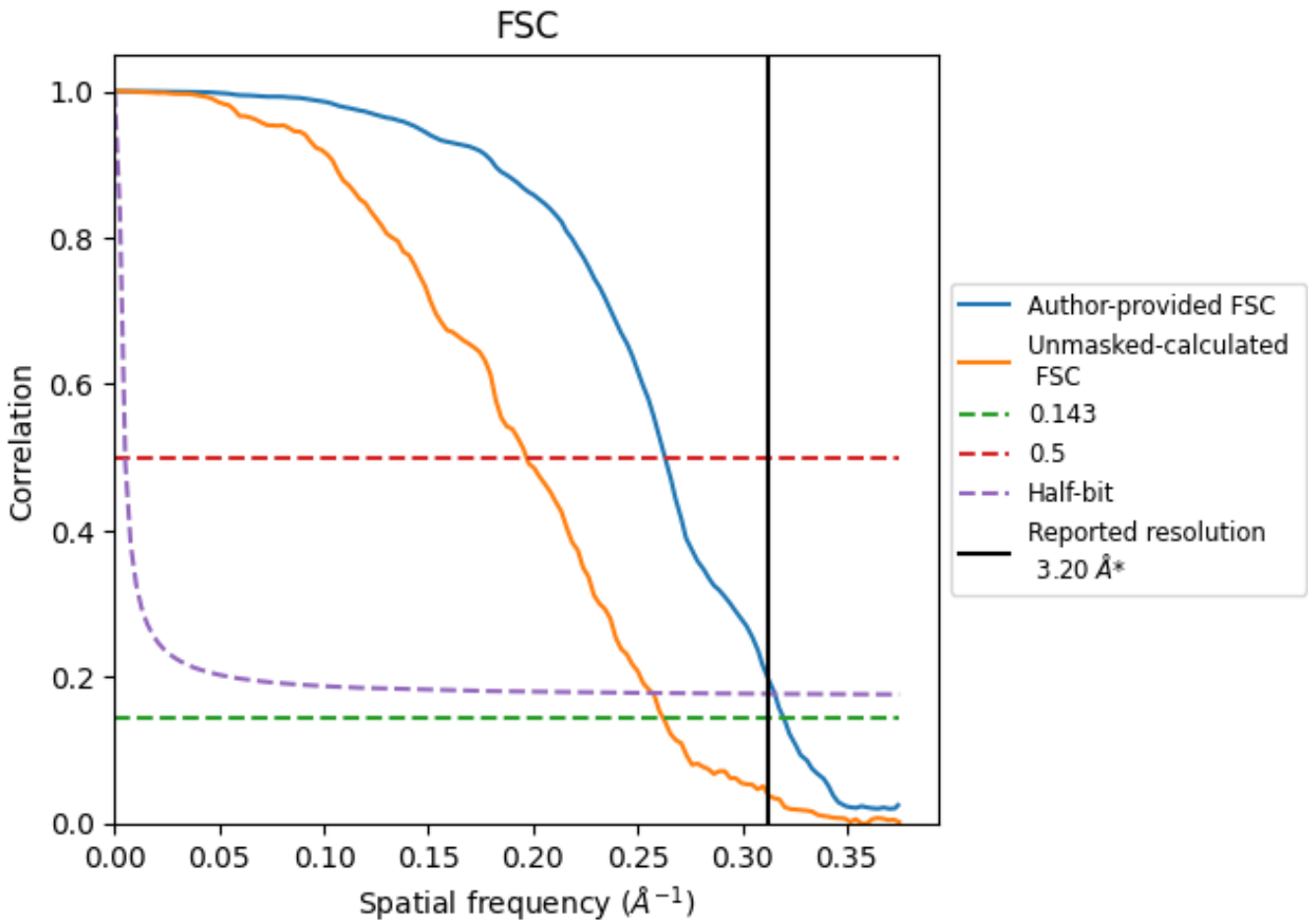


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



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

8.2 Resolution estimates (i)

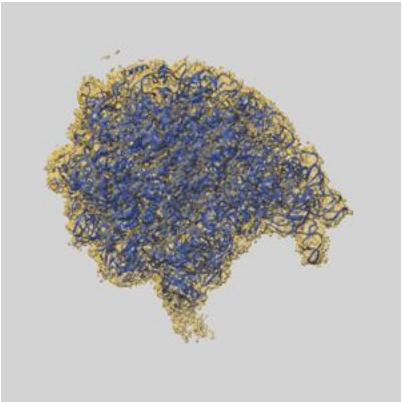
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.13	3.80	3.17
Unmasked-calculated*	3.81	5.08	3.89

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

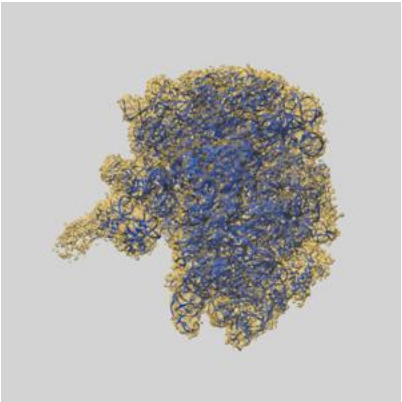
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21632 and PDB model 6WDD. Per-residue inclusion information can be found in section 3 on page 15.

