



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 08:45 PM EST

PDB ID : 6OFX
EMDB ID : EMD-20048
Title : Non-rotated ribosome (Structure I)
Authors : Svidritskiy, E.; Demo, G.; Loveland, A.B.; Xu, C.; Korostelev, A.A.
Deposited on : 2019-04-01
Resolution : 3.30 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 ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

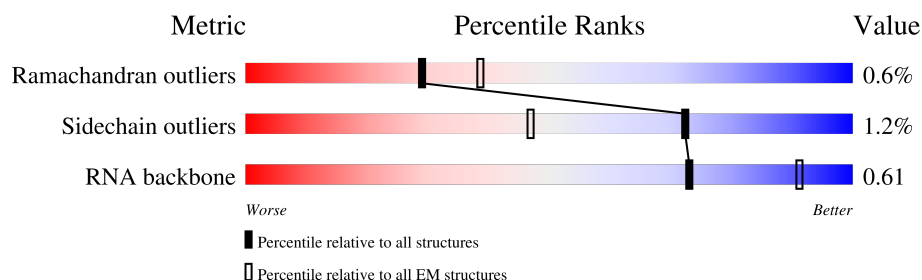
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



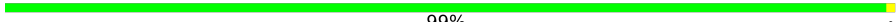
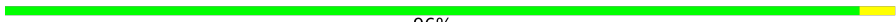













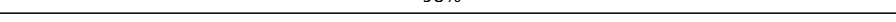
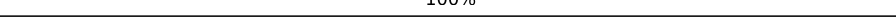
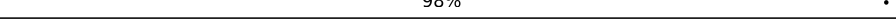

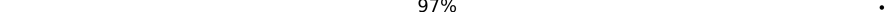
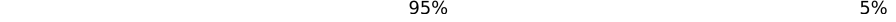

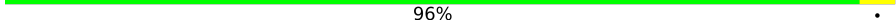
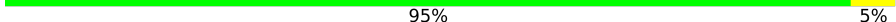

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	b	271	
2	c	209	
3	d	201	
4	e	177	
5	f	176	
6	g	149	
7	j	142	
8	k	122	

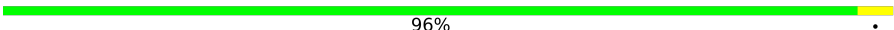
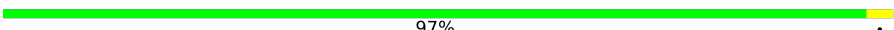
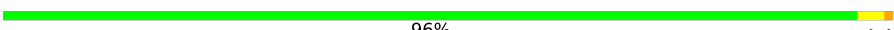
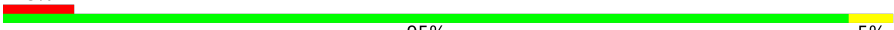








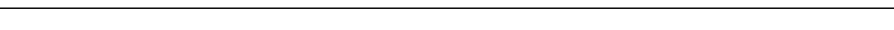
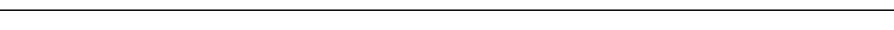
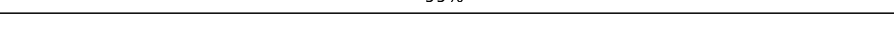






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Mol	Chain	Length	Quality of chain
9	l	143	 99% .
10	m	136	 96% .
11	n	120	 99% .
12	o	116	 95% 5%
13	p	114	 100%
14	q	117	 98% .
15	r	103	 100%
16	s	110	 99% .
17	t	93	 100%
18	u	102	 97% .
19	v	94	 99% .
20	w	75	 100%
21	x	77	 100%
22	y	63	 98% .
23	z	58	 98% .
24	B	56	 100%
25	C	50	 98% .
26	D	46	 100%
27	E	64	 97% .
28	F	38	 95% 5%
29	G	225	 93% 7%
30	H	206	 96% .
31	I	205	 95% 5%
32	J	157	 93% 5% .
33	K	101	 93% 7%

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Mol	Chain	Length	Quality of chain
34	L	151	 96% .
35	M	129	 97% .
36	N	127	 96% ..
37	O	98	 8% 95% 5%
38	P	116	 99% .
39	Q	123	 98% .
40	R	114	 95% 5%
41	S	100	 98% .
42	T	88	 90% 10%
43	U	82	 100%
44	V	80	 98% .
45	W	65	 97% .
46	X	79	 97% .
47	Y	85	 99% .
48	Z	65	 89% 11%
49	a	223	 26% 57% 40%
50	3	1539	 88% 12%
51	1	2903	 5% 84% 15%
52	2	120	 86% 13% .
53	5	77	 82% 18%
54	4	27	 56% 19% 26%

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 144986 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
1	b	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

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

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

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

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

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

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

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

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

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

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

- Molecule 7 is a protein called 50S ribosomal protein L13.

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

- Molecule 8 is a protein called 50S ribosomal protein L14.

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

- Molecule 9 is a protein called 50S ribosomal protein L15.

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

- Molecule 10 is a protein called 50S ribosomal protein L16.

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

- Molecule 11 is a protein called 50S ribosomal protein L17.

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

- Molecule 12 is a protein called 50S ribosomal protein L18.

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

- Molecule 13 is a protein called 50S ribosomal protein L19.

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

- Molecule 14 is a protein called 50S ribosomal protein L20.

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

- Molecule 15 is a protein called 50S ribosomal protein L21.

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

- Molecule 16 is a protein called 50S ribosomal protein L22.

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

- Molecule 17 is a protein called 50S ribosomal protein L23.

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

- Molecule 18 is a protein called 50S ribosomal protein L24.

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

- Molecule 19 is a protein called 50S ribosomal protein L25.

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

- Molecule 20 is a protein called 50S ribosomal protein L27.

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

- Molecule 21 is a protein called 50S ribosomal protein L28.

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

- Molecule 22 is a protein called 50S ribosomal protein L29.

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

- Molecule 23 is a protein called 50S ribosomal protein L30.

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

- Molecule 24 is a protein called 50S ribosomal protein L32.

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

- Molecule 25 is a protein called 50S ribosomal protein L33.

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

- Molecule 26 is a protein called 50S ribosomal protein L34.

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

- Molecule 27 is a protein called 50S ribosomal protein L35.

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

- Molecule 28 is a protein called 50S ribosomal protein L36.

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

- Molecule 29 is a protein called 30S ribosomal protein S2.

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

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

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

- Molecule 31 is a protein called 30S ribosomal protein S4.

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

- Molecule 32 is a protein called 30S ribosomal protein S5.

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

- Molecule 33 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	K	101	Total	C	N	O	S	0	0
			824	520	149	149	6		

- Molecule 34 is a protein called 30S ribosomal protein S7.

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

- Molecule 35 is a protein called 30S ribosomal protein S8.

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

- Molecule 36 is a protein called 30S ribosomal protein S9.

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

- Molecule 37 is a protein called 30S ribosomal protein S10.

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

- Molecule 38 is a protein called 30S ribosomal protein S11.

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

- Molecule 39 is a protein called 30S ribosomal protein S12.

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

- Molecule 40 is a protein called 30S ribosomal protein S13.

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

- Molecule 41 is a protein called 30S ribosomal protein S14.

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

- Molecule 42 is a protein called 30S ribosomal protein S15.

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

- Molecule 43 is a protein called 30S ribosomal protein S16.

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

- Molecule 44 is a protein called 30S ribosomal protein S17.

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

- Molecule 45 is a protein called 30S ribosomal protein S18.

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

- Molecule 46 is a protein called 30S ribosomal protein S19.

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

- Molecule 47 is a protein called 30S ribosomal protein S20.

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

- Molecule 48 is a protein called 30S ribosomal protein S21.

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

- Molecule 49 is a protein called 50S ribosomal protein L1.

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

- Molecule 50 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 51 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 52 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

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

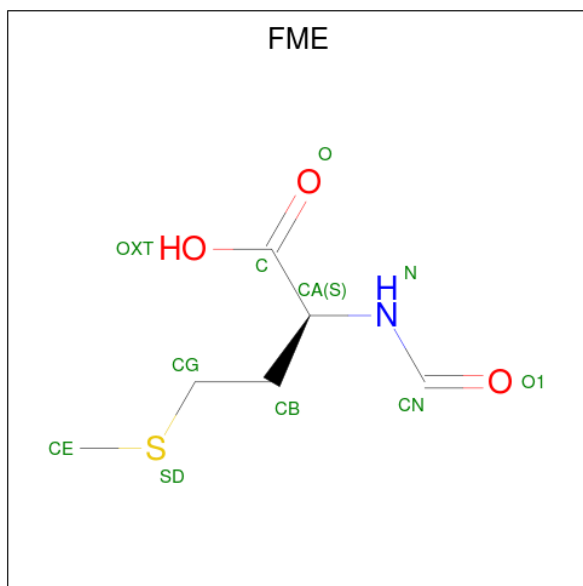
- Molecule 53 is a RNA chain called tRNA^{fMet}.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	20	Total	C	N	O	P	0	0
			437	197	91	130	19		

- Molecule 55 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
55	5	1	10	6	1	2	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%



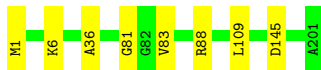
- Molecule 2: 50S ribosomal protein L3

Chain c:  96%



- Molecule 3: 50S ribosomal protein L4

Chain d:  96%



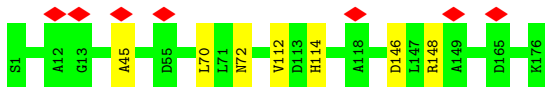
- Molecule 4: 50S ribosomal protein L5

Chain e:  95% 5%

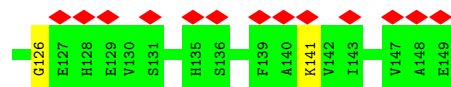
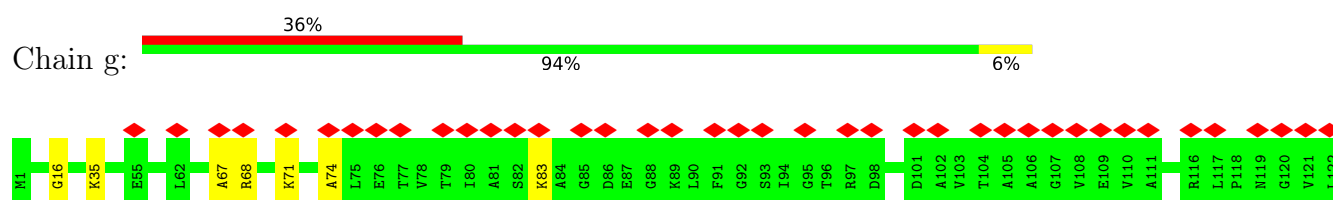


- Molecule 5: 50S ribosomal protein L6

Chain f:  96%



- Molecule 6: 50S ribosomal protein L9



- Molecule 7: 50S ribosomal protein L13



- Molecule 8: 50S ribosomal protein L14



- Molecule 9: 50S ribosomal protein L15



- Molecule 10: 50S ribosomal protein L16



- Molecule 11: 50S ribosomal protein L17



- Molecule 12: 50S ribosomal protein L18





- Molecule 13: 50S ribosomal protein L19

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 14: 50S ribosomal protein L20

Chain q:  98%



- Molecule 15: 50S ribosomal protein L21

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: 50S ribosomal protein L22

Chain s:  99%



- Molecule 17: 50S ribosomal protein L23

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: 50S ribosomal protein L24

Chain u:  97%



- Molecule 19: 50S ribosomal protein L25

Chain v:  99%



- Molecule 20: 50S ribosomal protein L27

Chain w:  100%

There are no outlier residues recorded for this chain.

