Full wwPDB EM Validation Report (i)

Mar 9, 2024 – 07:37 AM EST

PDB ID	:	6O8Z
EMDB ID	:	EMD-0659
Title	:	Cryo-EM image reconstruction of the 70S Ribosome Enterococcus faecalis Class04
Authors	:	Jogl, G.; Khayat, R.
Deposited on	:	2019-03-12
Resolution	:	3.49 Å(reported)
Based on initial models	:	5LI0, 4YBB

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:

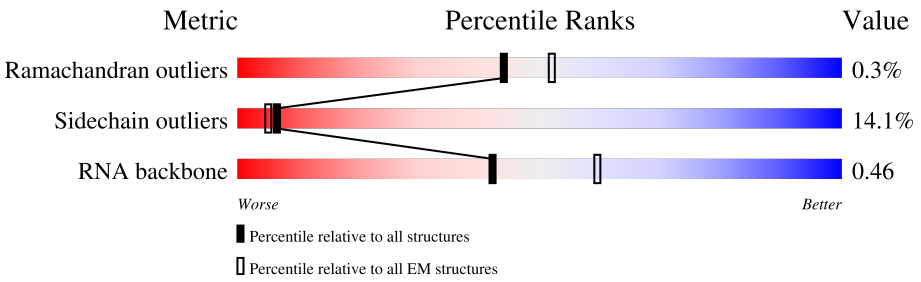
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.49 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	a	1528	79% 21%
2	c	204	• 89% 11%
3	d	201	89% 10%
4	e	163	88% 12%
5	f	97	91% 9%
6	g	154	93% 7%
7	h	131	85% 15%
8	i	128	84% 16%

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Mol	Chain	Length	Quality of chain
9	j	99	88% 12%
10	k	117	93% 7%
11	l	136	88% 12%
12	m	112	88% 12%
13	n	60	88% 12%
14	o	88	89% 11%
15	p	89	85% 15%
16	q	83	86% 14%
17	r	66	82% 18%
18	s	78	92% 8%
19	t	81	91% 9%
20	A	2909	75% 23%
21	B	116	69% 30%
22	C	275	84% 16%
23	D	207	88% 12%
24	E	206	84% 16%
25	F	177	90% 10%
26	G	176	93% 7%
27	K	145	86% 14%
28	L	122	86% 14%
29	M	146	86% 13%
30	N	141	87% 13%
31	O	123	83% 17%
32	P	117	91% 9%
33	Q	114	86% 14%

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Mol	Chain	Length	Quality of chain
34	R	118	88% 12%
35	S	102	91% 9%
36	T	112	91% 9%
37	U	89	82% 18%
38	V	101	87% 13%
39	W	94	48% 89% 11%
40	X	76	89% 11%
41	Y	54	80% 20%
42	Z	61	92% 8%
43	0	58	83% 17%
44	1	83	86% 14%
45	2	56	91% 9%
46	3	49	84% 16%
47	4	44	84% 16%
48	5	64	92% 8%
49	6	38	95% 5%

2 Entry composition (i)

There are 50 unique types of molecules in this entry. The entry contains 138498 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1523	32646	14564	5967	10592	1523	0	0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	c	204	1610	1012	303	292	3	0	0

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	d	201	1620	1016	303	297	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	e	163	1204	759	222	221	2	0	0

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	f	97	795	501	137	154	3	0	0

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	g	154	1229	765	236	222	6	0	0

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	h	131	1041	662	184	193	2	0	0

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	i	128	990	615	197	177	1	0	0

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	j	99	800	504	147	147	2	0	0

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	k	117	863	533	165	161	4	0	0

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	l	136	1065	661	214	188	2	0	0

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	m	112	884	540	180	163	1	0	0

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	n	60	492	310	100	77	5	0	0

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	o	88	741	455	152	133	1	0	0

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	p	89	708	448	131	127	2	0	0

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	q	83	681	427	127	124	3	0	0

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	r	66	537	343	99	94	1	0	0

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	s	78	634	410	113	109	2	0	0

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	t	81	610	372	119	117	2	0	0

- Molecule 20 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	A	2903	62311	27813	11458	20137	2903	0	0

- Molecule 21 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	B	116	2480	1106	444	814	116	0	0

- Molecule 22 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	C	275	2115	1311	416	381	7	0	0

- Molecule 23 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	D	207	1579	994	292	289	4	0	0

- Molecule 24 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	E	206	1574	984	290	298	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	F	177	1392	887	239	260	6	0	0

- Molecule 26 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	G	176	1345	842	244	255	4	0	0

- Molecule 27 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	K	145	1130	714	205	207	4	0	0

- Molecule 28 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	L	122	922	574	176	170	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	M	146	1095	677	212	205	1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	N	141	1118	710	216	185	7	0	0

- Molecule 31 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	O	123	979	603	190	183	3	0	0

- Molecule 32 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	P	117	899	556	175	167	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	Q	114	924	582	185	157	0	0

- Molecule 34 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	R	118	950	602	184	160	4	0	0

- Molecule 35 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	S	102	784	500	139	143	2	0	0

- Molecule 36 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	T	112	849	532	156	159	2	0	0

- Molecule 37 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	U	89	720	458	127	132	3	0	0

- Molecule 38 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	V	101	763	486	135	140	2	0	0

- Molecule 39 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	W	94	758	479	135	140	4	0	0

- Molecule 40 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	X	76	572	351	109	112	0	0

- Molecule 41 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Y	54	425	265	86	72	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	51	ALA	THR	conflict	UNP A0A1B4XRZ8

- Molecule 42 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Z	61	504	314	94	95	1	0	0

- Molecule 43 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	0	58	435	271	81	82	1	0	0

- Molecule 44 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	1	83	673	424	114	133	2	0	0

- Molecule 45 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	2	56	429	262	88	73	6	0	0

- Molecule 46 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	3	49	419	253	86	76	4	0	0

- Molecule 47 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	4	44	374	227	91	54	2	0	0

- Molecule 48 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	5	64	522	320	122	78	2	0	0

- Molecule 49 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	6	38	304	188	66	44	6	0	0

- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn).

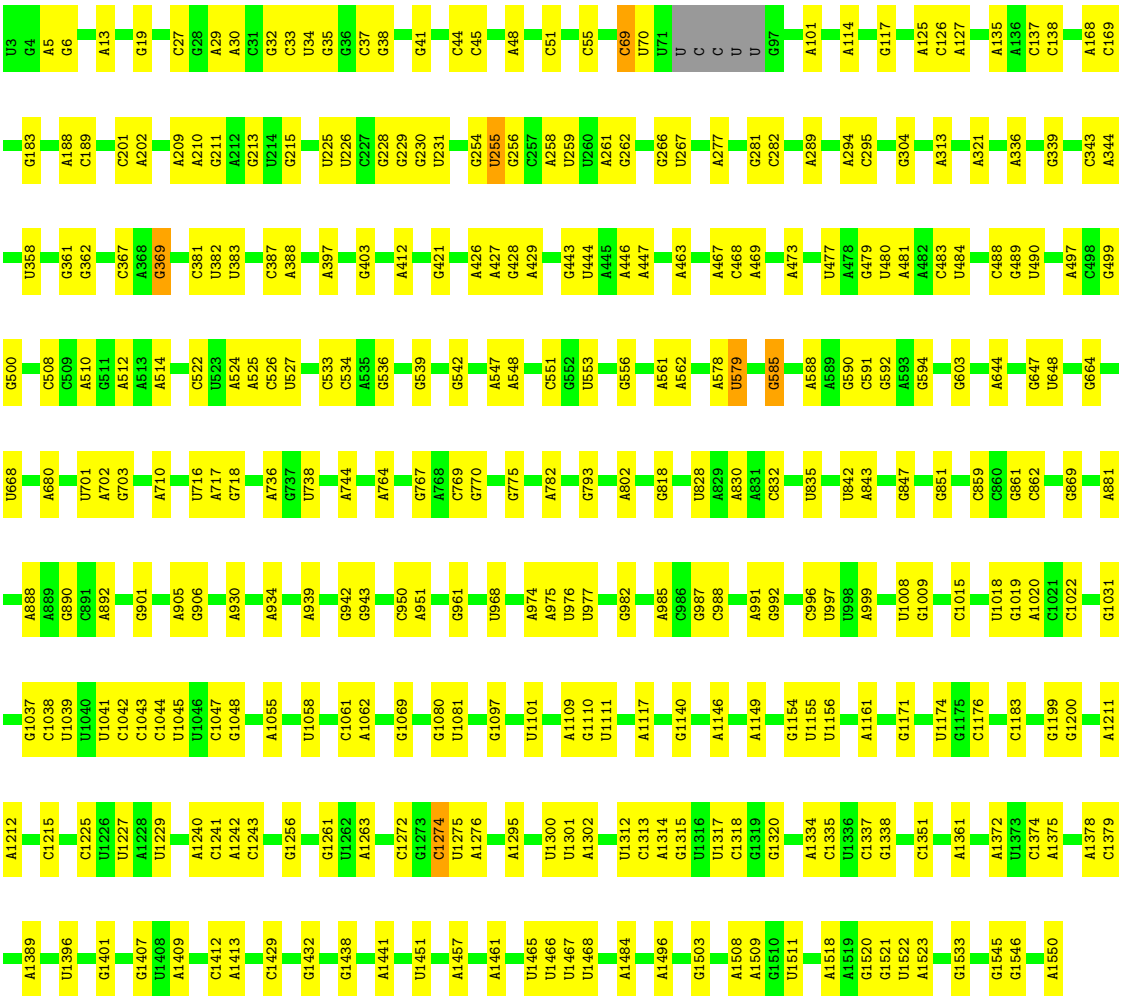
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
50	n	1	1	1	0
50	2	1	1	1	0
50	3	1	1	1	0
50	6	1	1	1	0

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.