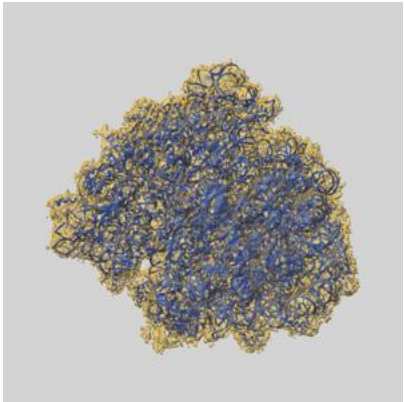
9.1 Map-model overlay (i)



X



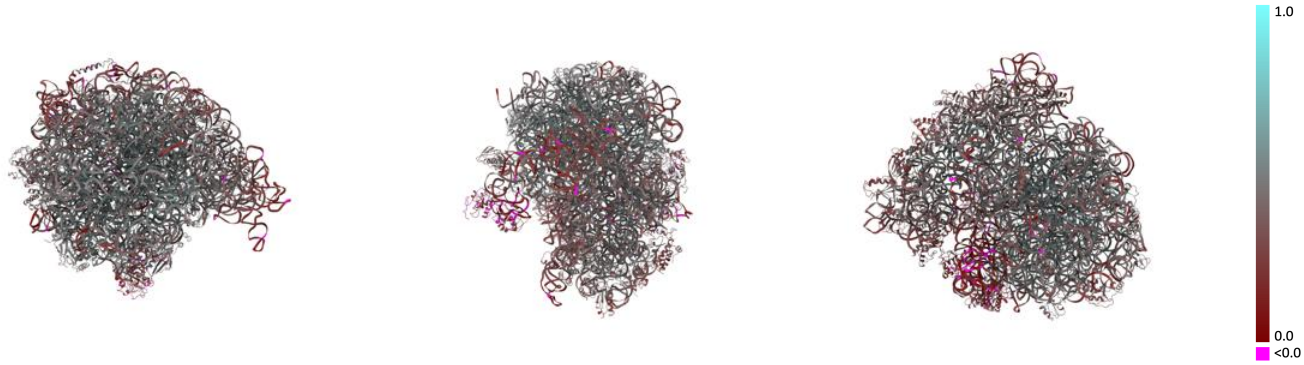
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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.

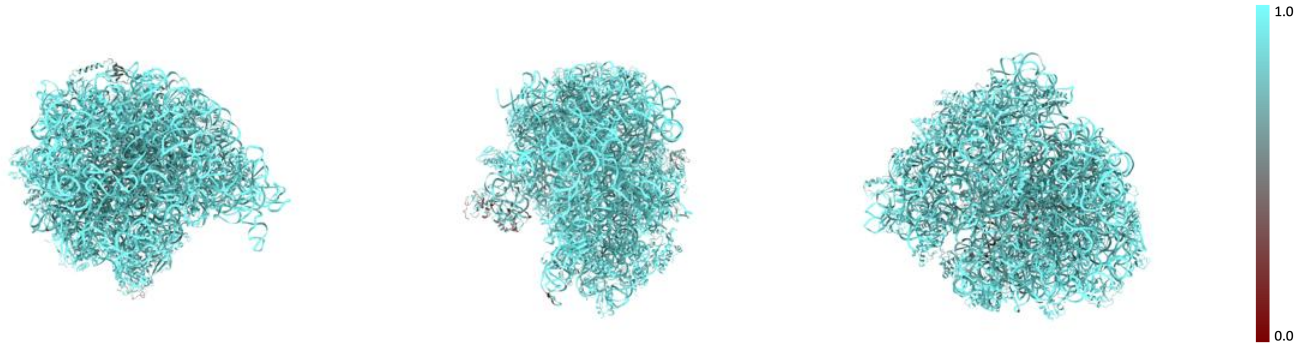
9.2 Q-score mapped to coordinate model (i)



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.