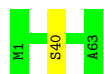
- Molecule 21: 50S ribosomal protein L28

Chain x:  100%

There are no outlier residues recorded for this chain.

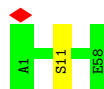
- Molecule 22: 50S ribosomal protein L29

Chain y:  98%



- Molecule 23: 50S ribosomal protein L30

Chain z:  98%



- Molecule 24: 50S ribosomal protein L32

Chain B:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: 50S ribosomal protein L33

Chain C:  98%



- Molecule 26: 50S ribosomal protein L34

Chain D:  100%

There are no outlier residues recorded for this chain.

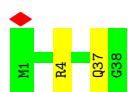
- Molecule 27: 50S ribosomal protein L35

Chain E:  97%



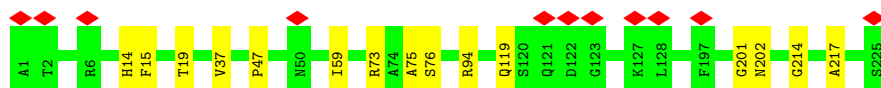
- Molecule 28: 50S ribosomal protein L36

Chain F:  95% 5%



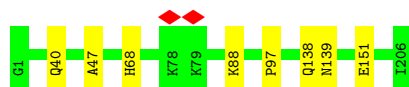
- Molecule 29: 30S ribosomal protein S2

Chain G:  5% 93% 7%



- Molecule 30: 30S ribosomal protein S3

Chain H:  96% .




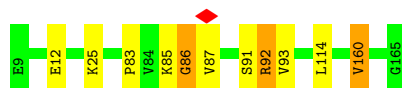
- Molecule 31: 30S ribosomal protein S4

Chain I:  95% 5%



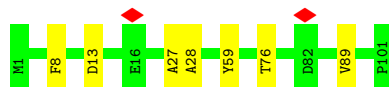
- Molecule 32: 30S ribosomal protein S5

Chain J:  93% 5% .



- Molecule 33: 30S ribosomal protein S6

Chain K:  93% 7%



- Molecule 34: 30S ribosomal protein S7

Chain L:  96% .



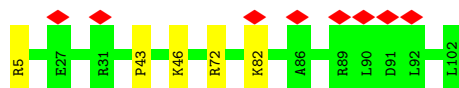
• Molecule 35: 30S ribosomal protein S8

Chain M:  97% .

• Molecule 36: 30S ribosomal protein S9

Chain N:  96% ..

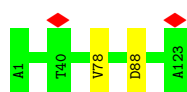
• Molecule 37: 30S ribosomal protein S10

Chain O:  8% 95% 5%

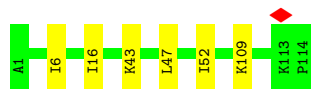
• Molecule 38: 30S ribosomal protein S11

Chain P:  99% .

• Molecule 39: 30S ribosomal protein S12

Chain Q:  98% .


• Molecule 40: 30S ribosomal protein S13

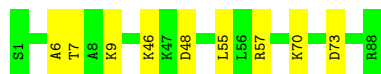
Chain R:  95% 5%

• Molecule 41: 30S ribosomal protein S14

Chain S:  98% .

- Molecule 42: 30S ribosomal protein S15

Chain T:  90% 10%



- Molecule 43: 30S ribosomal protein S16

Chain U:  100%



- Molecule 44: 30S ribosomal protein S17

Chain V:  98%



- Molecule 45: 30S ribosomal protein S18

Chain W:  97%



- Molecule 46: 30S ribosomal protein S19

Chain X:  97%




- Molecule 47: 30S ribosomal protein S20

Chain Y:  99%

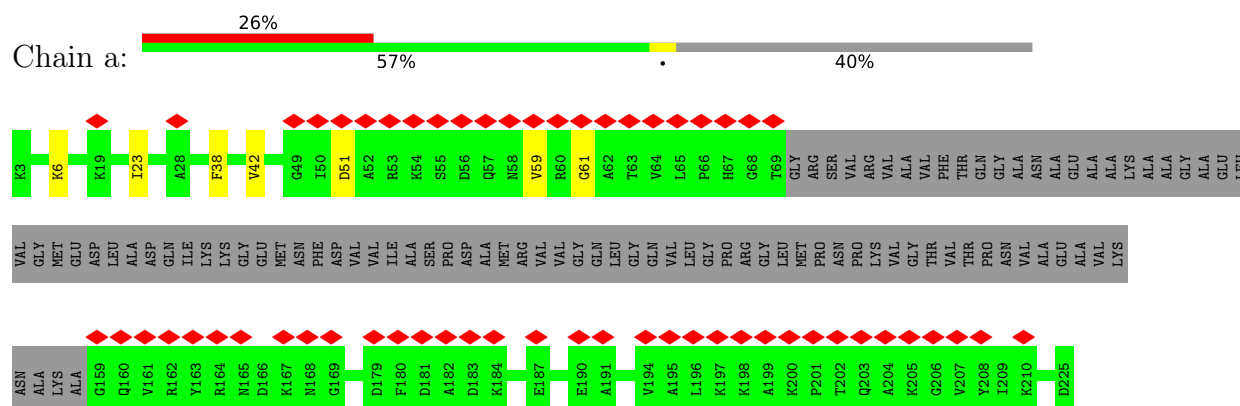


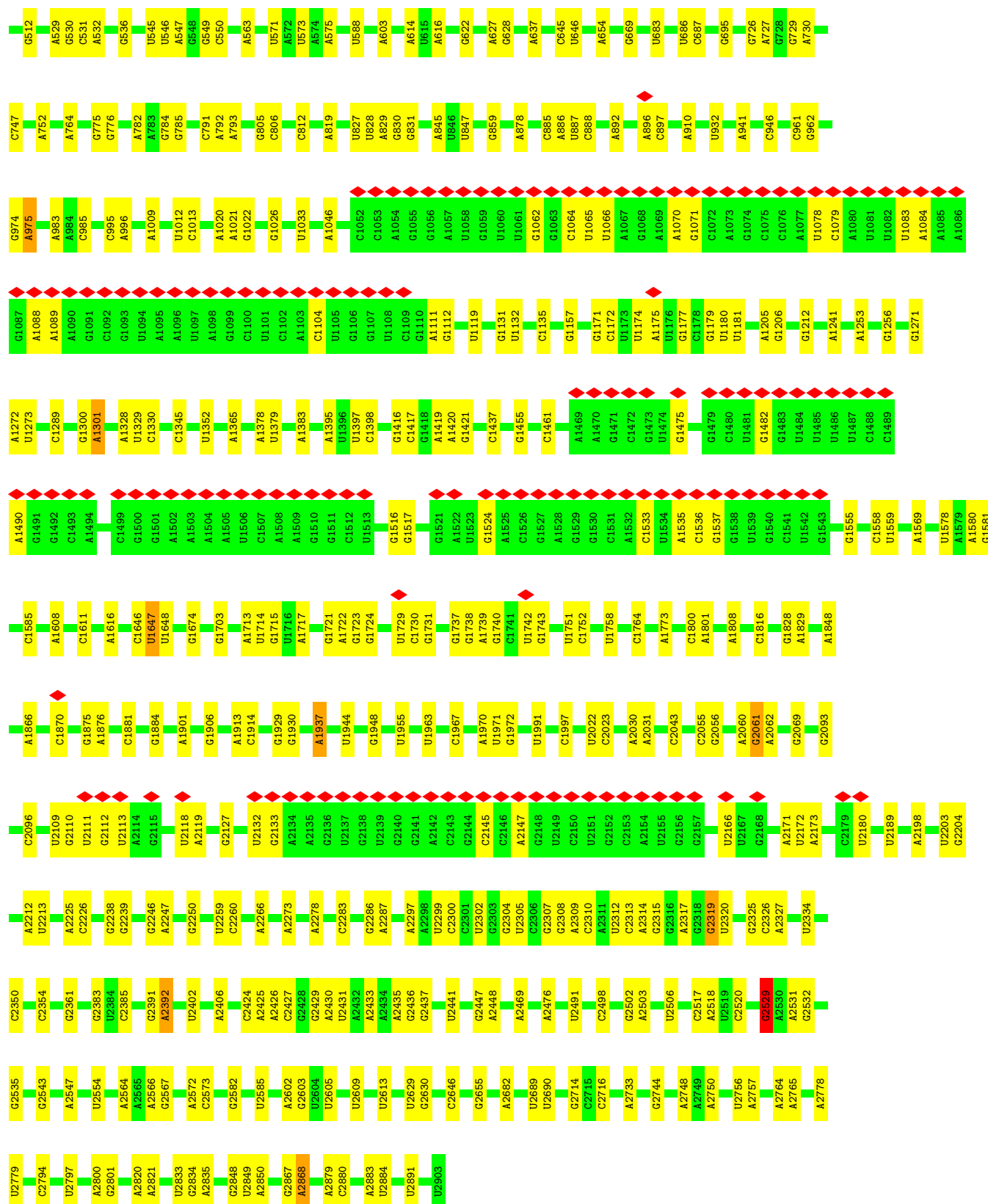
- Molecule 48: 30S ribosomal protein S21