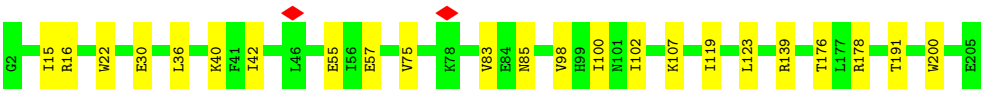
- Molecule 1: 16S rRNA

Chain a: 79% 21%



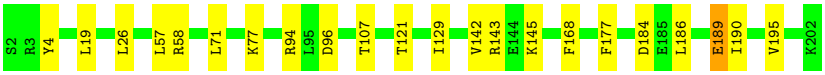
- Molecule 2: 30S ribosomal protein S3

Chain c: 89% 11%



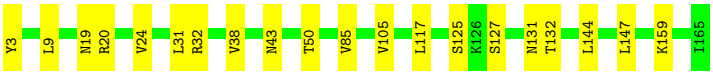
• Molecule 3: 30S ribosomal protein S4

Chain d:



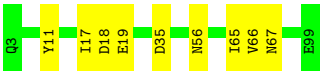
• Molecule 4: 30S ribosomal protein S5

Chain e:



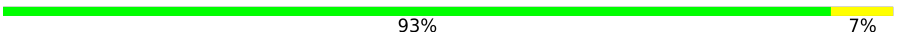
• Molecule 5: 30S ribosomal protein S6

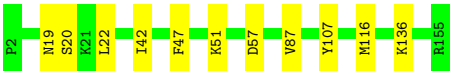
Chain f:



• Molecule 6: 30S ribosomal protein S7

Chain g:



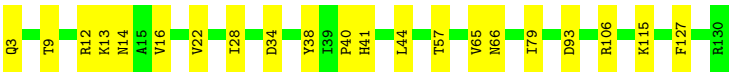


• Molecule 7: 30S ribosomal protein S8

Chain h:

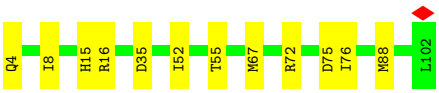
• Molecule 8: 30S ribosomal protein S9

Chain i:



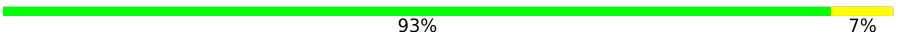
• Molecule 9: 30S ribosomal protein S10

Chain j:



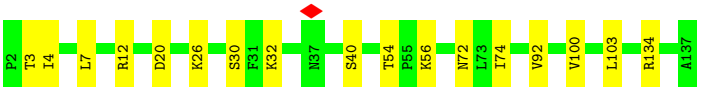
• Molecule 10: 30S ribosomal protein S11

Chain k:



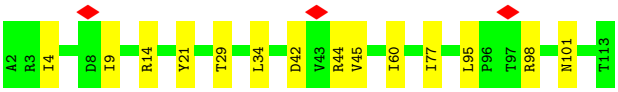
• Molecule 11: 30S ribosomal protein S12

Chain l:



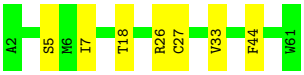
• Molecule 12: 30S ribosomal protein S13

Chain m:



• Molecule 13: 30S ribosomal protein S14 type Z

Chain n:

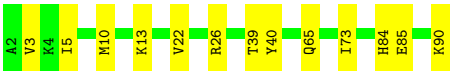


• Molecule 14: 30S ribosomal protein S15

Chain o:

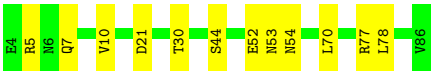
• Molecule 15: 30S ribosomal protein S16

Chain p:



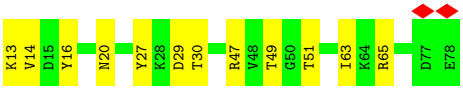
• Molecule 16: 30S ribosomal protein S17

Chain q:



• Molecule 17: 30S ribosomal protein S18

Chain r:

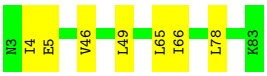


• Molecule 18: 30S ribosomal protein S19

Chain s:

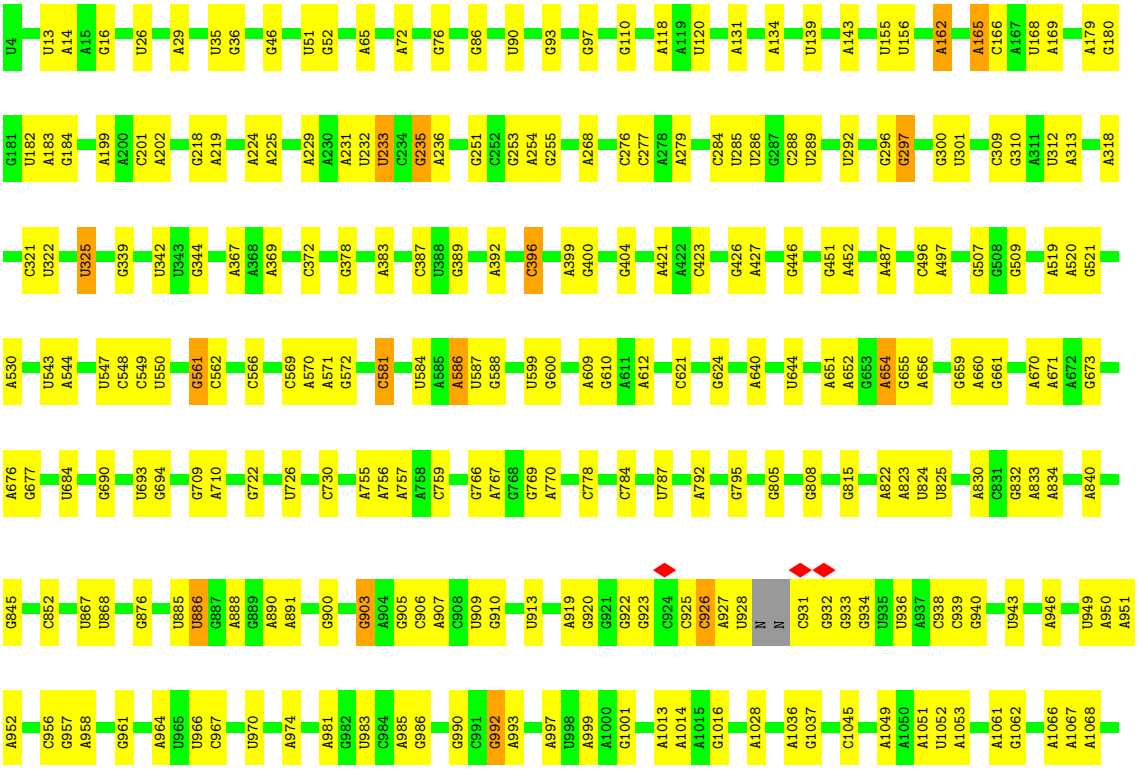
• Molecule 19: 30S ribosomal protein S20

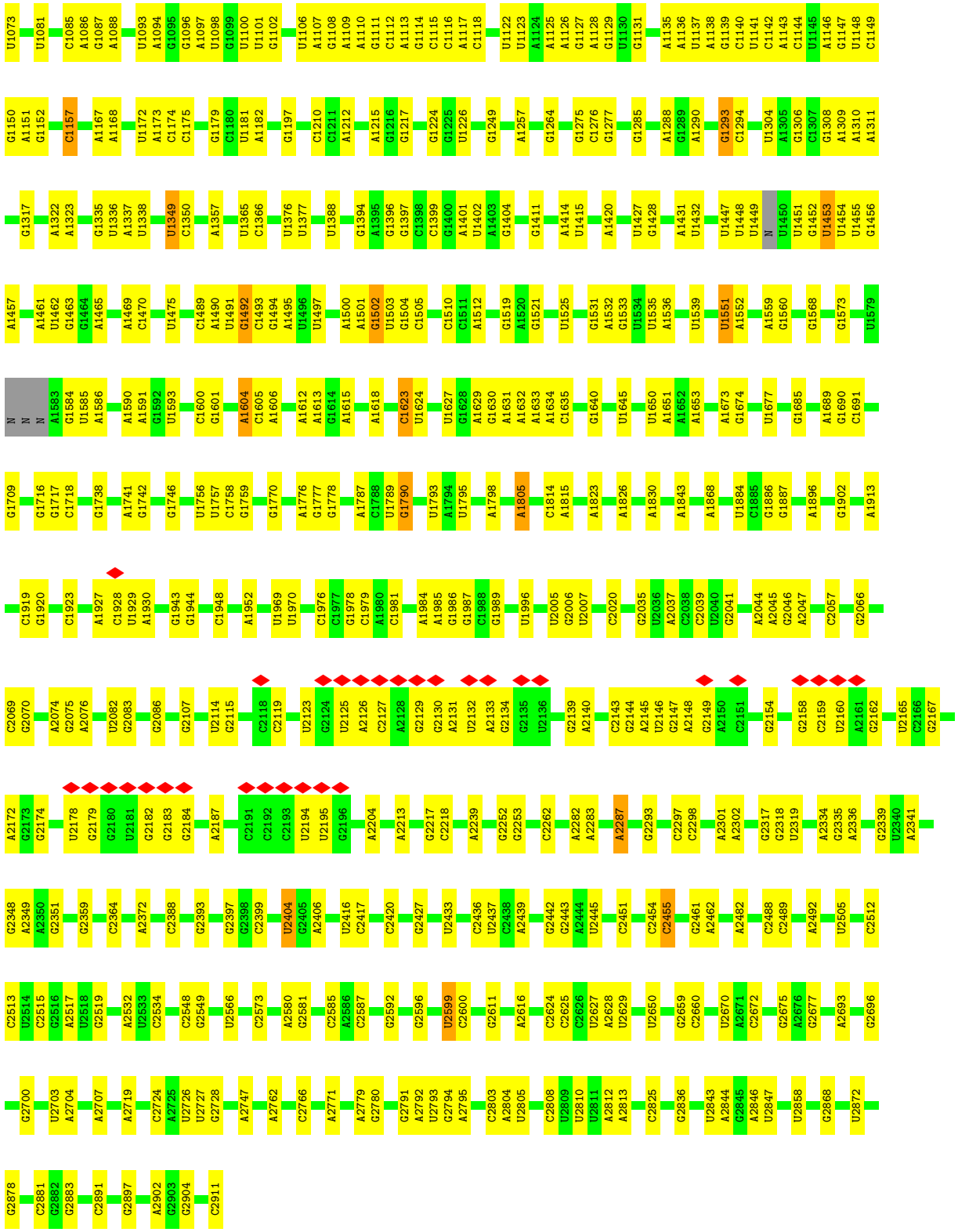
Chain t:



• Molecule 20: 23S rRNA

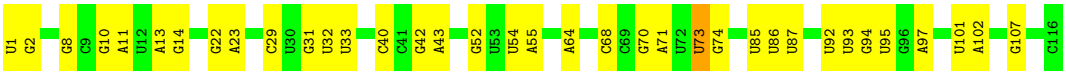
Chain A:





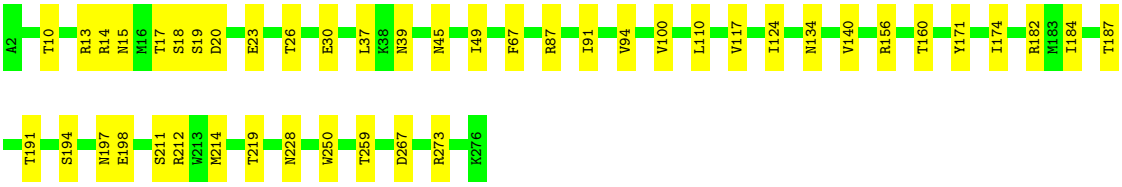
- Molecule 21: 5S rRNA

Chain B: 69% 30%



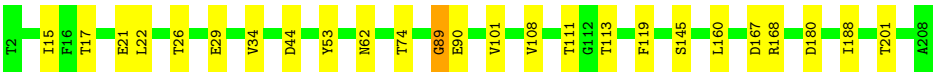
• Molecule 22: 50S ribosomal protein L2

Chain C: 84% 16%



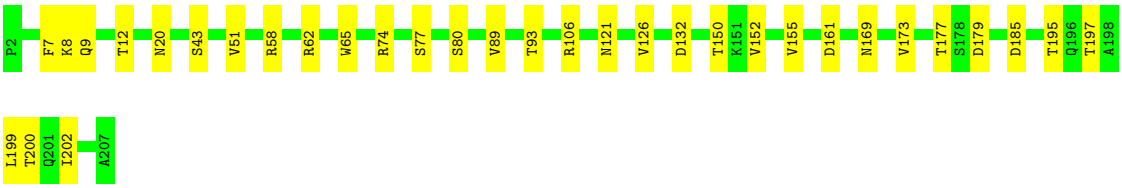
• Molecule 23: 50S ribosomal protein L3

Chain D: 88% 12%



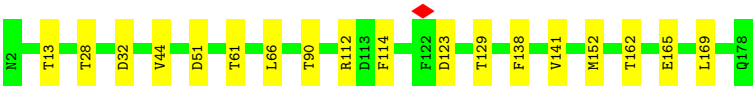
• Molecule 24: 50S ribosomal protein L4

Chain E: 84% 16%



• Molecule 25: 50S ribosomal protein L5

Chain F: 90% 10%

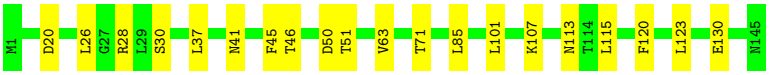


• Molecule 26: 50S ribosomal protein L6

Chain G: 93% 7%

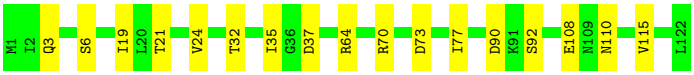
• Molecule 27: 50S ribosomal protein L13

Chain K: 86% 14%



• Molecule 28: 50S ribosomal protein L14

Chain L: 86% 14%

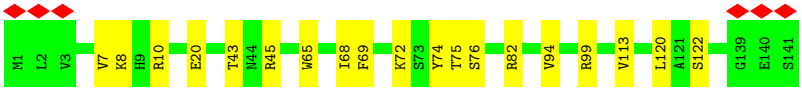


• Molecule 29: 50S ribosomal protein L15

Chain M: 86% 13%

• Molecule 30: 50S ribosomal protein L16

Chain N: 87% 13%



• Molecule 31: 50S ribosomal protein L17

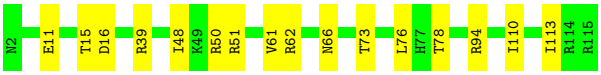
Chain O: 83% 17%

• Molecule 32: 50S ribosomal protein L18

Chain P: 91% 9%

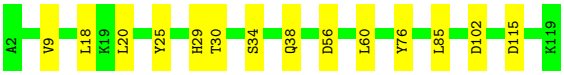
• Molecule 33: 50S ribosomal protein L19

Chain Q: 86% 14%



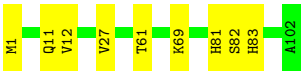
• Molecule 34: 50S ribosomal protein L20

Chain R: 88% 12%



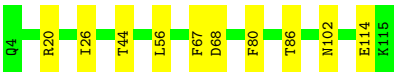
• Molecule 35: 50S ribosomal protein L21

Chain S: 91% 9%



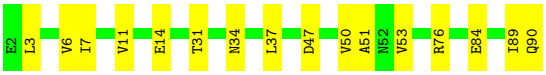
• Molecule 36: 50S ribosomal protein L22

Chain T: 91% 9%



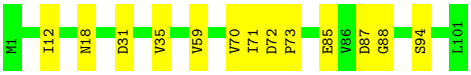
• Molecule 37: 50S ribosomal protein L23

Chain U: 82% 18%



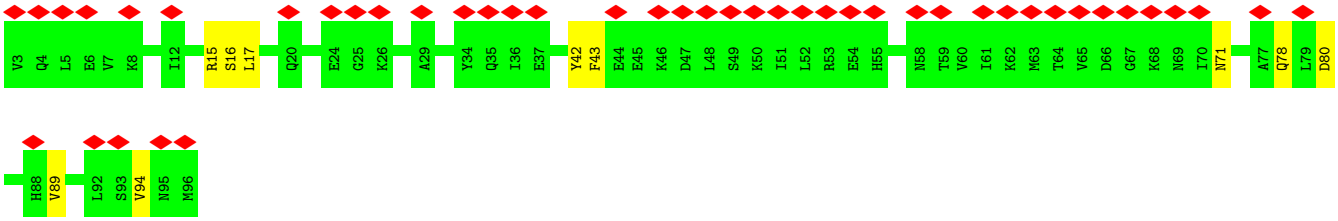
• Molecule 38: 50S ribosomal protein L24

Chain V: 87% 13%



• Molecule 39: 50S ribosomal protein L25

Chain W: 48% 89% 11%



• Molecule 40: 50S ribosomal protein L27

Chain X: 89% 11%

• Molecule 41: 50S ribosomal protein L28

Chain Y: 80% 20%

• Molecule 42: 50S ribosomal protein L29

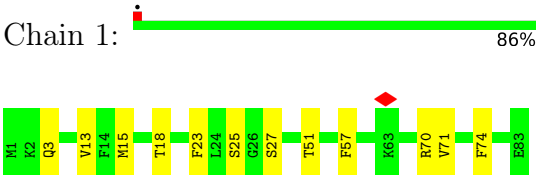
Chain Z: 92% 8%

• Molecule 43: 50S ribosomal protein L30

Chain 0: 83% 17%

• Molecule 44: 50S ribosomal protein L31 type B

Chain 1: 86% 14%

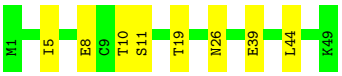


• Molecule 45: 50S ribosomal protein L32

Chain 2: 91% 9%

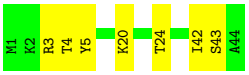
• Molecule 46: 50S ribosomal protein L33

Chain 3: 84% 16%



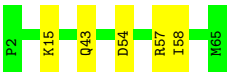
• Molecule 47: 50S ribosomal protein L34

Chain 4: 84% 16%

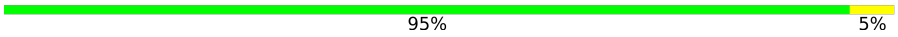


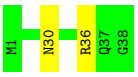
• Molecule 48: 50S ribosomal protein L35

Chain 5:



- Molecule 49: 50S ribosomal protein L36

Chain 6: 



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37183	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 ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.100	Depositor
Minimum map value	-0.938	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.238	Depositor
Map size (Å)	482.68, 482.68, 482.68	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.097, 1.097, 1.097	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: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	a	0.87	0/36547	0.98	22/57003 (0.0%)
2	c	0.38	0/1635	0.50	0/2197
3	d	0.41	0/1650	0.51	1/2217 (0.0%)
4	e	0.42	0/1217	0.51	0/1641
5	f	0.42	0/807	0.49	0/1087
6	g	0.33	0/1249	0.46	0/1682
7	h	0.44	0/1054	0.54	0/1417
8	i	0.35	0/1003	0.47	0/1343
9	j	0.35	0/812	0.53	0/1093
10	k	0.36	0/878	0.50	0/1185
11	l	0.40	0/1082	0.54	0/1453
12	m	0.33	0/890	0.55	0/1195
13	n	0.41	0/504	0.50	0/669
14	o	0.44	0/751	0.53	0/1001
15	p	0.43	0/720	0.49	0/966
16	q	0.45	0/689	0.51	0/920
17	r	0.41	0/544	0.54	0/728
18	s	0.35	0/650	0.49	0/872
19	t	0.34	0/612	0.48	0/818
20	A	1.08	5/69799 (0.0%)	1.08	116/108874 (0.1%)
21	B	0.88	1/2773 (0.0%)	1.02	4/4320 (0.1%)
22	C	0.54	0/2150	0.58	0/2892
23	D	0.57	0/1601	0.58	0/2150
24	E	0.49	0/1596	0.54	0/2159
25	F	0.38	0/1411	0.48	0/1897
26	G	0.41	0/1365	0.52	0/1839
27	K	2.78	7/1151 (0.6%)	0.67	2/1554 (0.1%)
28	L	0.53	0/929	0.55	0/1247
29	M	0.49	0/1105	0.63	0/1474
30	N	0.44	0/1141	0.53	0/1519
31	O	0.53	0/987	0.61	0/1323
32	P	0.43	0/908	0.54	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Q	0.56	0/938	0.53	0/1262
34	R	0.53	0/963	0.52	0/1280
35	S	0.51	0/796	0.56	0/1068
36	T	0.49	0/858	0.52	0/1157
37	U	0.51	0/727	0.59	0/972
38	V	0.42	0/772	0.55	1/1035 (0.1%)
39	W	0.30	0/769	0.54	0/1034
40	X	0.53	0/578	0.57	0/773
41	Y	0.45	0/431	0.55	0/574
42	Z	0.38	0/505	0.49	0/672
43	0	0.44	0/437	0.53	0/589
44	1	0.38	0/690	0.54	0/930
45	2	0.53	0/436	0.52	0/578
46	3	0.40	0/423	0.48	0/563
47	4	0.45	0/377	0.51	0/491
48	5	0.45	0/528	0.49	0/689
49	6	0.50	0/309	0.53	0/409
All	All	0.92	13/150747 (0.0%)	0.95	146/226027 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	d	0	1
19	t	0	1
23	D	0	2
26	G	0	1
29	M	0	2
30	N	0	1
31	O	0	2
37	U	0	1
38	V	0	2
39	W	0	1
All	All	0	14