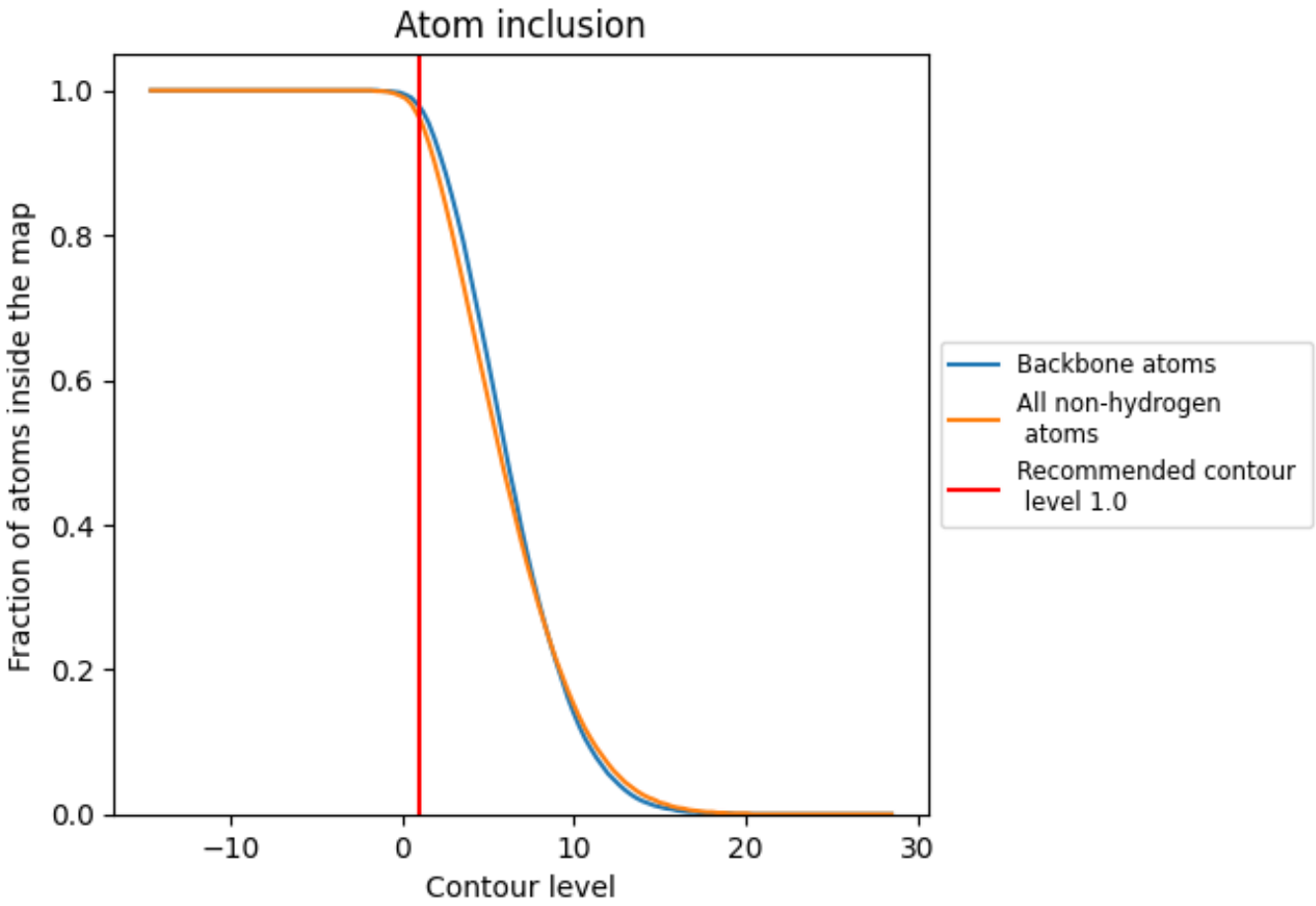
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9610	0.4100
1	0.9820	0.4400
2	0.9830	0.3580
3	0.9780	0.3940
4	0.9230	0.3160
5	0.8470	0.2010
6	0.8510	0.1520
7	0.9360	0.2670
B	0.9580	0.4890
C	0.8980	0.4300
D	0.9580	0.5150
E	0.9590	0.5090
F	0.9010	0.4580
G	0.9050	0.3700
H	0.9350	0.4320
I	0.9180	0.3740
J	0.9440	0.4360
K	0.9590	0.4070
L	0.9420	0.3480
M	0.9490	0.4310
N	0.9420	0.3840
O	0.8780	0.3620
P	0.9590	0.4170
Q	0.9520	0.4730
R	0.9460	0.3280
S	0.9170	0.3920
T	0.9680	0.4170
U	0.9030	0.3780
V	0.9590	0.4190
W	0.9280	0.3950
X	0.9570	0.3460
Y	0.9400	0.3790
Z	0.8650	0.3220
a	0.8970	0.1760
b	0.9700	0.5070

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Chain	Atom inclusion	Q-score
c	0.9630	0.4940
d	0.9500	0.4390
e	0.9210	0.2490
f	0.9650	0.3780
g	0.7640	0.2830
h	0.6460	0.1480
i	0.6350	0.1380
j	0.9630	0.4930
k	0.9650	0.4840
l	0.9510	0.4650
m	0.9440	0.4790
n	0.9660	0.4960
o	0.9570	0.3980
p	0.9580	0.4730
q	0.9640	0.4970
r	0.9640	0.4650
s	0.9460	0.4920
t	0.9470	0.4630
u	0.9440	0.4160
v	0.9620	0.4420
w	0.9640	0.4880
x	0.9800	0.4940
y	0.9400	0.3980
z	0.9680	0.4740