Chain Z:  89% 11%



- Molecule 49: 50S ribosomal protein L1



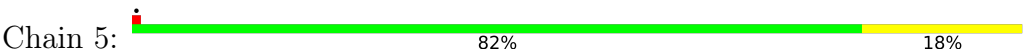


• Molecule 52: 5S ribosomal RNA

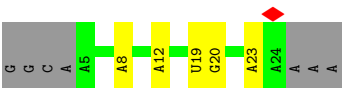
Chain 2: 86% 13%



• Molecule 53: tRNAfMet



• Molecule 54: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	102723	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	29.4	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	6.503	Depositor
Minimum map value	-1.639	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.401	Depositor
Recommended contour level	0.7	Depositor
Map size (\AA)	416.208, 416.208, 416.208	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.334, 1.334, 1.334	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	b	0.56	1/2122 (0.0%)	0.71	0/2852
2	c	0.57	1/1586 (0.1%)	0.72	1/2134 (0.0%)
3	d	0.58	3/1571 (0.2%)	0.67	1/2113 (0.0%)
4	e	0.68	2/1435 (0.1%)	0.72	1/1926 (0.1%)
5	f	0.68	5/1343 (0.4%)	0.74	1/1816 (0.1%)
6	g	0.86	4/1122 (0.4%)	0.84	2/1515 (0.1%)
7	j	0.56	1/1152 (0.1%)	0.67	1/1551 (0.1%)
8	k	0.61	1/948 (0.1%)	0.77	1/1268 (0.1%)
9	l	0.51	0/1054	0.71	0/1403
10	m	0.63	2/1093 (0.2%)	0.74	0/1460
11	n	0.55	0/974	0.66	0/1301
12	o	0.75	4/902 (0.4%)	0.71	1/1209 (0.1%)
13	p	0.48	0/929	0.61	0/1242
14	q	0.62	0/960	0.68	0/1278
15	r	0.53	0/829	0.66	0/1107
16	s	0.64	0/864	0.71	1/1156 (0.1%)
17	t	0.60	0/745	0.66	0/994
18	u	0.51	0/788	0.68	0/1051
19	v	0.53	0/766	0.64	0/1025
20	w	0.48	0/582	0.62	0/769
21	x	0.63	0/635	0.68	0/848
22	y	0.67	1/510 (0.2%)	0.72	0/677
23	z	0.48	0/453	0.58	0/605
24	B	0.50	0/450	0.63	0/599
25	C	0.51	1/417 (0.2%)	0.60	0/554
26	D	0.54	0/380	0.70	0/498
27	E	0.64	1/513 (0.2%)	0.69	0/676
28	F	0.74	1/303 (0.3%)	0.82	0/397
29	G	0.84	9/1788 (0.5%)	0.79	3/2408 (0.1%)
30	H	0.74	6/1652 (0.4%)	0.72	1/2225 (0.0%)
31	I	0.77	8/1665 (0.5%)	0.77	1/2227 (0.0%)
32	J	0.81	6/1170 (0.5%)	0.88	2/1573 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	K	0.87	6/843 (0.7%)	0.81	1/1140 (0.1%)
34	L	0.73	3/1196 (0.3%)	0.75	2/1602 (0.1%)
35	M	0.73	1/989 (0.1%)	0.73	1/1326 (0.1%)
36	N	0.71	3/1034 (0.3%)	0.75	1/1375 (0.1%)
37	O	0.67	1/797 (0.1%)	0.75	0/1077
38	P	0.58	0/886	0.68	0/1195
39	Q	0.56	1/969 (0.1%)	0.77	0/1300
40	R	0.77	3/893 (0.3%)	0.78	1/1193 (0.1%)
41	S	0.70	1/817 (0.1%)	0.73	1/1088 (0.1%)
42	T	0.78	4/722 (0.6%)	0.76	0/964
43	U	0.48	0/659	0.64	0/884
44	V	0.46	0/658	0.63	0/881
45	W	0.73	1/545 (0.2%)	0.76	0/731
46	X	0.66	2/653 (0.3%)	0.70	0/877
47	Y	0.74	0/671	0.70	0/888
48	Z	0.78	2/551 (0.4%)	0.83	1/728 (0.1%)
49	a	0.78	4/1034 (0.4%)	0.76	0/1387
50	3	0.30	0/36963	0.67	0/57662
51	1	0.29	0/69796	0.67	1/108888 (0.0%)
52	2	0.30	0/2872	0.66	0/4479
53	5	0.33	0/1832	0.70	0/2855
54	4	0.28	0/493	0.66	0/769
All	All	0.43	89/157574 (0.1%)	0.68	26/235746 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	e	0	1
29	G	0	1
32	J	0	2
50	3	0	10
51	1	0	41
52	2	0	1
All	All	0	56

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	o	58	ILE	C-O	9.62	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	I	61	ARG	C-O	9.59	1.41	1.23
32	J	92	ARG	C-O	9.48	1.41	1.23
2	c	157	LYS	C-O	9.39	1.41	1.23
49	a	59	VAL	C-O	9.18	1.40	1.23
45	W	12	PHE	C-O	8.80	1.40	1.23
29	G	73	ARG	C-O	-8.43	1.07	1.23
41	S	14	ALA	C-O	8.38	1.39	1.23
31	I	60	VAL	C-O	8.37	1.39	1.23
32	J	86	GLY	C-N	-7.90	1.15	1.34
6	g	126	GLY	C-O	7.76	1.36	1.23
4	e	132	ARG	C-O	7.37	1.37	1.23
40	R	16	ILE	C-O	7.28	1.37	1.23
32	J	114	LEU	C-O	7.21	1.37	1.23
48	Z	19	LYS	C-O	7.02	1.36	1.23
49	a	42	VAL	C-O	7.01	1.36	1.23
33	K	13	ASP	C-O	6.95	1.36	1.23
28	F	4	ARG	C-O	6.88	1.36	1.23
33	K	76	THR	C-O	6.88	1.36	1.23
29	G	202	ASN	N-CA	6.86	1.60	1.46
30	H	68	HIS	C-O	6.82	1.36	1.23
27	E	53	ASP	C-O	6.80	1.36	1.23
5	f	148	ARG	C-O	6.77	1.36	1.23
6	g	68	ARG	C-O	6.73	1.36	1.23
3	d	36	ALA	C-O	6.70	1.36	1.23
33	K	59	TYR	C-O	6.70	1.36	1.23
5	f	72	ASN	C-O	6.64	1.35	1.23
32	J	160	VAL	C-O	6.64	1.35	1.23
29	G	217	ALA	C-O	6.59	1.35	1.23
10	m	119	LEU	C-O	6.57	1.35	1.23
40	R	43	LYS	C-O	6.55	1.35	1.23
30	H	97	PRO	C-O	6.54	1.36	1.23
6	g	67	ALA	C-O	6.49	1.35	1.23
39	Q	78	VAL	C-O	6.46	1.35	1.23
6	g	35	LYS	C-O	6.41	1.35	1.23
10	m	53	MET	C-O	6.38	1.35	1.23
29	G	47	PRO	C-O	6.35	1.35	1.23
36	N	61	ASP	C-O	6.24	1.35	1.23
31	I	201	GLU	C-O	6.16	1.35	1.23
49	a	23	ILE	C-O	6.13	1.34	1.23
30	H	138	GLN	C-O	6.09	1.34	1.23
36	N	64	ILE	C-O	6.05	1.34	1.23
42	T	70	LYS	C-O	6.04	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G	76	SER	C-O	5.99	1.34	1.23
7	j	81	ILE	N-CA	5.98	1.58	1.46
31	I	101	VAL	C-O	5.97	1.34	1.23
42	T	55	LEU	C-O	5.92	1.34	1.23
5	f	114	HIS	N-CA	5.81	1.57	1.46
30	H	139	ASN	C-O	5.80	1.34	1.23
1	b	66	PHE	N-CA	5.73	1.57	1.46
30	H	40	GLN	C-O	5.71	1.34	1.23
35	M	39	LEU	C-O	5.71	1.34	1.23
40	R	52	ILE	C-O	5.70	1.34	1.23
29	G	75	ALA	C-O	5.68	1.34	1.23
48	Z	56	ALA	C-O	5.67	1.34	1.23
8	k	37	ASP	C-O	5.66	1.34	1.23
12	o	77	ALA	C-O	5.66	1.34	1.23
30	H	88	LYS	C-O	5.62	1.34	1.23
31	I	64	TYR	N-CA	5.61	1.57	1.46
12	o	30	ARG	N-CA	5.58	1.57	1.46
32	J	85	LYS	C-N	5.58	1.43	1.33
29	G	37	VAL	C-O	5.56	1.33	1.23
49	a	61	GLY	C-O	5.55	1.32	1.23
33	K	27	ALA	C-O	5.55	1.33	1.23
12	o	75	GLY	C-O	5.54	1.32	1.23
25	C	33	LEU	C-O	5.53	1.33	1.23
36	N	15	ALA	N-CA	5.50	1.57	1.46
31	I	200	VAL	C-O	5.46	1.33	1.23
33	K	28	ALA	C-O	5.44	1.33	1.23
31	I	169	TRP	C-O	5.39	1.33	1.23
5	f	70	LEU	C-O	5.36	1.33	1.23
22	y	40	SER	C-O	5.31	1.33	1.23
31	I	199	ILE	C-O	5.29	1.33	1.23
29	G	214	GLY	C-O	5.27	1.32	1.23
3	d	109	LEU	C-O	5.26	1.33	1.23
46	X	66	VAL	C-O	5.26	1.33	1.23
5	f	146	ASP	C-O	5.26	1.33	1.23
34	L	133	ALA	C-O	5.25	1.33	1.23
46	X	9	PHE	C-O	5.25	1.33	1.23
42	T	7	THR	C-O	5.25	1.33	1.23
37	O	46	LYS	N-CA	5.23	1.56	1.46
3	d	145	ASP	C-O	5.22	1.33	1.23
42	T	6	ALA	C-O	5.19	1.33	1.23
34	L	100	MET	C-O	5.16	1.33	1.23
4	e	145	VAL	N-CA	5.14	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G	59	ILE	C-O	5.14	1.33	1.23
34	L	147	ASN	C-O	5.09	1.33	1.23
33	K	8	PHE	C-O	5.07	1.32	1.23
32	J	91	SER	C-O	5.06	1.32	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	J	85	LYS	C-N-CA	-8.75	103.92	122.30
29	G	201	GLY	C-N-CA	-7.90	101.95	121.70
32	J	86	GLY	C-N-CA	7.52	140.49	121.70
7	j	80	HIS	C-N-CA	-7.10	103.95	121.70
29	G	75	ALA	C-N-CA	-6.92	104.39	121.70
34	L	147	ASN	C-N-CA	-6.71	104.93	121.70
31	I	63	ILE	C-N-CA	-6.64	105.10	121.70
34	L	145	GLU	O-C-N	-6.50	112.31	122.70
41	S	17	ASP	C-N-CA	-6.19	106.23	121.70
6	g	16	GLY	N-CA-C	6.02	128.14	113.10
40	R	109	LYS	C-N-CA	-5.93	109.84	122.30
2	c	157	LYS	O-C-N	5.92	133.27	123.20
3	d	81	GLY	N-CA-C	-5.83	98.52	113.10
5	f	112	VAL	O-C-N	-5.81	113.40	122.70
6	g	71	LYS	C-N-CA	-5.71	107.42	121.70
29	G	202	ASN	N-CA-C	5.67	126.30	111.00
30	H	68	HIS	O-C-N	5.62	131.69	122.70
35	M	36	ALA	C-N-CA	-5.41	108.17	121.70
12	o	28	VAL	O-C-N	-5.35	114.14	122.70
8	k	112	PHE	C-N-CA	-5.32	108.40	121.70
36	N	90	ASP	N-CA-C	5.29	125.29	111.00
4	e	144	LYS	C-N-CA	-5.17	108.76	121.70
33	K	59	TYR	O-C-N	5.17	130.98	122.70
16	s	38	TYR	C-N-CA	-5.11	108.92	121.70
48	Z	10	PRO	N-CA-C	5.09	125.34	112.10
51	1	2529	G	N9-C1'-C2'	5.02	120.52	114.00

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	1	1171	G	Sidechain
51	1	1241	A	Sidechain
51	1	1301	A	Sidechain