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	K	107	LYS	CD-CE	63.90	3.11	1.51
27	K	120	PHE	CE1-CZ	32.03	1.98	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	K	120	PHE	CE2-CZ	30.54	1.95	1.37
27	K	120	PHE	CD1-CE1	29.43	1.98	1.39
27	K	120	PHE	CD2-CE2	29.43	1.98	1.39
27	K	120	PHE	CG-CD2	19.79	1.68	1.38
27	K	120	PHE	CG-CD1	19.33	1.67	1.38
21	B	1	U	OP3-P	-10.89	1.48	1.61
20	A	903	G	C6-N1	-10.13	1.32	1.39
20	A	956	C	C4-N4	-5.46	1.29	1.33
20	A	1805	A	N3-C4	-5.42	1.31	1.34
20	A	1288	A	N7-C5	-5.23	1.36	1.39
20	A	956	C	N3-C4	-5.09	1.30	1.33

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	956	C	N3-C4-N4	-28.67	97.93	118.00
20	A	956	C	C5-C4-N4	22.28	135.79	120.20
20	A	903	G	N1-C6-O6	-21.42	107.05	119.90
20	A	903	G	C5-C6-O6	19.35	140.21	128.60
20	A	956	C	N3-C4-C5	10.47	126.09	121.90
20	A	956	C	C4-C5-C6	-9.27	112.77	117.40
20	A	2454	C	O4'-C1'-N1	9.01	115.41	108.20
27	K	107	LYS	CD-CE-NZ	8.74	131.81	111.70
20	A	1157	C	C2-N1-C1'	7.95	127.55	118.80
20	A	1551	U	C2-N1-C1'	7.90	127.18	117.70
20	A	931	C	N1-C2-O2	7.86	123.61	118.90
20	A	926	C	C6-N1-C2	-7.83	117.17	120.30
20	A	992	G	N3-C4-N9	7.79	130.67	126.00
20	A	926	C	C5-C6-N1	7.18	124.59	121.00
20	A	1551	U	N1-C2-O2	7.15	127.80	122.80
20	A	931	C	C2-N1-C1'	7.12	126.63	118.80
1	a	996	C	C6-N1-C2	-7.10	117.46	120.30
20	A	1197	G	C6-C5-N7	-7.09	126.14	130.40
20	A	586	A	N1-C6-N6	-7.04	114.37	118.60
20	A	2287	A	O4'-C1'-N9	6.99	113.79	108.20
20	A	1758	C	C2-N1-C1'	6.98	126.47	118.80
1	a	267	U	C2-N1-C1'	6.88	125.96	117.70
27	K	107	LYS	CG-CD-CE	6.67	131.92	111.90
20	A	1157	C	C6-N1-C1'	-6.66	112.81	120.80
20	A	1350	C	C2-N1-C1'	6.54	125.99	118.80
20	A	1623	C	N3-C2-O2	-6.50	117.35	121.90
1	a	383	U	C2-N1-C1'	6.42	125.41	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	769	C	C2-N1-C1'	6.36	125.80	118.80
20	A	769	G	N3-C4-N9	-6.33	122.20	126.00
20	A	1293	G	C4-N9-C1'	6.25	134.63	126.50
1	a	1465	U	N1-C2-O2	6.24	127.17	122.80
20	A	1758	C	N1-C2-O2	6.22	122.63	118.90
20	A	769	G	N3-C4-C5	6.21	131.70	128.60
20	A	1197	G	C4-N9-C1'	6.16	134.51	126.50
20	A	581	C	C2-N1-C1'	6.16	125.57	118.80
20	A	1197	G	N3-C4-N9	6.14	129.69	126.00
1	a	1225	C	N1-C2-O2	6.10	122.56	118.90
20	A	903	G	C4-N9-C1'	6.09	134.42	126.50
20	A	654	A	C8-N9-C4	6.06	108.22	105.80
20	A	1349	U	N3-C2-O2	-6.05	117.97	122.20
20	A	1293	G	N3-C4-N9	6.00	129.60	126.00
20	A	992	G	C8-N9-C1'	-6.00	119.20	127.00
21	B	73	U	C2-N1-C1'	6.00	124.90	117.70
20	A	2020	C	C2-N1-C1'	5.96	125.36	118.80
20	A	423	C	C2-N1-C1'	5.93	125.32	118.80
20	A	1197	G	C4-C5-N7	5.92	113.17	110.80
20	A	1789	U	C5-C4-O4	-5.92	122.35	125.90
20	A	2670	U	C2-N1-C1'	5.91	124.79	117.70
21	B	68	C	C2-N1-C1'	5.90	125.29	118.80
20	A	550	U	C2-N1-C1'	5.88	124.75	117.70
20	A	1551	U	N3-C2-O2	-5.86	118.10	122.20
20	A	2262	C	C2-N1-C1'	5.85	125.24	118.80
20	A	1902	G	C4-N9-C1'	5.83	134.08	126.50
20	A	992	G	C6-C5-N7	-5.83	126.90	130.40
20	A	1492	G	N3-C4-N9	-5.81	122.51	126.00
20	A	1197	G	C8-N9-C1'	-5.81	119.45	127.00
1	a	508	C	N3-C2-O2	-5.80	117.84	121.90
1	a	255	U	O4'-C1'-N1	5.77	112.82	108.20
20	A	1293	G	C8-N9-C1'	-5.76	119.51	127.00
20	A	233	U	C2-N1-C1'	5.74	124.59	117.70
20	A	2404	U	C2-N1-C1'	5.71	124.55	117.70
20	A	2700	G	N3-C4-C5	-5.70	125.75	128.60
20	A	1293	G	C6-C5-N7	-5.69	126.99	130.40
1	a	996	C	O4'-C1'-N1	5.65	112.72	108.20
20	A	931	C	N3-C2-O2	-5.64	117.95	121.90
3	d	26	LEU	CA-CB-CG	5.63	128.26	115.30
1	a	579	U	N3-C2-O2	-5.63	118.26	122.20
20	A	2724	C	N3-C2-O2	-5.62	117.96	121.90
1	a	1274	C	N3-C2-O2	-5.61	117.97	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1225	C	N3-C2-O2	-5.61	117.98	121.90
1	a	1465	U	N3-C2-O2	-5.61	118.28	122.20
20	A	1317	G	C4-N9-C1'	5.60	133.78	126.50
20	A	1902	G	O4'-C1'-N9	5.59	112.67	108.20
20	A	1790	G	N3-C4-N9	5.58	129.35	126.00
20	A	396	C	C2-N1-C1'	5.58	124.94	118.80
21	B	52	G	N1-C6-O6	-5.56	116.56	119.90
1	a	996	C	N3-C2-O2	-5.55	118.02	121.90
1	a	69	C	C2-N1-C1'	5.53	124.88	118.80
20	A	1317	G	N3-C4-N9	5.51	129.31	126.00
20	A	201	C	C2-N1-C1'	5.50	124.85	118.80
20	A	1709	G	N1-C6-O6	-5.49	116.61	119.90
20	A	992	G	C4-N9-C1'	5.48	133.63	126.50
20	A	621	C	C2-N1-C1'	5.48	124.82	118.80
20	A	1349	U	C2-N1-C1'	5.47	124.26	117.70
20	A	1790	G	C4-N9-C1'	5.46	133.59	126.50
1	a	769	C	C6-N1-C1'	-5.45	114.26	120.80
20	A	1551	U	C6-N1-C1'	-5.45	113.57	121.20
20	A	886	U	N1-C2-O2	5.43	126.60	122.80
1	a	483	C	P-O3'-C3'	5.41	126.20	119.70
20	A	1304	U	C2-N1-C1'	5.41	124.19	117.70
20	A	2451	C	N3-C2-O2	-5.41	118.11	121.90
20	A	1492	G	N3-C4-C5	5.41	131.30	128.60
20	A	2599	U	C2-N1-C1'	5.40	124.18	117.70
20	A	509	G	O4'-C1'-N9	5.39	112.51	108.20
20	A	2287	A	N7-C8-N9	5.39	116.49	113.80
20	A	1492	G	C2-N3-C4	-5.39	109.21	111.90
20	A	392	A	N7-C8-N9	5.37	116.49	113.80
20	A	2585	C	C6-N1-C2	-5.36	118.16	120.30
20	A	769	G	C2-N3-C4	-5.35	109.23	111.90
20	A	1453	U	N1-C2-O2	5.33	126.53	122.80
1	a	33	C	N1-C2-O2	5.32	122.09	118.90
20	A	730	C	C6-N1-C2	-5.32	118.17	120.30
20	A	2573	C	N3-C2-O2	-5.30	118.19	121.90
1	a	1465	U	C2-N1-C1'	5.27	124.03	117.70
20	A	992	G	N9-C4-C5	-5.26	103.30	105.40
20	A	561	G	C4-N9-C1'	5.25	133.32	126.50
38	V	71	ILE	C-N-CA	5.24	134.81	121.70
20	A	235	G	C6-C5-N7	-5.24	127.26	130.40
20	A	1902	G	C6-C5-N7	-5.21	127.27	130.40
20	A	2672	C	N3-C2-O2	-5.20	118.26	121.90
20	A	644	U	N3-C2-O2	-5.20	118.56	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1604	A	P-O3'-C3'	5.19	125.93	119.70
20	A	1790	G	C6-C5-N7	-5.19	127.29	130.40
20	A	325	U	N1-C2-O2	5.19	126.43	122.80
20	A	581	C	C6-N1-C1'	-5.19	114.58	120.80
20	A	1197	G	N9-C4-C5	-5.17	103.33	105.40
20	A	2165	U	C2-N1-C1'	5.17	123.90	117.70
20	A	992	G	N3-C4-C5	-5.15	126.02	128.60
20	A	1157	C	N1-C2-O2	5.14	121.98	118.90
20	A	2825	C	N3-C2-O2	-5.14	118.30	121.90
20	A	2881	C	C6-N1-C2	-5.13	118.25	120.30
20	A	1987	G	N3-C4-N9	5.13	129.08	126.00
20	A	561	G	C8-N9-C1'	-5.13	120.33	127.00
20	A	1502	G	N3-C4-N9	5.13	129.08	126.00
20	A	162	A	C8-N9-C4	-5.12	103.75	105.80
20	A	165	A	O4'-C1'-N9	5.12	112.29	108.20
20	A	1317	G	C8-N9-C1'	-5.10	120.38	127.00
1	a	33	C	N3-C2-O2	-5.08	118.34	121.90
20	A	823	A	C8-N9-C4	-5.08	103.77	105.80
20	A	922	G	N3-C4-N9	5.08	129.05	126.00
1	a	369	G	C4-N9-C1'	5.08	133.11	126.50
20	A	2455	C	N3-C2-O2	-5.08	118.34	121.90
20	A	1399	C	C2-N1-C1'	5.08	124.39	118.80
20	A	876	G	C8-N9-C4	-5.08	104.37	106.40
20	A	297	G	O4'-C1'-N9	-5.06	104.15	108.20
20	A	1591	A	C8-N9-C4	-5.05	103.78	105.80
20	A	2041	G	C8-N9-C1'	-5.05	120.44	127.00
20	A	983	U	N3-C2-O2	-5.04	118.67	122.20
21	B	73	U	N3-C2-O2	-5.04	118.67	122.20
20	A	561	G	N3-C4-N9	5.04	129.02	126.00
20	A	1505	C	N3-C2-O2	-5.04	118.37	121.90
20	A	931	C	C5-C6-N1	5.03	123.52	121.00
1	a	585	G	C4-N9-C1'	5.02	133.03	126.50
20	A	1969	U	C5-C6-N1	-5.02	120.19	122.70
20	A	2388	C	N3-C2-O2	-5.01	118.39	121.90
20	A	2513	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	D	53	TYR	Peptide
23	D	89	GLY	Peptide

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Mol	Chain	Res	Type	Group
26	G	47	GLY	Peptide
29	M	85	PHE	Peptide
29	M	97	LYS	Peptide
30	N	8	LYS	Peptide
31	O	22	THR	Peptide
31	O	77	ASP	Peptide
37	U	84	GLU	Peptide
38	V	72	ASP	Peptide
38	V	87	ASP	Peptide
39	W	42	TYR	Peptide
3	d	189	GLU	Peptide
19	t	66	ILE	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	c	202/204 (99%)	177 (88%)	25 (12%)	0	100 100
3	d	199/201 (99%)	159 (80%)	39 (20%)	1 (0%)	29 68
4	e	161/163 (99%)	140 (87%)	21 (13%)	0	100 100
5	f	95/97 (98%)	79 (83%)	16 (17%)	0	100 100
6	g	152/154 (99%)	129 (85%)	23 (15%)	0	100 100
7	h	129/131 (98%)	106 (82%)	23 (18%)	0	100 100
8	i	126/128 (98%)	109 (86%)	15 (12%)	2 (2%)	9 43
9	j	97/99 (98%)	76 (78%)	21 (22%)	0	100 100
10	k	115/117 (98%)	93 (81%)	22 (19%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	134/136 (98%)	105 (78%)	29 (22%)	0	100	100
12	m	110/112 (98%)	81 (74%)	29 (26%)	0	100	100
13	n	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
14	o	86/88 (98%)	75 (87%)	10 (12%)	1 (1%)	13	50
15	p	87/89 (98%)	72 (83%)	15 (17%)	0	100	100
16	q	81/83 (98%)	68 (84%)	13 (16%)	0	100	100
17	r	64/66 (97%)	56 (88%)	8 (12%)	0	100	100
18	s	76/78 (97%)	60 (79%)	16 (21%)	0	100	100
19	t	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
22	C	273/275 (99%)	219 (80%)	54 (20%)	0	100	100
23	D	205/207 (99%)	163 (80%)	40 (20%)	2 (1%)	15	54
24	E	204/206 (99%)	167 (82%)	37 (18%)	0	100	100
25	F	175/177 (99%)	144 (82%)	31 (18%)	0	100	100
26	G	174/176 (99%)	133 (76%)	39 (22%)	2 (1%)	14	52
27	K	143/145 (99%)	112 (78%)	31 (22%)	0	100	100
28	L	120/122 (98%)	97 (81%)	23 (19%)	0	100	100
29	M	144/146 (99%)	101 (70%)	40 (28%)	3 (2%)	7	38
30	N	139/141 (99%)	111 (80%)	28 (20%)	0	100	100
31	O	121/123 (98%)	92 (76%)	29 (24%)	0	100	100
32	P	115/117 (98%)	90 (78%)	25 (22%)	0	100	100
33	Q	112/114 (98%)	101 (90%)	11 (10%)	0	100	100
34	R	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
35	S	100/102 (98%)	85 (85%)	15 (15%)	0	100	100
36	T	110/112 (98%)	94 (86%)	16 (14%)	0	100	100
37	U	87/89 (98%)	66 (76%)	19 (22%)	2 (2%)	6	36
38	V	99/101 (98%)	68 (69%)	29 (29%)	2 (2%)	7	39
39	W	92/94 (98%)	67 (73%)	23 (25%)	2 (2%)	6	37
40	X	74/76 (97%)	63 (85%)	11 (15%)	0	100	100
41	Y	52/54 (96%)	39 (75%)	13 (25%)	0	100	100
42	Z	59/61 (97%)	54 (92%)	5 (8%)	0	100	100
43	0	56/58 (97%)	50 (89%)	6 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	1	81/83 (98%)	52 (64%)	29 (36%)	0	100	100
45	2	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
46	3	47/49 (96%)	40 (85%)	7 (15%)	0	100	100
47	4	42/44 (96%)	36 (86%)	6 (14%)	0	100	100
48	5	62/64 (97%)	47 (76%)	15 (24%)	0	100	100
49	6	36/38 (95%)	28 (78%)	8 (22%)	0	100	100
All	All	5143/5235 (98%)	4173 (81%)	953 (18%)	17 (0%)	44	75

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	G	48	ASN
29	M	95	VAL
29	M	98	GLU
38	V	73	PRO
39	W	16	SER
8	i	41	HIS
26	G	47	GLY
37	U	50	VAL
38	V	88	GLY
23	D	90	GLU
37	U	51	ALA
39	W	17	LEU
14	o	25	PRO
23	D	89	GLY
29	M	16	ARG
3	d	190	ILE
8	i	40	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	c	162/162 (100%)	139 (86%)	23 (14%)	3 19
3	d	175/175 (100%)	155 (89%)	20 (11%)	5 26
4	e	126/126 (100%)	106 (84%)	20 (16%)	2 14
5	f	86/86 (100%)	77 (90%)	9 (10%)	7 31
6	g	131/131 (100%)	120 (92%)	11 (8%)	11 40
7	h	112/112 (100%)	92 (82%)	20 (18%)	2 9
8	i	101/101 (100%)	82 (81%)	19 (19%)	1 8
9	j	90/90 (100%)	78 (87%)	12 (13%)	4 21
10	k	91/91 (100%)	83 (91%)	8 (9%)	10 38
11	l	118/118 (100%)	101 (86%)	17 (14%)	3 18
12	m	95/95 (100%)	81 (85%)	14 (15%)	3 18
13	n	51/51 (100%)	44 (86%)	7 (14%)	3 20
14	o	78/78 (100%)	69 (88%)	9 (12%)	5 26
15	p	79/79 (100%)	66 (84%)	13 (16%)	2 13
16	q	76/76 (100%)	64 (84%)	12 (16%)	2 15
17	r	57/57 (100%)	45 (79%)	12 (21%)	1 5
18	s	68/68 (100%)	62 (91%)	6 (9%)	10 38
19	t	62/62 (100%)	56 (90%)	6 (10%)	8 33
22	C	225/225 (100%)	180 (80%)	45 (20%)	1 7
23	D	170/170 (100%)	148 (87%)	22 (13%)	4 22
24	E	172/172 (100%)	139 (81%)	33 (19%)	1 7
25	F	154/154 (100%)	136 (88%)	18 (12%)	5 26
26	G	146/146 (100%)	135 (92%)	11 (8%)	13 43
27	K	122/122 (100%)	104 (85%)	18 (15%)	3 17
28	L	98/98 (100%)	81 (83%)	17 (17%)	2 11
29	M	112/112 (100%)	94 (84%)	18 (16%)	2 14
30	N	112/112 (100%)	94 (84%)	18 (16%)	2 14
31	O	105/105 (100%)	86 (82%)	19 (18%)	1 9
32	P	91/91 (100%)	81 (89%)	10 (11%)	6 29
33	Q	97/97 (100%)	81 (84%)	16 (16%)	2 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	R	94/94 (100%)	80 (85%)	14 (15%)	3	17
35	S	83/83 (100%)	74 (89%)	9 (11%)	6	30
36	T	95/95 (100%)	85 (90%)	10 (10%)	7	31
37	U	80/80 (100%)	67 (84%)	13 (16%)	2	13
38	V	85/85 (100%)	77 (91%)	8 (9%)	8	35
39	W	85/85 (100%)	78 (92%)	7 (8%)	11	40
40	X	61/61 (100%)	53 (87%)	8 (13%)	4	21
41	Y	47/47 (100%)	36 (77%)	11 (23%)	1	4
42	Z	55/55 (100%)	50 (91%)	5 (9%)	9	36
43	0	49/49 (100%)	39 (80%)	10 (20%)	1	6
44	1	75/75 (100%)	63 (84%)	12 (16%)	2	14
45	2	46/46 (100%)	41 (89%)	5 (11%)	6	29
46	3	49/49 (100%)	41 (84%)	8 (16%)	2	13
47	4	39/39 (100%)	32 (82%)	7 (18%)	2	9
48	5	51/51 (100%)	46 (90%)	5 (10%)	8	33
49	6	35/35 (100%)	33 (94%)	2 (6%)	20	53
All	All	4391/4391 (100%)	3774 (86%)	617 (14%)	6	19

All (617) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	c	15	ILE
2	c	16	ARG
2	c	22	TRP
2	c	30	GLU
2	c	36	LEU
2	c	40	LYS
2	c	42	ILE
2	c	55	GLU
2	c	57	GLU
2	c	75	VAL
2	c	83	VAL
2	c	85	ASN
2	c	98	VAL
2	c	100	ILE
2	c	102	ILE