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Mol	Chain	Res	Type	Group
51	1	1328	A	Sidechain
51	1	1558	C	Sidechain
51	1	1580	A	Sidechain
51	1	1647	U	Sidechain
51	1	1713	A	Sidechain
51	1	1717	A	Sidechain
51	1	1828	G	Sidechain
51	1	1937	A	Sidechain
51	1	196	A	Sidechain
51	1	2061	G	Sidechain
51	1	2109	U	Sidechain
51	1	2180	U	Sidechain
51	1	2266	A	Sidechain
51	1	2273	A	Sidechain
51	1	2319	G	Sidechain
51	1	2391	G	Sidechain
51	1	2392	A	Sidechain
51	1	2447	G	Sidechain
51	1	2529	G	Sidechain
51	1	2532	G	Sidechain
51	1	27	G	Sidechain
51	1	2848	G	Sidechain
51	1	2868	A	Sidechain
51	1	328	U	Sidechain
51	1	446	G	Sidechain
51	1	450	G	Sidechain
51	1	476	G	Sidechain
51	1	477	A	Sidechain
51	1	500	G	Sidechain
51	1	501	A	Sidechain
51	1	506	G	Sidechain
51	1	51	G	Sidechain
51	1	512	G	Sidechain
51	1	683	U	Sidechain
51	1	726	G	Sidechain
51	1	727	A	Sidechain
51	1	775	G	Sidechain
51	1	975	A	Sidechain
52	2	24	G	Sidechain
50	3	1057	G	Sidechain
50	3	1182	G	Sidechain
50	3	1316	G	Sidechain

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Mol	Chain	Res	Type	Group
50	3	297	G	Sidechain
50	3	413	G	Sidechain
50	3	428	G	Sidechain
50	3	532	A	Sidechain
50	3	872	A	Sidechain
50	3	898	G	Sidechain
50	3	938	A	Sidechain
29	G	14	HIS	Mainchain
32	J	86	GLY	Mainchain
32	J	92	ARG	Mainchain
4	e	149	ARG	Mainchain

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%)	248 (92%)	21 (8%)	0	100	100
2	c	207/209 (99%)	188 (91%)	17 (8%)	2 (1%)	15	46
3	d	199/201 (99%)	187 (94%)	11 (6%)	1 (0%)	29	61
4	e	175/177 (99%)	156 (89%)	18 (10%)	1 (1%)	25	57
5	f	174/176 (99%)	152 (87%)	21 (12%)	1 (1%)	25	57
6	g	147/149 (99%)	125 (85%)	21 (14%)	1 (1%)	22	54
7	j	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
8	k	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	9	35
9	l	141/143 (99%)	125 (89%)	14 (10%)	2 (1%)	11	38
10	m	134/136 (98%)	121 (90%)	10 (8%)	3 (2%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	n	118/120 (98%)	107 (91%)	11 (9%)	0	100	100
12	o	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
13	p	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
14	q	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
15	r	101/103 (98%)	89 (88%)	12 (12%)	0	100	100
16	s	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
17	t	91/93 (98%)	80 (88%)	11 (12%)	0	100	100
18	u	100/102 (98%)	84 (84%)	15 (15%)	1 (1%)	15	46
19	v	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
20	w	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
21	x	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
22	y	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
23	z	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
24	B	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
25	C	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
26	D	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
27	E	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	9	36
28	F	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	5	25
29	G	223/225 (99%)	194 (87%)	27 (12%)	2 (1%)	17	48
30	H	204/206 (99%)	196 (96%)	7 (3%)	1 (0%)	29	61
31	I	203/205 (99%)	177 (87%)	26 (13%)	0	100	100
32	J	155/157 (99%)	128 (83%)	22 (14%)	5 (3%)	4	22
33	K	99/101 (98%)	83 (84%)	16 (16%)	0	100	100
34	L	149/151 (99%)	135 (91%)	13 (9%)	1 (1%)	22	54
35	M	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
36	N	125/127 (98%)	102 (82%)	22 (18%)	1 (1%)	19	51
37	O	96/98 (98%)	85 (88%)	10 (10%)	1 (1%)	15	46
38	P	114/116 (98%)	103 (90%)	11 (10%)	0	100	100
39	Q	121/123 (98%)	97 (80%)	24 (20%)	0	100	100
40	R	112/114 (98%)	95 (85%)	15 (13%)	2 (2%)	8	35
41	S	98/100 (98%)	92 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	T	86/88 (98%)	78 (91%)	7 (8%)	1 (1%)	13	42
43	U	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
44	V	78/80 (98%)	67 (86%)	11 (14%)	0	100	100
45	W	63/65 (97%)	60 (95%)	2 (3%)	1 (2%)	9	36
46	X	77/79 (98%)	70 (91%)	7 (9%)	0	100	100
47	Y	83/85 (98%)	81 (98%)	1 (1%)	1 (1%)	13	42
48	Z	63/65 (97%)	40 (64%)	21 (33%)	2 (3%)	4	22
49	a	130/223 (58%)	124 (95%)	6 (5%)	0	100	100
All	All	5652/5841 (97%)	5093 (90%)	525 (9%)	34 (1%)	29	57

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	d	83	VAL
8	k	92	GLU
9	l	15	ALA
10	m	11	LYS
10	m	70	ASP
18	u	99	SER
27	E	31	ILE
29	G	15	PHE
30	H	47	ALA
32	J	93	VAL
36	N	90	ASP
40	R	6	ILE
42	T	46	LYS
48	Z	8	ASN
6	g	74	ALA
10	m	10	ARG
32	J	160	VAL
5	f	45	ALA
37	O	43	PRO
40	R	47	LEU
2	c	149	ASN
8	k	93	GLN
9	l	31	GLY
28	F	37	GLN
29	G	19	THR
47	Y	68	LYS

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Mol	Chain	Res	Type
32	J	25	LYS
32	J	87	VAL
45	W	17	VAL
48	Z	65	ARG
2	c	152	PRO
34	L	80	GLY
32	J	83	PRO
4	e	61	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	216/216 (100%)	213 (99%)	3 (1%)	67	82
2	c	164/164 (100%)	158 (96%)	6 (4%)	34	63
3	d	165/165 (100%)	162 (98%)	3 (2%)	59	78
4	e	148/148 (100%)	145 (98%)	3 (2%)	55	76
5	f	137/137 (100%)	137 (100%)	0	100	100
6	g	114/114 (100%)	112 (98%)	2 (2%)	59	78
7	j	116/116 (100%)	115 (99%)	1 (1%)	78	87
8	k	103/103 (100%)	102 (99%)	1 (1%)	76	86
9	l	102/102 (100%)	102 (100%)	0	100	100
10	m	109/109 (100%)	108 (99%)	1 (1%)	78	87
11	n	100/100 (100%)	99 (99%)	1 (1%)	76	86
12	o	86/86 (100%)	85 (99%)	1 (1%)	71	83
13	p	99/99 (100%)	99 (100%)	0	100	100
14	q	89/89 (100%)	87 (98%)	2 (2%)	52	74
15	r	84/84 (100%)	84 (100%)	0	100	100
16	s	93/93 (100%)	93 (100%)	0	100	100
17	t	80/80 (100%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	u	83/83 (100%)	81 (98%)	2 (2%)	49	73
19	v	78/78 (100%)	77 (99%)	1 (1%)	69	82
20	w	57/57 (100%)	57 (100%)	0	100	100
21	x	67/67 (100%)	67 (100%)	0	100	100
22	y	55/55 (100%)	55 (100%)	0	100	100
23	z	48/48 (100%)	47 (98%)	1 (2%)	53	75
24	B	47/47 (100%)	47 (100%)	0	100	100
25	C	45/45 (100%)	45 (100%)	0	100	100
26	D	38/38 (100%)	38 (100%)	0	100	100
27	E	51/51 (100%)	51 (100%)	0	100	100
28	F	34/34 (100%)	34 (100%)	0	100	100
29	G	186/186 (100%)	184 (99%)	2 (1%)	73	85
30	H	170/170 (100%)	169 (99%)	1 (1%)	86	91
31	I	172/172 (100%)	170 (99%)	2 (1%)	71	83
32	J	119/119 (100%)	118 (99%)	1 (1%)	81	89
33	K	88/88 (100%)	87 (99%)	1 (1%)	73	85
34	L	124/124 (100%)	123 (99%)	1 (1%)	81	89
35	M	104/104 (100%)	102 (98%)	2 (2%)	57	77
36	N	105/105 (100%)	104 (99%)	1 (1%)	76	86
37	O	86/86 (100%)	83 (96%)	3 (4%)	36	64
38	P	89/89 (100%)	88 (99%)	1 (1%)	73	85
39	Q	103/103 (100%)	102 (99%)	1 (1%)	76	86
40	R	92/92 (100%)	92 (100%)	0	100	100
41	S	83/83 (100%)	83 (100%)	0	100	100
42	T	76/76 (100%)	72 (95%)	4 (5%)	22	53
43	U	65/65 (100%)	65 (100%)	0	100	100
44	V	74/74 (100%)	72 (97%)	2 (3%)	44	71
45	W	56/56 (100%)	56 (100%)	0	100	100
46	X	70/70 (100%)	70 (100%)	0	100	100
47	Y	65/65 (100%)	65 (100%)	0	100	100
48	Z	55/55 (100%)	53 (96%)	2 (4%)	35	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
49	a	110/174 (63%)	107 (97%)	3 (3%)	44 71
All	All	4700/4764 (99%)	4645 (99%)	55 (1%)	72 83

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	35	LYS
1	b	47	ARG
1	b	212	TRP
2	c	33	ARG
2	c	42	ASN
2	c	77	ARG
2	c	148	GLN
2	c	151	THR
2	c	183	GLU
3	d	1	MET
3	d	6	LYS
3	d	88	ARG
4	e	117	SER
4	e	120	SER
4	e	148	VAL
6	g	83	LYS
6	g	141	LYS
7	j	13	ARG
8	k	92	GLU
10	m	13	HIS
11	n	1	MET
12	o	111	ARG
14	q	48	ASP
14	q	65	ASN
18	u	21	ARG
18	u	36	GLU
19	v	1	MET
23	z	11	SER
29	G	94	ARG
29	G	119	GLN
30	H	151	GLU
31	I	49	ASP
31	I	151	GLN
32	J	12	GLU
33	K	89	VAL
34	L	110	ARG

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Mol	Chain	Res	Type
35	M	61	THR
35	M	74	ILE
36	N	45	MET
37	O	5	ARG
37	O	72	ARG
37	O	82	LYS
38	P	124	LYS
39	Q	88	ASP
42	T	9	LYS
42	T	48	ASP
42	T	57	ARG
42	T	73	ASP
44	V	37	ILE
44	V	62	GLU
48	Z	35	GLU
48	Z	44	ARG
49	a	6	LYS
49	a	38	PHE
49	a	51	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	43	ASN
1	b	44	ASN
1	b	45	ASN
1	b	85	ASN
1	b	89	ASN
1	b	133	ASN
1	b	196	ASN
1	b	199	HIS
1	b	259	ASN
2	c	36	GLN
2	c	42	ASN
2	c	130	GLN
2	c	150	GLN
2	c	164	GLN
3	d	24	ASN
3	d	92	HIS
3	d	94	GLN
3	d	136	GLN
3	d	163	ASN

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Mol	Chain	Res	Type
3	d	195	GLN
4	e	26	GLN
4	e	36	ASN
4	e	51	ASN
5	f	47	ASN
5	f	142	GLN
6	g	43	ASN
6	g	73	ASN
7	j	40	HIS
7	j	58	ASN
7	j	80	HIS
7	j	136	GLN
7	j	138	GLN
9	l	35	HIS
9	l	54	GLN
10	m	3	GLN
10	m	13	HIS
11	n	9	GLN
11	n	23	ASN
11	n	62	ASN
12	o	104	GLN
13	p	11	GLN
13	p	40	GLN
13	p	65	ASN
13	p	114	ASN
14	q	51	GLN
14	q	55	GLN
14	q	65	ASN
15	r	18	GLN
15	r	43	ASN
16	s	7	HIS
16	s	40	ASN
17	t	59	ASN
18	u	68	ASN
18	u	98	ASN
19	v	78	GLN
21	x	15	ASN
21	x	16	ASN
21	x	22	ASN
22	y	20	ASN
23	z	8	GLN
24	B	5	ASN