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Mol	Chain	Res	Type
2	c	107	LYS
2	c	119	ILE
2	c	123	LEU
2	c	139	ARG
2	c	176	THR
2	c	178	ARG
2	c	191	THR
2	c	200	TRP
3	d	4	TYR
3	d	19	LEU
3	d	57	LEU
3	d	58	ARG
3	d	71	LEU
3	d	77	LYS
3	d	94	ARG
3	d	96	ASP
3	d	107	THR
3	d	121	THR
3	d	129	ILE
3	d	142	VAL
3	d	143	ARG
3	d	145	LYS
3	d	168	PHE
3	d	177	PHE
3	d	184	ASP
3	d	186	LEU
3	d	189	GLU
3	d	195	VAL
4	e	3	TYR
4	e	9	LEU
4	e	19	ASN
4	e	20	ARG
4	e	24	VAL
4	e	31	LEU
4	e	32	ARG
4	e	38	VAL
4	e	43	ASN
4	e	50	THR
4	e	85	VAL
4	e	105	VAL
4	e	117	LEU
4	e	125	SER

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Mol	Chain	Res	Type
4	e	127	SER
4	e	131	ASN
4	e	132	THR
4	e	144	LEU
4	e	147	LEU
4	e	159	LYS
5	f	11	TYR
5	f	17	ILE
5	f	18	ASP
5	f	19	GLU
5	f	35	ASP
5	f	56	ASN
5	f	65	ILE
5	f	66	VAL
5	f	67	ASN
6	g	19	ASN
6	g	20	SER
6	g	22	LEU
6	g	42	ILE
6	g	47	PHE
6	g	51	LYS
6	g	57	ASP
6	g	87	VAL
6	g	107	TYR
6	g	116	MET
6	g	136	LYS
7	h	7	ILE
7	h	20	VAL
7	h	22	HIS
7	h	32	ILE
7	h	59	VAL
7	h	60	ILE
7	h	69	ASN
7	h	70	GLU
7	h	73	VAL
7	h	74	ILE
7	h	78	LYS
7	h	79	ARG
7	h	86	ARG
7	h	92	ASP
7	h	98	LEU
7	h	99	ASN

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Mol	Chain	Res	Type
7	h	103	ILE
7	h	112	VAL
7	h	114	THR
7	h	127	VAL
8	i	3	GLN
8	i	9	THR
8	i	12	ARG
8	i	13	LYS
8	i	14	ASN
8	i	16	VAL
8	i	22	VAL
8	i	28	ILE
8	i	34	ASP
8	i	38	TYR
8	i	44	LEU
8	i	57	THR
8	i	65	VAL
8	i	66	ASN
8	i	79	ILE
8	i	93	ASP
8	i	106	ARG
8	i	115	LYS
8	i	127	PHE
9	j	4	GLN
9	j	8	ILE
9	j	15	HIS
9	j	16	ARG
9	j	35	ASP
9	j	52	ILE
9	j	55	THR
9	j	67	MET
9	j	72	ARG
9	j	75	ASP
9	j	76	ILE
9	j	88	MET
10	k	35	THR
10	k	53	LYS
10	k	55	SER
10	k	58	SER
10	k	65	MET
10	k	83	ASP
10	k	108	THR

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Mol	Chain	Res	Type
10	k	122	ARG
11	l	3	THR
11	l	4	ILE
11	l	7	LEU
11	l	12	ARG
11	l	20	ASP
11	l	26	LYS
11	l	30	SER
11	l	32	LYS
11	l	40	SER
11	l	54	THR
11	l	56	LYS
11	l	72	ASN
11	l	74	ILE
11	l	92	VAL
11	l	100	VAL
11	l	103	LEU
11	l	134	ARG
12	m	4	ILE
12	m	9	ILE
12	m	14	ARG
12	m	21	TYR
12	m	29	THR
12	m	34	LEU
12	m	42	ASP
12	m	44	ARG
12	m	45	VAL
12	m	60	ILE
12	m	77	ILE
12	m	95	LEU
12	m	98	ARG
12	m	101	ASN
13	n	5	SER
13	n	7	ILE
13	n	18	THR
13	n	26	ARG
13	n	27	CYS
13	n	33	VAL
13	n	44	PHE
14	o	10	GLU
14	o	24	SER
14	o	26	GLU

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Mol	Chain	Res	Type
14	o	37	ASN
14	o	52	SER
14	o	54	ARG
14	o	80	GLU
14	o	87	LEU
14	o	89	ARG
15	p	3	VAL
15	p	5	ILE
15	p	10	MET
15	p	13	LYS
15	p	22	VAL
15	p	26	ARG
15	p	39	THR
15	p	40	TYR
15	p	65	GLN
15	p	73	ILE
15	p	84	HIS
15	p	85	GLU
15	p	90	LYS
16	q	5	ARG
16	q	7	GLN
16	q	10	VAL
16	q	21	ASP
16	q	30	THR
16	q	44	SER
16	q	52	GLU
16	q	53	ASN
16	q	54	ASN
16	q	70	LEU
16	q	77	ARG
16	q	78	LEU
17	r	13	LYS
17	r	14	VAL
17	r	16	TYR
17	r	20	ASN
17	r	27	TYR
17	r	29	ASP
17	r	30	THR
17	r	47	ARG
17	r	49	THR
17	r	51	THR
17	r	63	ILE

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Mol	Chain	Res	Type
17	r	65	ARG
18	s	6	LYS
18	s	14	HIS
18	s	32	LYS
18	s	33	THR
18	s	65	ASP
18	s	78	ARG
19	t	4	ILE
19	t	5	GLU
19	t	46	VAL
19	t	49	LEU
19	t	65	LEU
19	t	78	LEU
22	C	10	THR
22	C	13	ARG
22	C	14	ARG
22	C	15	ASN
22	C	17	THR
22	C	18	SER
22	C	19	SER
22	C	20	ASP
22	C	23	GLU
22	C	26	THR
22	C	30	GLU
22	C	37	LEU
22	C	39	ASN
22	C	45	ASN
22	C	49	ILE
22	C	67	PHE
22	C	87	ARG
22	C	91	ILE
22	C	94	VAL
22	C	100	VAL
22	C	110	LEU
22	C	117	VAL
22	C	124	ILE
22	C	134	ASN
22	C	140	VAL
22	C	156	ARG
22	C	160	THR
22	C	171	TYR
22	C	174	ILE

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Mol	Chain	Res	Type
22	C	182	ARG
22	C	184	ILE
22	C	187	THR
22	C	191	THR
22	C	194	SER
22	C	197	ASN
22	C	198	GLU
22	C	211	SER
22	C	212	ARG
22	C	214	MET
22	C	219	THR
22	C	228	ASN
22	C	250	TRP
22	C	259	THR
22	C	267	ASP
22	C	273	ARG
23	D	15	ILE
23	D	17	THR
23	D	21	GLU
23	D	22	LEU
23	D	26	THR
23	D	29	GLU
23	D	34	VAL
23	D	44	ASP
23	D	62	ASN
23	D	74	THR
23	D	101	VAL
23	D	108	VAL
23	D	111	THR
23	D	113	THR
23	D	119	PHE
23	D	145	SER
23	D	160	LEU
23	D	167	ASP
23	D	168	ARG
23	D	180	ASP
23	D	188	ILE
23	D	201	THR
24	E	7	PHE
24	E	8	LYS
24	E	9	GLN
24	E	12	THR

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Mol	Chain	Res	Type
24	E	20	ASN
24	E	43	SER
24	E	51	VAL
24	E	58	ARG
24	E	62	ARG
24	E	65	TRP
24	E	74	ARG
24	E	77	SER
24	E	80	SER
24	E	89	VAL
24	E	93	THR
24	E	106	ARG
24	E	121	ASN
24	E	126	VAL
24	E	132	ASP
24	E	150	THR
24	E	152	VAL
24	E	155	VAL
24	E	161	ASP
24	E	169	ASN
24	E	173	VAL
24	E	177	THR
24	E	179	ASP
24	E	185	ASP
24	E	195	THR
24	E	197	THR
24	E	199	LEU
24	E	200	THR
24	E	202	ILE
25	F	13	THR
25	F	28	THR
25	F	32	ASP
25	F	44	VAL
25	F	51	ASP
25	F	61	THR
25	F	66	LEU
25	F	90	THR
25	F	112	ARG
25	F	114	PHE
25	F	123	ASP
25	F	129	THR
25	F	138	PHE

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Mol	Chain	Res	Type
25	F	141	VAL
25	F	152	MET
25	F	162	THR
25	F	165	GLU
25	F	169	LEU
26	G	8	VAL
26	G	25	THR
26	G	43	MET
26	G	45	ILE
26	G	52	PHE
26	G	65	HIS
26	G	74	ASN
26	G	89	LEU
26	G	107	VAL
26	G	116	THR
26	G	149	ARG
27	K	20	ASP
27	K	26	LEU
27	K	28	ARG
27	K	30	SER
27	K	37	LEU
27	K	41	ASN
27	K	45	PHE
27	K	46	THR
27	K	50	ASP
27	K	51	THR
27	K	63	VAL
27	K	71	THR
27	K	85	LEU
27	K	101	LEU
27	K	113	ASN
27	K	115	LEU
27	K	123	LEU
27	K	130	GLU
28	L	3	GLN
28	L	6	SER
28	L	19	ILE
28	L	21	THR
28	L	24	VAL
28	L	32	THR
28	L	35	ILE
28	L	37	ASP

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Mol	Chain	Res	Type
28	L	64	ARG
28	L	70	ARG
28	L	73	ASP
28	L	77	ILE
28	L	90	ASP
28	L	92	SER
28	L	108	GLU
28	L	110	ASN
28	L	115	VAL
29	M	18	ARG
29	M	23	THR
29	M	73	ASP
29	M	76	VAL
29	M	77	VAL
29	M	79	LEU
29	M	80	ASP
29	M	84	ARG
29	M	92	THR
29	M	95	VAL
29	M	96	LEU
29	M	97	LYS
29	M	103	LYS
29	M	105	GLU
29	M	117	LEU
29	M	122	THR
29	M	127	LYS
29	M	143	ILE
30	N	7	VAL
30	N	10	ARG
30	N	20	GLU
30	N	43	THR
30	N	45	ARG
30	N	65	TRP
30	N	68	ILE
30	N	69	PHE
30	N	72	LYS
30	N	74	TYR
30	N	75	THR
30	N	76	SER
30	N	82	ARG
30	N	94	VAL
30	N	99	ARG