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Mol	Chain	Res	Type
26	D	13	ASN
28	F	13	ASN
29	G	23	ASN
29	G	41	ASN
29	G	57	ASN
29	G	121	GLN
29	G	145	ASN
29	G	176	ASN
29	G	189	ASN
30	H	2	GLN
30	H	31	ASN
30	H	138	GLN
30	H	139	ASN
30	H	184	ASN
31	I	73	ASN
31	I	88	ASN
31	I	115	GLN
31	I	130	ASN
31	I	195	ASN
32	J	69	ASN
32	J	96	GLN
33	K	17	GLN
33	K	52	ASN
33	K	63	ASN
34	L	27	ASN
34	L	67	ASN
34	L	96	ASN
34	L	121	ASN
35	M	15	ASN
35	M	37	ASN
35	M	66	GLN
35	M	75	GLN
36	N	49	GLN
36	N	109	GLN
36	N	125	GLN
37	O	64	GLN
38	P	118	ASN
40	R	7	ASN
40	R	51	GLN
41	S	42	ASN
41	S	48	GLN
41	S	59	GLN

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Mol	Chain	Res	Type
41	S	65	GLN
42	T	36	ASN
42	T	61	GLN
43	U	26	ASN
43	U	40	ASN
43	U	79	ASN
44	V	30	HIS
45	W	73	HIS
46	X	51	HIS
46	X	68	HIS
47	Y	2	ASN
47	Y	19	HIS
47	Y	69	ASN
47	Y	83	ASN
49	a	67	HIS
49	a	160	GLN
49	a	165	ASN
49	a	172	HIS
49	a	188	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	3	1538/1539 (99%)	182 (11%)	2 (0%)
51	1	2902/2903 (99%)	422 (14%)	13 (0%)
52	2	119/120 (99%)	16 (13%)	1 (0%)
53	5	76/77 (98%)	14 (18%)	0
54	4	19/27 (70%)	5 (26%)	0
All	All	4654/4666 (99%)	639 (13%)	16 (0%)

All (639) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	3	3	A
50	3	9	G
50	3	22	G
50	3	31	G
50	3	32	A
50	3	39	G
50	3	47	C
50	3	48	C

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Mol	Chain	Res	Type
50	3	51	A
50	3	71	A
50	3	72	A
50	3	75	G
50	3	82	G
50	3	85	U
50	3	87	C
50	3	122	G
50	3	130	A
50	3	144	G
50	3	181	A
50	3	183	C
50	3	184	G
50	3	197	A
50	3	207	C
50	3	209	U
50	3	210	C
50	3	226	G
50	3	244	U
50	3	247	G
50	3	251	G
50	3	253	A
50	3	266	G
50	3	267	C
50	3	269	C
50	3	280	C
50	3	281	G
50	3	289	G
50	3	296	U
50	3	316	C
50	3	328	C
50	3	345	C
50	3	351	G
50	3	352	C
50	3	367	U
50	3	372	C
50	3	373	A
50	3	397	A
50	3	411	A
50	3	412	A
50	3	413	G
50	3	414	A

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Mol	Chain	Res	Type
50	3	422	C
50	3	428	G
50	3	429	U
50	3	467	U
50	3	468	A
50	3	474	G
50	3	485	U
50	3	486	U
50	3	495	A
50	3	509	A
50	3	518	C
50	3	531	U
50	3	532	A
50	3	547	A
50	3	561	U
50	3	564	C
50	3	572	A
50	3	573	A
50	3	575	G
50	3	576	C
50	3	577	G
50	3	615	G
50	3	633	G
50	3	650	G
50	3	654	G
50	3	665	A
50	3	666	G
50	3	688	G
50	3	692	U
50	3	702	A
50	3	703	G
50	3	713	G
50	3	723	U
50	3	724	G
50	3	755	G
50	3	777	A
50	3	790	A
50	3	809	G
50	3	815	A
50	3	817	C
50	3	818	G
50	3	819	A

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Mol	Chain	Res	Type
50	3	821	G
50	3	842	U
50	3	843	U
50	3	844	G
50	3	845	A
50	3	846	G
50	3	851	G
50	3	873	A
50	3	890	G
50	3	902	G
50	3	926	G
50	3	934	C
50	3	935	A
50	3	960	U
50	3	961	U
50	3	966	G
50	3	969	A
50	3	975	A
50	3	976	G
50	3	977	A
50	3	992	U
50	3	993	G
50	3	1004	A
50	3	1022	A
50	3	1028	C
50	3	1031	C
50	3	1033	G
50	3	1034	G
50	3	1053	G
50	3	1055	A
50	3	1094	G
50	3	1096	C
50	3	1101	A
50	3	1127	G
50	3	1130	A
50	3	1132	C
50	3	1135	U
50	3	1137	C
50	3	1138	G
50	3	1139	G
50	3	1159	U
50	3	1168	U

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Mol	Chain	Res	Type
50	3	1169	A
50	3	1182	G
50	3	1184	G
50	3	1191	A
50	3	1196	A
50	3	1197	A
50	3	1201	A
50	3	1202	U
50	3	1212	U
50	3	1225	A
50	3	1238	A
50	3	1240	U
50	3	1241	G
50	3	1253	G
50	3	1258	G
50	3	1260	G
50	3	1262	C
50	3	1275	A
50	3	1278	G
50	3	1280	A
50	3	1286	U
50	3	1287	A
50	3	1300	G
50	3	1302	C
50	3	1312	G
50	3	1317	C
50	3	1336	C
50	3	1346	A
50	3	1347	G
50	3	1363	A
50	3	1379	G
50	3	1395	C
50	3	1397	C
50	3	1398	A
50	3	1446	A
50	3	1448	C
50	3	1452	C
50	3	1493	A
50	3	1499	A
50	3	1503	A
50	3	1506	U
50	3	1517	G

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Mol	Chain	Res	Type
50	3	1519	A
50	3	1529	G
50	3	1530	G
50	3	1536	C
50	3	1539	C
50	3	1540	U
51	1	10	A
51	1	34	U
51	1	35	G
51	1	46	G
51	1	51	G
51	1	63	A
51	1	71	A
51	1	74	A
51	1	75	G
51	1	86	G
51	1	96	C
51	1	118	A
51	1	120	U
51	1	137	U
51	1	138	U
51	1	139	U
51	1	140	C
51	1	141	G
51	1	142	A
51	1	146	A
51	1	162	U
51	1	163	C
51	1	196	A
51	1	215	G
51	1	216	A
51	1	221	A
51	1	222	A
51	1	229	C
51	1	248	G
51	1	255	A
51	1	265	A
51	1	266	G
51	1	271	G
51	1	276	U
51	1	278	A
51	1	281	C

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Mol	Chain	Res	Type
51	1	284	U
51	1	285	G
51	1	323	C
51	1	324	A
51	1	329	G
51	1	330	A
51	1	361	G
51	1	367	G
51	1	371	A
51	1	372	G
51	1	386	G
51	1	387	U
51	1	389	G
51	1	391	A
51	1	404	A
51	1	406	G
51	1	411	G
51	1	421	C
51	1	424	G
51	1	457	A
51	1	458	G
51	1	481	G
51	1	491	G
51	1	504	A
51	1	505	A
51	1	529	A
51	1	530	G
51	1	531	C
51	1	532	A
51	1	536	G
51	1	545	U
51	1	546	U
51	1	547	A
51	1	549	G
51	1	550	C
51	1	563	A
51	1	571	U
51	1	573	U
51	1	575	A
51	1	588	U
51	1	603	A
51	1	614	A

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Mol	Chain	Res	Type
51	1	616	A
51	1	622	G
51	1	627	A
51	1	628	G
51	1	637	A
51	1	645	C
51	1	646	U
51	1	654	A
51	1	669	G
51	1	686	U
51	1	687	C
51	1	695	G
51	1	729	G
51	1	730	A
51	1	747	C
51	1	752	A
51	1	764	A
51	1	776	G
51	1	782	A
51	1	784	G
51	1	785	G
51	1	791	C
51	1	792	A
51	1	793	A
51	1	805	G
51	1	806	C
51	1	812	C
51	1	819	A
51	1	827	U
51	1	828	U
51	1	829	A
51	1	830	G
51	1	831	G
51	1	845	A
51	1	847	U
51	1	859	G
51	1	878	A
51	1	885	C
51	1	886	A
51	1	887	U
51	1	888	C
51	1	892	A

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Mol	Chain	Res	Type
51	1	896	A
51	1	897	C
51	1	910	A
51	1	932	U
51	1	941	A
51	1	946	C
51	1	961	C
51	1	962	G
51	1	974	G
51	1	975	A
51	1	983	A
51	1	985	C
51	1	995	C
51	1	996	A
51	1	1009	A
51	1	1012	U
51	1	1013	C
51	1	1021	A
51	1	1022	G
51	1	1026	G
51	1	1033	U
51	1	1046	A
51	1	1062	G
51	1	1064	C
51	1	1065	U
51	1	1066	U
51	1	1070	A
51	1	1071	G
51	1	1078	U
51	1	1079	C
51	1	1083	U
51	1	1084	A
51	1	1088	A
51	1	1089	A
51	1	1104	C
51	1	1111	A
51	1	1112	G
51	1	1119	U
51	1	1131	G
51	1	1132	U
51	1	1135	C
51	1	1157	G

Continued on next page...