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Mol	Chain	Res	Type
30	N	113	VAL
30	N	120	LEU
30	N	122	SER
31	O	4	ARG
31	O	24	LEU
31	O	27	ASN
31	O	30	ILE
31	O	41	ARG
31	O	42	SER
31	O	43	THR
31	O	56	LEU
31	O	70	VAL
31	O	75	GLU
31	O	81	VAL
31	O	89	LEU
31	O	104	TYR
31	O	110	THR
31	O	114	ARG
31	O	116	ASP
31	O	121	VAL
31	O	122	VAL
31	O	125	PHE
32	P	3	THR
32	P	22	ILE
32	P	23	SER
32	P	31	LEU
32	P	33	ILE
32	P	48	VAL
32	P	62	GLU
32	P	71	THR
32	P	101	HIS
32	P	103	ARG
33	Q	11	GLU
33	Q	15	THR
33	Q	16	ASP
33	Q	39	ARG
33	Q	48	ILE
33	Q	50	ARG
33	Q	51	ARG
33	Q	61	VAL
33	Q	62	ARG
33	Q	66	ASN

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Mol	Chain	Res	Type
33	Q	73	THR
33	Q	76	LEU
33	Q	78	THR
33	Q	94	ARG
33	Q	110	ILE
33	Q	113	ILE
34	R	9	VAL
34	R	18	LEU
34	R	20	LEU
34	R	25	TYR
34	R	29	HIS
34	R	30	THR
34	R	34	SER
34	R	38	GLN
34	R	56	ASP
34	R	60	LEU
34	R	76	TYR
34	R	85	LEU
34	R	102	ASP
34	R	115	ASP
35	S	1	MET
35	S	11	GLN
35	S	12	VAL
35	S	27	VAL
35	S	61	THR
35	S	69	LYS
35	S	81	HIS
35	S	82	SER
35	S	83	HIS
36	T	20	ARG
36	T	26	ILE
36	T	44	THR
36	T	56	LEU
36	T	67	PHE
36	T	68	ASP
36	T	80	PHE
36	T	86	THR
36	T	102	ASN
36	T	114	GLU
37	U	3	LEU
37	U	6	VAL
37	U	7	ILE

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Mol	Chain	Res	Type
37	U	11	VAL
37	U	14	GLU
37	U	31	THR
37	U	34	ASN
37	U	37	LEU
37	U	47	ASP
37	U	53	VAL
37	U	76	ARG
37	U	89	ILE
37	U	90	GLN
38	V	12	ILE
38	V	18	ASN
38	V	31	ASP
38	V	35	VAL
38	V	59	VAL
38	V	70	VAL
38	V	85	GLU
38	V	94	SER
39	W	15	ARG
39	W	43	PHE
39	W	71	ASN
39	W	78	GLN
39	W	80	ASP
39	W	89	VAL
39	W	94	VAL
40	X	34	SER
40	X	36	ASP
40	X	50	ARG
40	X	67	THR
40	X	73	ASP
40	X	77	ARG
40	X	80	ARG
40	X	88	VAL
41	Y	8	THR
41	Y	10	ARG
41	Y	12	THR
41	Y	14	SER
41	Y	16	ASN
41	Y	25	THR
41	Y	32	ASN
41	Y	36	VAL
41	Y	43	LYS

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Mol	Chain	Res	Type
41	Y	47	VAL
41	Y	55	LYS
42	Z	32	LEU
42	Z	39	ASN
42	Z	50	ILE
42	Z	57	LEU
42	Z	62	ASN
43	0	8	LEU
43	0	13	ILE
43	0	22	THR
43	0	34	THR
43	0	40	ASN
43	0	43	ILE
43	0	47	VAL
43	0	49	THR
43	0	50	ILE
43	0	53	LEU
44	1	3	GLN
44	1	13	VAL
44	1	15	MET
44	1	18	THR
44	1	23	PHE
44	1	25	SER
44	1	27	SER
44	1	51	THR
44	1	57	PHE
44	1	70	ARG
44	1	71	VAL
44	1	74	PHE
45	2	7	ARG
45	2	9	SER
45	2	18	THR
45	2	32	ASN
45	2	37	LYS
46	3	5	ILE
46	3	8	GLU
46	3	10	THR
46	3	11	SER
46	3	19	THR
46	3	26	ASN
46	3	39	GLU
46	3	44	LEU

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Mol	Chain	Res	Type
47	4	3	ARG
47	4	4	THR
47	4	5	TYR
47	4	20	LYS
47	4	24	THR
47	4	42	ILE
47	4	43	SER
48	5	15	LYS
48	5	43	GLN
48	5	54	ASP
48	5	57	ARG
48	5	58	ILE
49	6	30	ASN
49	6	36	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
2	c	125	ASN
3	d	39	ASN
3	d	113	GLN
6	g	28	ASN
7	h	122	ASN
8	i	126	GLN
9	j	20	GLN
9	j	56	HIS
11	l	5	ASN
12	m	104	ASN
13	n	10	ASN
13	n	16	HIS
13	n	19	GLN
13	n	38	HIS
13	n	52	GLN
14	o	28	GLN
15	p	65	GLN
15	p	72	ASN
16	q	12	GLN
16	q	50	HIS
17	r	21	HIS
17	r	56	GLN
18	s	22	GLN
18	s	23	GLN

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Mol	Chain	Res	Type
18	s	63	GLN
19	t	18	ASN
22	C	228	ASN
22	C	232	HIS
23	D	33	ASN
23	D	37	GLN
23	D	54	GLN
23	D	62	ASN
23	D	68	HIS
24	E	75	GLN
24	E	169	ASN
25	F	37	ASN
25	F	178	GLN
26	G	23	ASN
26	G	44	ASN
26	G	56	ASN
26	G	84	GLN
26	G	130	GLN
27	K	48	HIS
27	K	131	HIS
29	M	4	HIS
29	M	38	GLN
29	M	54	GLN
31	O	61	GLN
31	O	68	ASN
32	P	101	HIS
33	Q	83	GLN
34	R	29	HIS
34	R	81	HIS
34	R	91	ASN
35	S	11	GLN
35	S	26	ASN
35	S	68	GLN
35	S	83	HIS
35	S	88	HIS
37	U	90	GLN
38	V	18	ASN
38	V	44	HIS
39	W	88	HIS
40	X	87	GLN
41	Y	20	HIS
42	Z	36	GLN

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Mol	Chain	Res	Type
45	2	32	ASN
45	2	40	HIS
45	2	48	HIS
48	5	60	GLN
48	5	61	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1521/1528 (99%)	312 (20%)	0
20	A	2899/2909 (99%)	654 (22%)	27 (0%)
21	B	115/116 (99%)	30 (26%)	3 (2%)
All	All	4535/4553 (99%)	996 (21%)	30 (0%)

All (996) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	5	A
1	a	6	G
1	a	13	A
1	a	19	G
1	a	27	C
1	a	29	A
1	a	30	A
1	a	32	G
1	a	34	U
1	a	35	G
1	a	37	C
1	a	38	G
1	a	41	G
1	a	44	C
1	a	45	C
1	a	48	A
1	a	51	C
1	a	55	C
1	a	69	C
1	a	70	U
1	a	101	A
1	a	114	A
1	a	117	G
1	a	125	A

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Mol	Chain	Res	Type
1	a	126	C
1	a	127	A
1	a	135	A
1	a	137	C
1	a	138	C
1	a	168	A
1	a	169	C
1	a	183	G
1	a	188	A
1	a	189	C
1	a	201	C
1	a	202	A
1	a	209	A
1	a	210	A
1	a	211	G
1	a	213	G
1	a	215	G
1	a	225	U
1	a	226	U
1	a	228	G
1	a	229	G
1	a	230	G
1	a	231	U
1	a	254	G
1	a	255	U
1	a	256	G
1	a	258	A
1	a	259	U
1	a	261	A
1	a	262	G
1	a	266	G
1	a	277	A
1	a	281	G
1	a	282	C
1	a	289	A
1	a	294	A
1	a	295	C
1	a	304	G
1	a	313	A
1	a	321	A
1	a	336	A
1	a	339	G

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Mol	Chain	Res	Type
1	a	343	C
1	a	344	A
1	a	358	U
1	a	361	G
1	a	362	G
1	a	367	C
1	a	369	G
1	a	381	C
1	a	382	U
1	a	387	C
1	a	388	A
1	a	397	A
1	a	403	G
1	a	412	A
1	a	421	G
1	a	426	A
1	a	427	A
1	a	428	G
1	a	429	A
1	a	443	G
1	a	444	U
1	a	446	A
1	a	447	A
1	a	463	A
1	a	467	A
1	a	468	C
1	a	469	A
1	a	473	A
1	a	477	U
1	a	479	G
1	a	480	U
1	a	481	A
1	a	484	U
1	a	488	C
1	a	489	G
1	a	490	U
1	a	497	A
1	a	499	G
1	a	500	G
1	a	510	A
1	a	512	A
1	a	514	A

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Mol	Chain	Res	Type
1	a	522	C
1	a	524	A
1	a	525	A
1	a	526	C
1	a	527	U
1	a	533	C
1	a	534	C
1	a	536	G
1	a	539	G
1	a	542	G
1	a	547	A
1	a	548	A
1	a	551	C
1	a	553	U
1	a	556	G
1	a	561	A
1	a	562	A
1	a	578	A
1	a	579	U
1	a	585	G
1	a	588	A
1	a	590	G
1	a	591	C
1	a	592	G
1	a	594	G
1	a	603	G
1	a	644	A
1	a	647	G
1	a	648	U
1	a	664	G
1	a	668	U
1	a	680	A
1	a	701	U
1	a	702	A
1	a	703	G
1	a	710	A
1	a	716	U
1	a	717	A
1	a	718	G
1	a	736	A
1	a	738	U
1	a	744	A