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Mol	Chain	Res	Type
51	1	1172	C
51	1	1174	U
51	1	1175	A
51	1	1177	G
51	1	1179	G
51	1	1180	U
51	1	1181	U
51	1	1205	A
51	1	1206	G
51	1	1212	G
51	1	1253	A
51	1	1256	G
51	1	1271	G
51	1	1272	A
51	1	1273	U
51	1	1289	C
51	1	1300	G
51	1	1301	A
51	1	1329	U
51	1	1330	C
51	1	1345	C
51	1	1352	U
51	1	1365	A
51	1	1378	A
51	1	1379	U
51	1	1383	A
51	1	1395	A
51	1	1397	U
51	1	1398	C
51	1	1416	G
51	1	1417	C
51	1	1419	A
51	1	1420	A
51	1	1421	G
51	1	1437	C
51	1	1455	G
51	1	1461	C
51	1	1475	G
51	1	1482	G
51	1	1490	A
51	1	1516	G
51	1	1517	G

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Mol	Chain	Res	Type
51	1	1524	G
51	1	1533	C
51	1	1535	A
51	1	1536	C
51	1	1537	G
51	1	1555	G
51	1	1559	U
51	1	1569	A
51	1	1578	U
51	1	1581	G
51	1	1585	C
51	1	1608	A
51	1	1611	C
51	1	1616	A
51	1	1646	C
51	1	1647	U
51	1	1648	U
51	1	1674	G
51	1	1703	G
51	1	1714	U
51	1	1715	G
51	1	1721	G
51	1	1722	A
51	1	1723	G
51	1	1724	G
51	1	1729	U
51	1	1730	C
51	1	1731	G
51	1	1737	G
51	1	1738	G
51	1	1739	A
51	1	1740	G
51	1	1742	U
51	1	1743	G
51	1	1751	U
51	1	1752	C
51	1	1758	U
51	1	1764	C
51	1	1773	A
51	1	1800	C
51	1	1801	A
51	1	1808	A

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Mol	Chain	Res	Type
51	1	1816	C
51	1	1829	A
51	1	1848	A
51	1	1866	A
51	1	1870	C
51	1	1875	G
51	1	1876	A
51	1	1881	C
51	1	1884	G
51	1	1901	A
51	1	1906	G
51	1	1913	A
51	1	1914	C
51	1	1929	G
51	1	1930	G
51	1	1937	A
51	1	1944	U
51	1	1948	G
51	1	1955	U
51	1	1963	U
51	1	1967	C
51	1	1970	A
51	1	1971	U
51	1	1972	G
51	1	1991	U
51	1	1997	C
51	1	2022	U
51	1	2023	C
51	1	2030	A
51	1	2031	A
51	1	2043	C
51	1	2055	C
51	1	2056	G
51	1	2060	A
51	1	2061	G
51	1	2062	A
51	1	2069	G
51	1	2093	G
51	1	2096	C
51	1	2110	G
51	1	2111	U
51	1	2112	G

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Mol	Chain	Res	Type
51	1	2113	U
51	1	2118	U
51	1	2119	A
51	1	2127	G
51	1	2132	U
51	1	2133	G
51	1	2145	C
51	1	2147	A
51	1	2166	U
51	1	2171	A
51	1	2172	U
51	1	2173	A
51	1	2189	U
51	1	2198	A
51	1	2203	U
51	1	2204	G
51	1	2212	A
51	1	2213	U
51	1	2225	A
51	1	2226	C
51	1	2238	G
51	1	2239	G
51	1	2246	G
51	1	2247	A
51	1	2250	G
51	1	2259	U
51	1	2260	C
51	1	2278	A
51	1	2283	C
51	1	2287	A
51	1	2297	A
51	1	2299	U
51	1	2300	C
51	1	2302	U
51	1	2304	G
51	1	2305	U
51	1	2307	G
51	1	2308	G
51	1	2309	A
51	1	2310	C
51	1	2312	U
51	1	2313	C

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Mol	Chain	Res	Type
51	1	2314	A
51	1	2315	G
51	1	2317	A
51	1	2319	G
51	1	2320	U
51	1	2325	G
51	1	2327	A
51	1	2334	U
51	1	2350	C
51	1	2354	C
51	1	2361	G
51	1	2383	G
51	1	2385	C
51	1	2392	A
51	1	2402	U
51	1	2406	A
51	1	2424	C
51	1	2425	A
51	1	2426	A
51	1	2427	C
51	1	2429	G
51	1	2430	A
51	1	2431	U
51	1	2433	A
51	1	2435	A
51	1	2437	G
51	1	2441	U
51	1	2448	A
51	1	2469	A
51	1	2476	A
51	1	2491	U
51	1	2498	C
51	1	2502	G
51	1	2503	A
51	1	2506	U
51	1	2517	C
51	1	2518	A
51	1	2520	C
51	1	2529	G
51	1	2531	A
51	1	2535	G
51	1	2543	G

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Mol	Chain	Res	Type
51	1	2547	A
51	1	2554	U
51	1	2564	A
51	1	2566	A
51	1	2567	G
51	1	2572	A
51	1	2573	C
51	1	2582	G
51	1	2585	U
51	1	2602	A
51	1	2603	G
51	1	2605	U
51	1	2609	U
51	1	2613	U
51	1	2629	U
51	1	2630	G
51	1	2646	C
51	1	2655	G
51	1	2682	A
51	1	2689	U
51	1	2690	U
51	1	2714	G
51	1	2716	C
51	1	2733	A
51	1	2744	G
51	1	2748	A
51	1	2750	A
51	1	2757	A
51	1	2764	A
51	1	2765	A
51	1	2778	A
51	1	2779	U
51	1	2794	C
51	1	2797	U
51	1	2800	A
51	1	2801	G
51	1	2820	A
51	1	2821	A
51	1	2833	U
51	1	2834	G
51	1	2835	A
51	1	2849	U

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Mol	Chain	Res	Type
51	1	2850	A
51	1	2867	G
51	1	2868	A
51	1	2879	A
51	1	2880	C
51	1	2883	A
51	1	2884	U
51	1	2891	U
52	2	4	C
52	2	13	G
52	2	15	A
52	2	18	G
52	2	24	G
52	2	25	U
52	2	35	C
52	2	41	G
52	2	44	G
52	2	67	G
52	2	89	U
52	2	90	C
52	2	91	C
52	2	108	A
52	2	109	A
52	2	116	G
53	5	8	U
53	5	9	G
53	5	14	A
53	5	15	G
53	5	17	C
53	5	18	G
53	5	19	G
53	5	20	U
53	5	47	U
53	5	48	C
53	5	49	G
53	5	59	A
53	5	61	C
53	5	76	A
54	4	8	A
54	4	12	A
54	4	19	U
54	4	20	G

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Mol	Chain	Res	Type
54	4	23	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	3	1190	G
50	3	1201	A
51	1	490	C
51	1	784	G
51	1	792	A
51	1	1020	A
51	1	1738	G
51	1	1875	G
51	1	2286	G
51	1	2299	U
51	1	2326	C
51	1	2430	A
51	1	2436	G
51	1	2529	G
51	1	2756	U
52	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](#)

1 ligand is 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
55	FME	5	101	-	8,9,10	1.36	1 (12%)	7,9,11	1.21	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	FME	5	101	-	-	1/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	5	101	FME	CA-N	3.13	1.50	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	5	101	FME	CA-N-CN	2.31	126.37	122.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	5	101	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	86:GLY	C	87:VAL	N	1.15

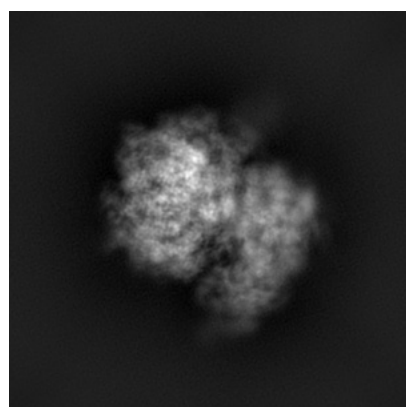
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20048. These allow visual inspection of the internal detail of the map and identification of artifacts.

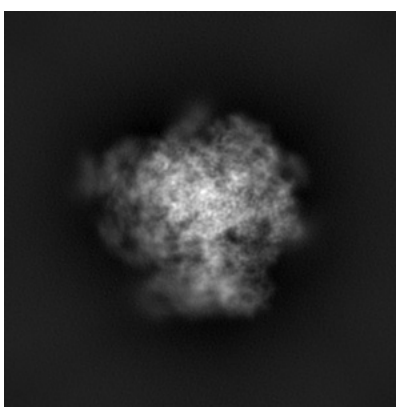
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

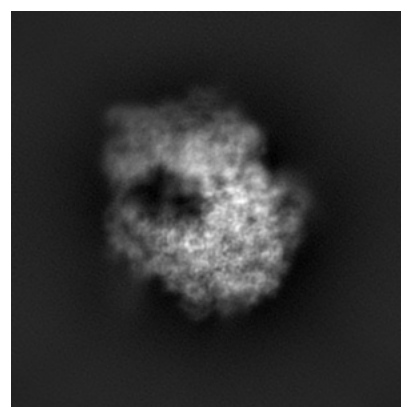
6.1.1 Primary map



X



Y

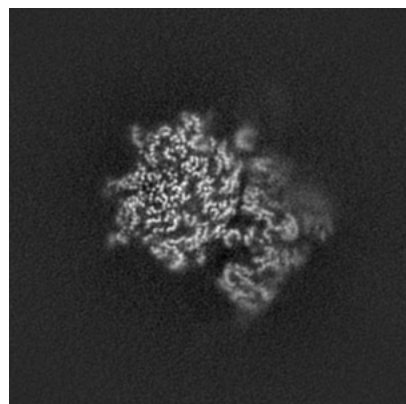


Z

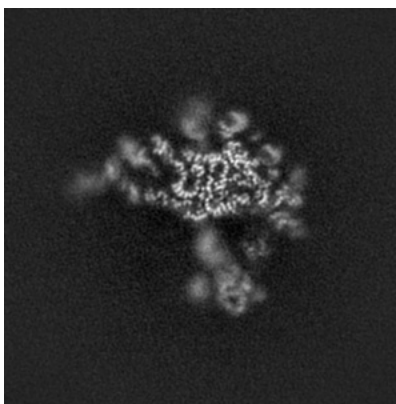
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

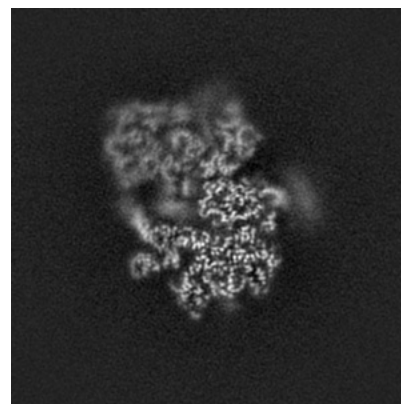
6.2.1 Primary map



X Index: 156



Y Index: 156

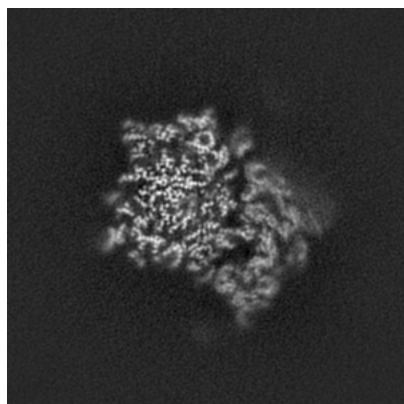


Z Index: 156

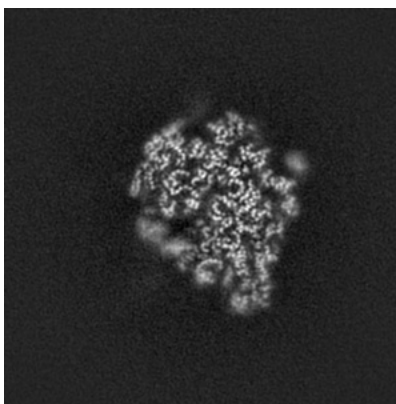
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

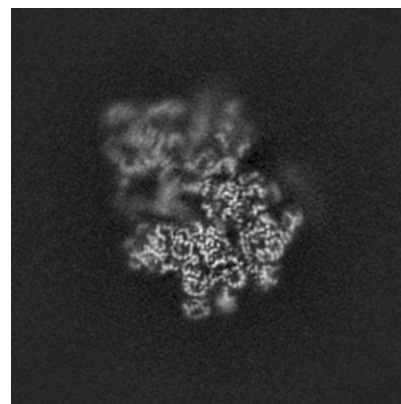
6.3.1 Primary map



X Index: 161



Y Index: 139



Z Index: 164

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

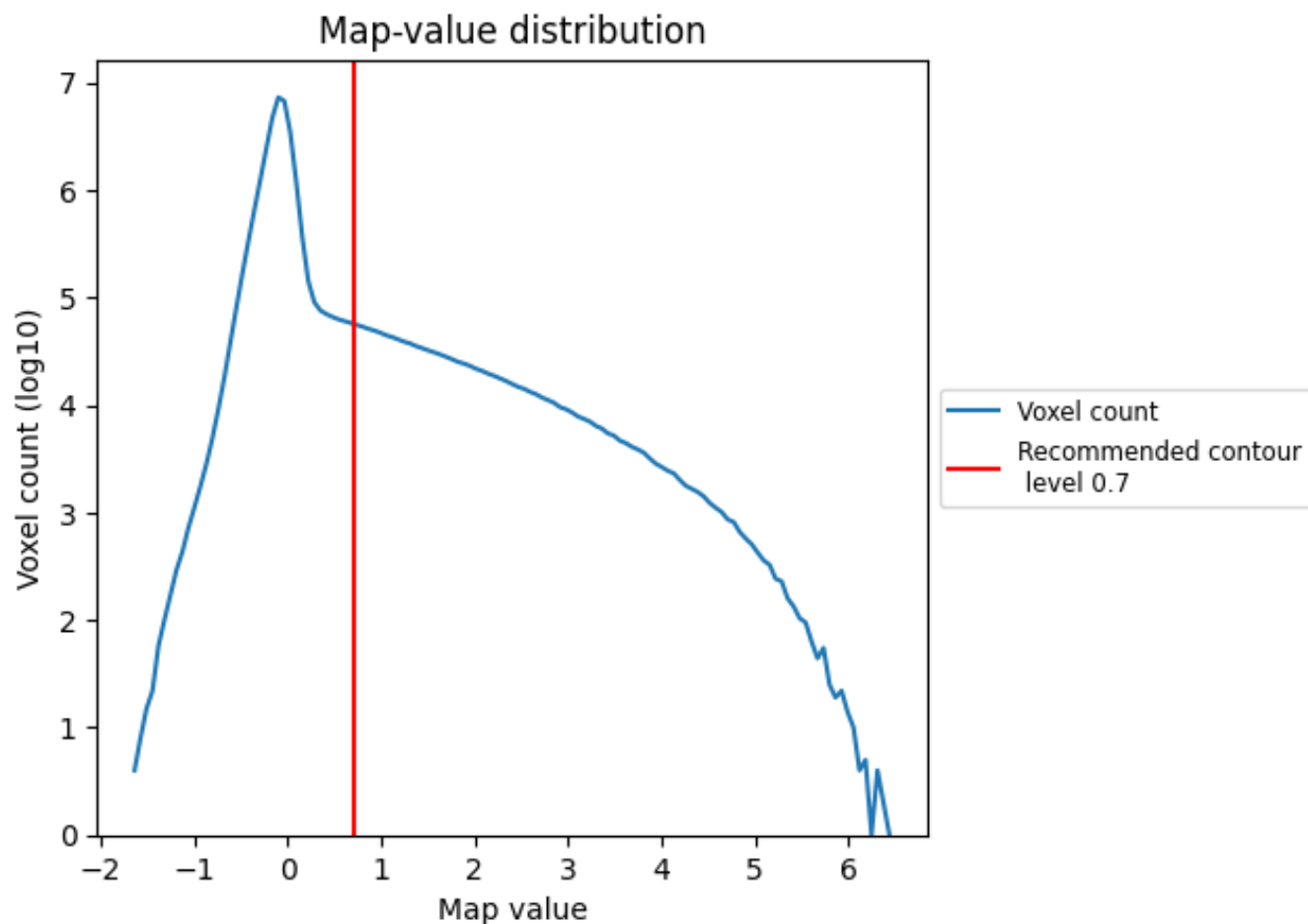
6.5 Mask visualisation

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

7 Map analysis [i](#)

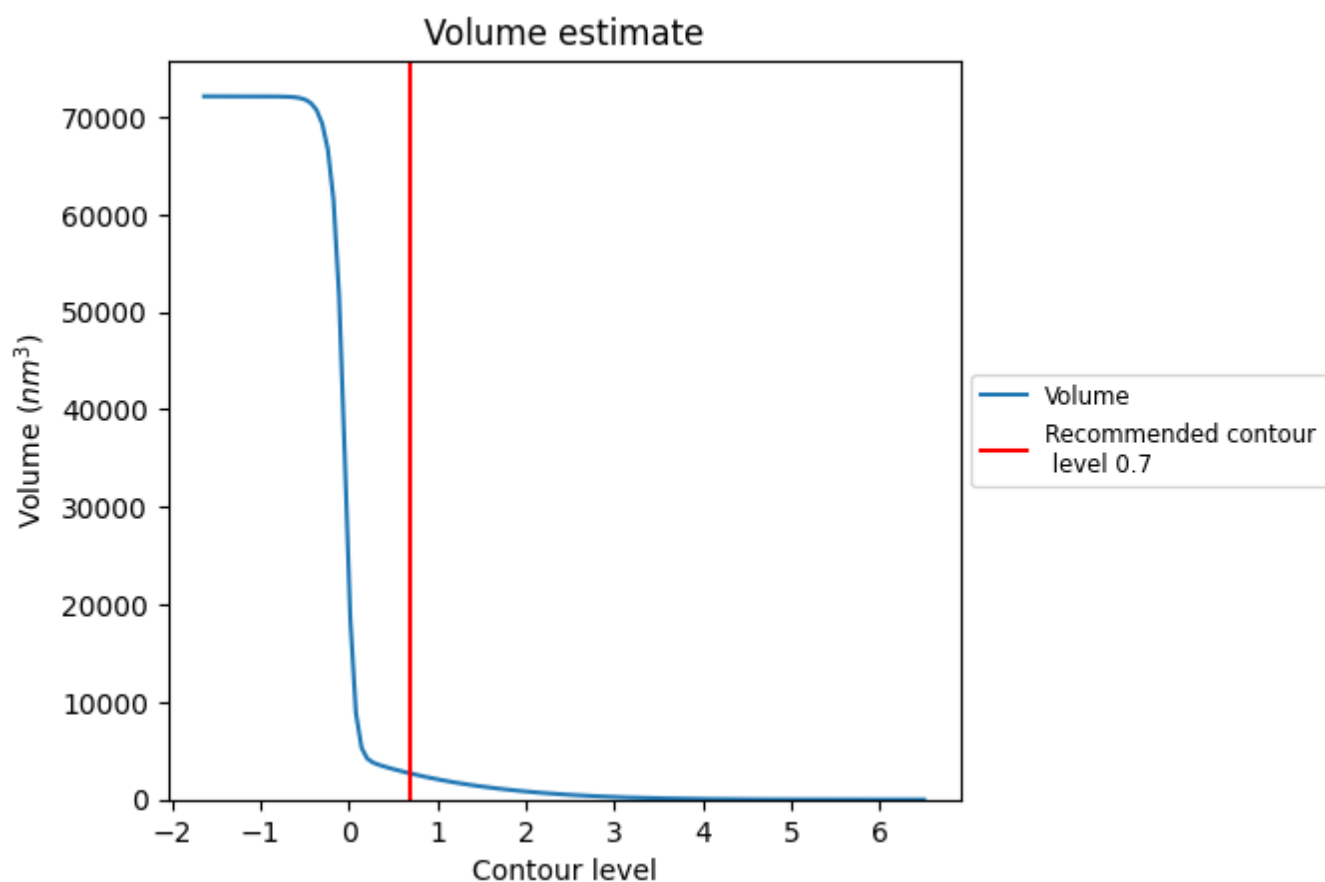
This section contains the results of statistical analysis of the map.

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.

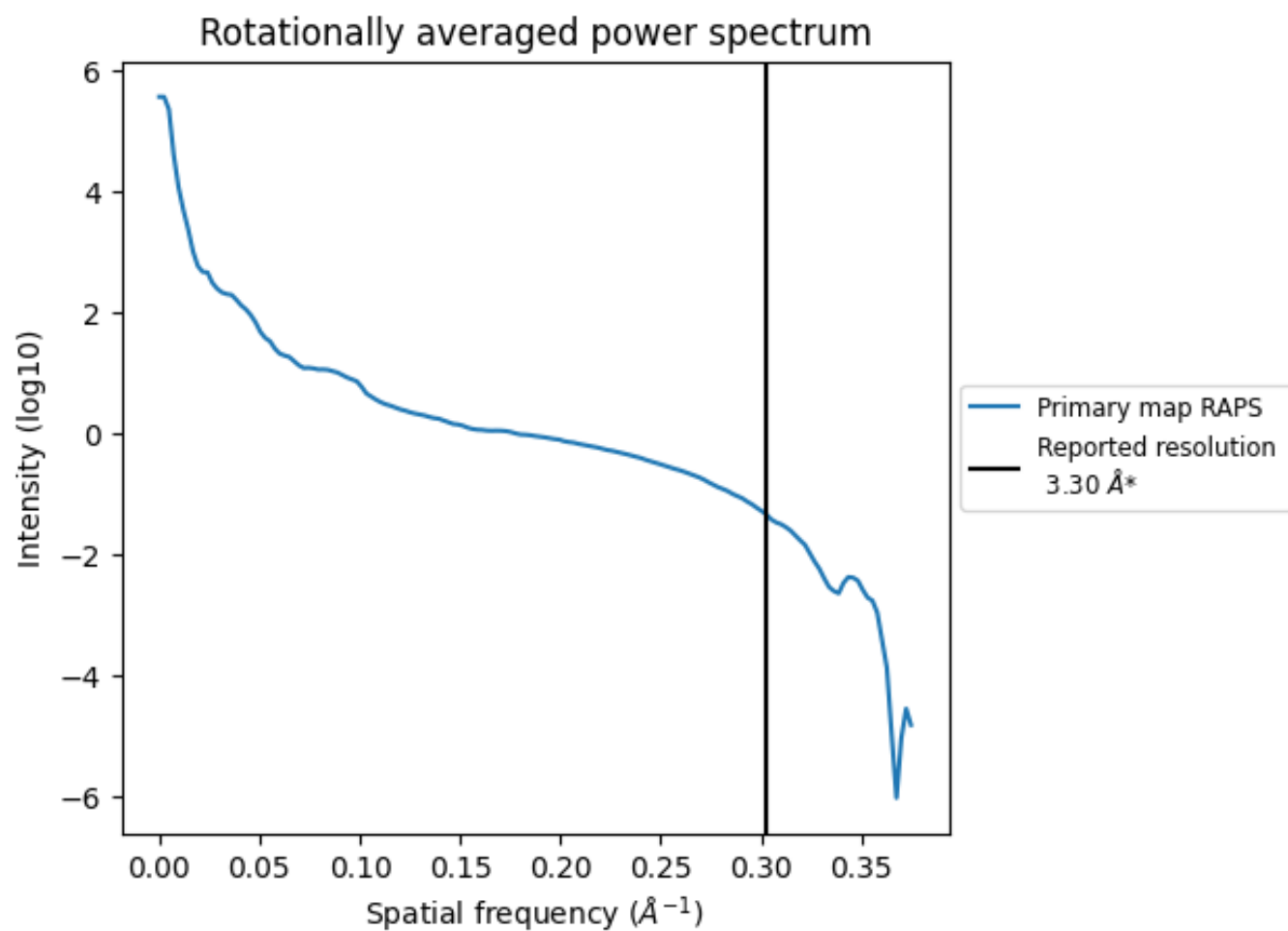
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2665 nm³; this corresponds to an approximate mass of 2407 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

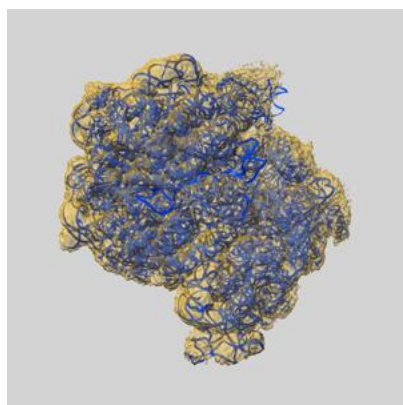
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

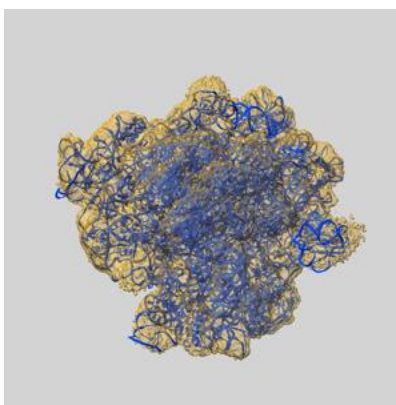
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20048 and PDB model 6OFX. Per-residue inclusion information can be found in section 3 on page 14.

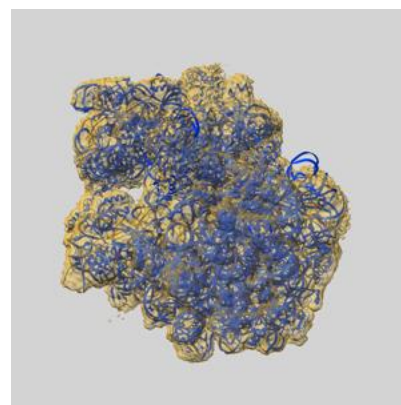
9.1 Map-model overlay [i](#)



X



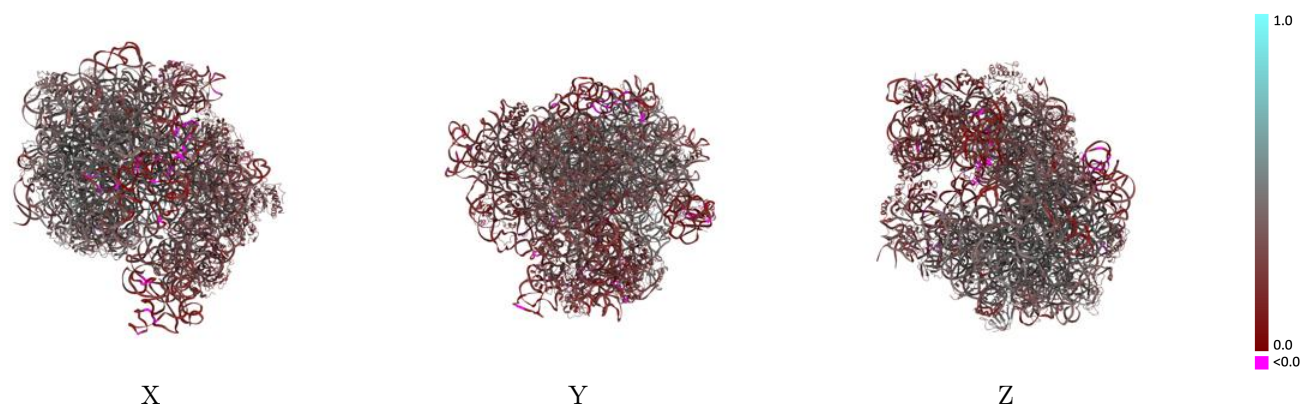
Y



Z

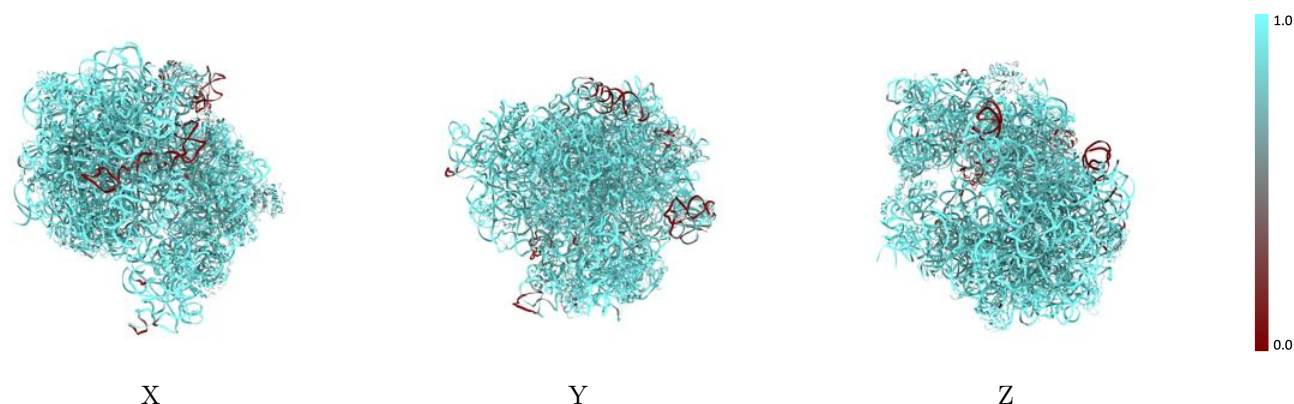
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



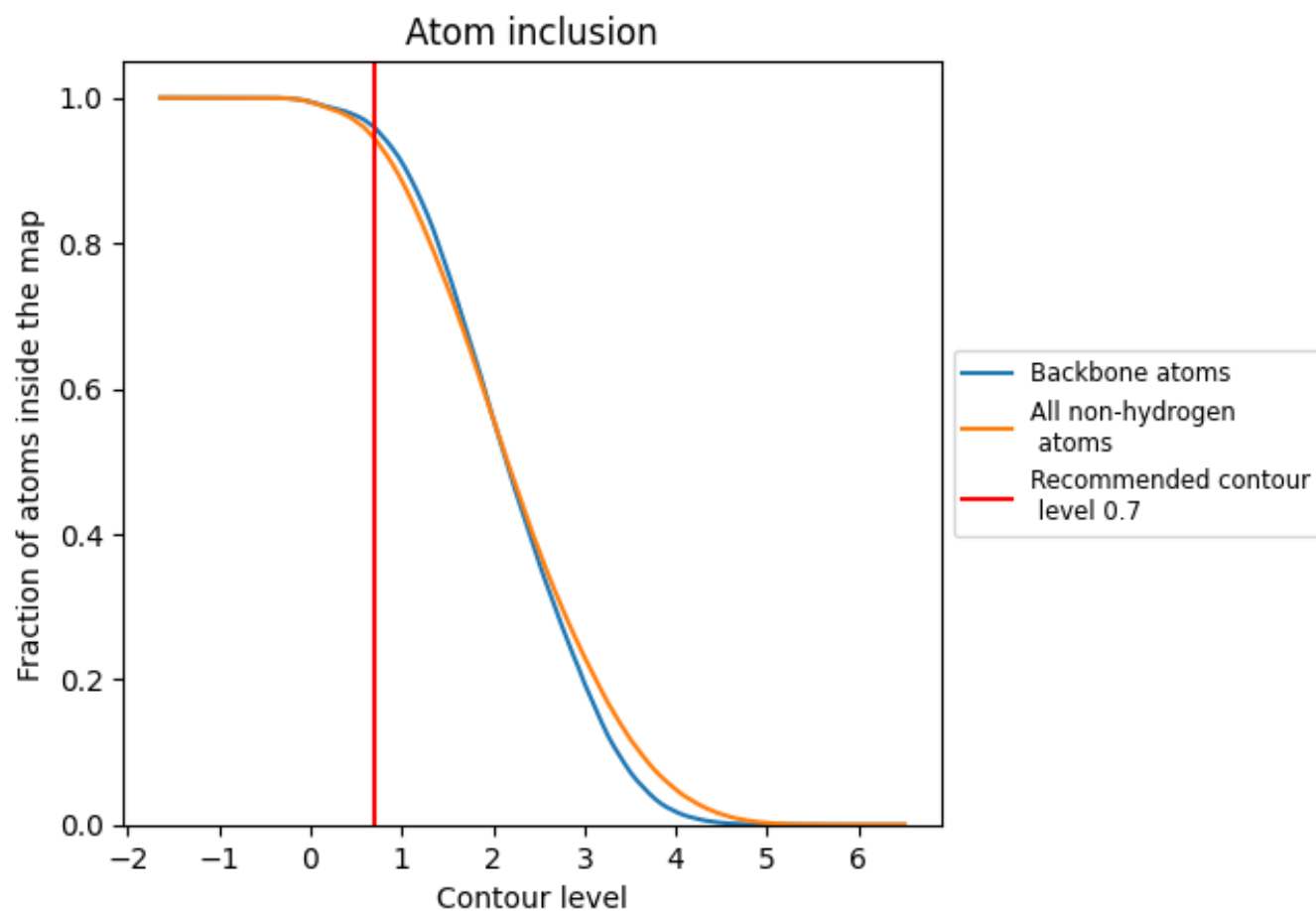
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.7).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 96% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9445	 0.3350
1	 0.9381	 0.3650
2	 0.9977	 0.3280
3	 0.9754	 0.2890
4	 0.8970	 0.2230
5	 0.9509	 0.1920
B	 0.9696	 0.4130
C	 0.9303	 0.3790
D	 0.9690	 0.4370
E	 0.9654	 0.4330
F	 0.9349	 0.3190
G	 0.8204	 0.2840
H	 0.9113	 0.2960
I	 0.9226	 0.2240
J	 0.9595	 0.3240
K	 0.9365	 0.2930
L	 0.9345	 0.2570
M	 0.9781	 0.3140
N	 0.9765	 0.2350
O	 0.8517	 0.2740
P	 0.9752	 0.3330
Q	 0.9251	 0.2930
R	 0.9366	 0.2130
S	 0.9574	 0.2380
T	 0.9522	 0.2810
U	 0.9506	 0.3060
V	 0.9810	 0.2880
W	 0.9903	 0.3060
X	 0.9791	 0.2080
Y	 0.9631	 0.2760
Z	 0.9363	 0.2700
a	 0.5139	 0.1640
b	 0.9742	 0.4110
c	 0.9831	 0.4350
d	 0.9579	 0.3950



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Chain	Atom inclusion	Q-score
e	 0.9585	 0.2200
f	 0.7980	 0.3080
g	 0.5648	 0.3070
j	 0.9782	 0.4150
k	 0.9716	 0.4170
l	 0.9656	 0.4170
m	 0.9741	 0.4140
n	 0.9783	 0.4270
o	 0.9699	 0.3360
p	 0.9718	 0.4040
q	 0.9714	 0.4200
r	 0.9674	 0.4170
s	 0.9545	 0.4250
t	 0.9696	 0.4020
u	 0.9701	 0.3850
v	 0.9688	 0.3650
w	 0.9678	 0.4410
x	 0.9634	 0.3870
y	 0.9517	 0.3250
z	 0.9474	 0.4070