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Mol	Chain	Res	Type
1	a	764	A
1	a	767	G
1	a	770	G
1	a	775	G
1	a	782	A
1	a	793	G
1	a	802	A
1	a	818	G
1	a	828	U
1	a	830	A
1	a	832	C
1	a	835	U
1	a	842	U
1	a	843	A
1	a	847	G
1	a	851	G
1	a	859	C
1	a	861	G
1	a	862	C
1	a	869	G
1	a	881	A
1	a	888	A
1	a	890	G
1	a	892	A
1	a	901	G
1	a	905	A
1	a	906	G
1	a	930	A
1	a	934	A
1	a	939	A
1	a	942	G
1	a	943	G
1	a	950	C
1	a	951	A
1	a	961	G
1	a	968	U
1	a	974	A
1	a	975	A
1	a	976	U
1	a	977	U
1	a	982	G
1	a	985	A

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Mol	Chain	Res	Type
1	a	987	G
1	a	988	C
1	a	991	A
1	a	992	G
1	a	997	U
1	a	999	A
1	a	1008	U
1	a	1009	G
1	a	1015	C
1	a	1018	U
1	a	1019	G
1	a	1020	A
1	a	1022	C
1	a	1031	G
1	a	1037	G
1	a	1038	C
1	a	1039	U
1	a	1041	U
1	a	1042	C
1	a	1043	C
1	a	1044	C
1	a	1045	U
1	a	1047	C
1	a	1048	G
1	a	1055	A
1	a	1058	U
1	a	1061	C
1	a	1062	A
1	a	1069	G
1	a	1080	G
1	a	1081	U
1	a	1097	G
1	a	1101	U
1	a	1109	A
1	a	1110	G
1	a	1111	U
1	a	1117	A
1	a	1140	G
1	a	1146	A
1	a	1149	A
1	a	1154	G
1	a	1155	U

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Mol	Chain	Res	Type
1	a	1156	U
1	a	1161	A
1	a	1171	G
1	a	1174	U
1	a	1176	C
1	a	1183	C
1	a	1199	G
1	a	1200	G
1	a	1211	A
1	a	1212	A
1	a	1215	C
1	a	1227	U
1	a	1229	U
1	a	1240	A
1	a	1241	C
1	a	1242	A
1	a	1243	C
1	a	1256	G
1	a	1261	G
1	a	1263	A
1	a	1272	C
1	a	1274	C
1	a	1275	U
1	a	1276	A
1	a	1295	A
1	a	1300	U
1	a	1301	U
1	a	1302	A
1	a	1312	U
1	a	1313	C
1	a	1314	A
1	a	1315	G
1	a	1317	U
1	a	1318	C
1	a	1320	G
1	a	1334	A
1	a	1335	C
1	a	1337	C
1	a	1338	G
1	a	1351	C
1	a	1361	A
1	a	1372	A

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Mol	Chain	Res	Type
1	a	1374	C
1	a	1375	A
1	a	1378	A
1	a	1379	C
1	a	1389	A
1	a	1396	U
1	a	1401	G
1	a	1407	G
1	a	1409	A
1	a	1412	C
1	a	1413	A
1	a	1429	C
1	a	1432	G
1	a	1438	G
1	a	1441	A
1	a	1451	U
1	a	1457	A
1	a	1461	A
1	a	1466	U
1	a	1467	U
1	a	1468	U
1	a	1484	A
1	a	1496	A
1	a	1503	G
1	a	1508	A
1	a	1509	A
1	a	1511	U
1	a	1518	A
1	a	1520	G
1	a	1521	G
1	a	1522	U
1	a	1523	A
1	a	1533	G
1	a	1545	G
1	a	1546	G
1	a	1550	A
20	A	14	A
20	A	16	G
20	A	26	U
20	A	29	A
20	A	35	U
20	A	36	G

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Mol	Chain	Res	Type
20	A	46	G
20	A	51	U
20	A	52	G
20	A	65	A
20	A	72	A
20	A	76	G
20	A	86	G
20	A	90	U
20	A	93	G
20	A	97	G
20	A	110	G
20	A	118	A
20	A	120	U
20	A	131	A
20	A	134	A
20	A	139	U
20	A	143	A
20	A	155	U
20	A	156	U
20	A	162	A
20	A	165	A
20	A	166	C
20	A	168	U
20	A	169	A
20	A	180	G
20	A	183	A
20	A	184	G
20	A	199	A
20	A	202	A
20	A	218	G
20	A	219	A
20	A	224	A
20	A	225	A
20	A	229	A
20	A	231	A
20	A	232	U
20	A	233	U
20	A	235	G
20	A	236	A
20	A	251	G
20	A	253	G
20	A	254	A

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Mol	Chain	Res	Type
20	A	255	G
20	A	268	A
20	A	276	C
20	A	277	C
20	A	279	A
20	A	284	C
20	A	285	U
20	A	286	U
20	A	288	C
20	A	289	U
20	A	292	U
20	A	296	G
20	A	297	G
20	A	300	G
20	A	301	U
20	A	309	C
20	A	310	G
20	A	313	A
20	A	318	A
20	A	321	C
20	A	322	U
20	A	325	U
20	A	339	G
20	A	342	U
20	A	344	G
20	A	367	A
20	A	369	A
20	A	372	C
20	A	378	G
20	A	383	A
20	A	387	C
20	A	389	G
20	A	396	C
20	A	399	A
20	A	400	G
20	A	404	G
20	A	421	A
20	A	426	G
20	A	446	G
20	A	451	G
20	A	452	A
20	A	487	A

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Mol	Chain	Res	Type
20	A	496	C
20	A	497	A
20	A	507	G
20	A	520	A
20	A	521	G
20	A	530	A
20	A	543	U
20	A	544	A
20	A	547	U
20	A	548	C
20	A	549	C
20	A	561	G
20	A	562	C
20	A	566	C
20	A	569	C
20	A	570	A
20	A	571	A
20	A	572	G
20	A	581	C
20	A	584	U
20	A	586	A
20	A	587	U
20	A	588	G
20	A	599	U
20	A	600	G
20	A	609	A
20	A	610	G
20	A	612	A
20	A	624	G
20	A	640	A
20	A	651	A
20	A	652	A
20	A	654	A
20	A	655	G
20	A	656	A
20	A	659	G
20	A	660	A
20	A	661	G
20	A	670	A
20	A	671	A
20	A	673	G
20	A	676	A

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Mol	Chain	Res	Type
20	A	677	G
20	A	684	U
20	A	690	G
20	A	693	U
20	A	694	G
20	A	709	G
20	A	710	A
20	A	722	G
20	A	726	U
20	A	756	A
20	A	757	A
20	A	759	C
20	A	766	G
20	A	767	A
20	A	770	A
20	A	778	C
20	A	784	C
20	A	787	U
20	A	792	A
20	A	795	G
20	A	805	G
20	A	808	G
20	A	815	G
20	A	822	A
20	A	824	U
20	A	825	U
20	A	830	A
20	A	832	G
20	A	833	A
20	A	834	A
20	A	840	A
20	A	845	G
20	A	852	C
20	A	867	U
20	A	868	U
20	A	885	U
20	A	886	U
20	A	888	A
20	A	891	A
20	A	900	G
20	A	903	G
20	A	905	G

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Mol	Chain	Res	Type
20	A	906	C
20	A	907	A
20	A	909	U
20	A	910	G
20	A	913	U
20	A	919	A
20	A	920	G
20	A	923	G
20	A	925	C
20	A	926	C
20	A	927	A
20	A	928	U
20	A	932	G
20	A	933	G
20	A	934	G
20	A	936	U
20	A	938	C
20	A	939	C
20	A	940	G
20	A	943	U
20	A	946	A
20	A	950	A
20	A	951	A
20	A	952	A
20	A	957	G
20	A	958	A
20	A	961	G
20	A	964	A
20	A	966	U
20	A	967	C
20	A	970	U
20	A	981	A
20	A	985	A
20	A	986	G
20	A	990	G
20	A	992	G
20	A	993	A
20	A	997	A
20	A	999	A
20	A	1001	G
20	A	1013	A
20	A	1014	A

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Mol	Chain	Res	Type
20	A	1016	G
20	A	1028	A
20	A	1036	A
20	A	1037	G
20	A	1045	C
20	A	1049	A
20	A	1051	A
20	A	1052	U
20	A	1053	A
20	A	1061	A
20	A	1062	G
20	A	1066	A
20	A	1067	A
20	A	1068	A
20	A	1073	U
20	A	1081	U
20	A	1085	C
20	A	1086	A
20	A	1087	G
20	A	1088	A
20	A	1093	U
20	A	1094	A
20	A	1096	G
20	A	1097	A
20	A	1098	U
20	A	1100	U
20	A	1101	U
20	A	1102	G
20	A	1106	U
20	A	1107	A
20	A	1108	G
20	A	1109	A
20	A	1110	A
20	A	1111	G
20	A	1112	C
20	A	1113	A
20	A	1114	G
20	A	1115	C
20	A	1116	C
20	A	1117	A
20	A	1118	C
20	A	1122	U

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Mol	Chain	Res	Type
20	A	1123	U
20	A	1125	A
20	A	1126	A
20	A	1127	G
20	A	1128	A
20	A	1129	G
20	A	1131	G
20	A	1135	A
20	A	1136	A
20	A	1137	U
20	A	1138	A
20	A	1139	G
20	A	1140	C
20	A	1141	U
20	A	1142	C
20	A	1143	A
20	A	1144	C
20	A	1146	A
20	A	1147	G
20	A	1148	U
20	A	1149	C
20	A	1150	G
20	A	1151	A
20	A	1152	G
20	A	1157	C
20	A	1167	A
20	A	1168	A
20	A	1172	U
20	A	1173	A
20	A	1174	C
20	A	1175	C
20	A	1179	G
20	A	1181	U
20	A	1182	A
20	A	1210	C
20	A	1212	A
20	A	1215	A
20	A	1217	G
20	A	1224	G
20	A	1249	G
20	A	1257	A
20	A	1264	G

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Mol	Chain	Res	Type
20	A	1275	G
20	A	1276	C
20	A	1277	G
20	A	1285	G
20	A	1290	A
20	A	1293	G
20	A	1294	C
20	A	1306	G
20	A	1308	G
20	A	1309	A
20	A	1310	A
20	A	1311	A
20	A	1322	A
20	A	1323	A
20	A	1335	G
20	A	1336	U
20	A	1337	A
20	A	1338	U
20	A	1349	U
20	A	1357	A
20	A	1365	U
20	A	1366	C
20	A	1376	U
20	A	1377	U
20	A	1388	U
20	A	1394	G
20	A	1396	G
20	A	1397	G
20	A	1401	A
20	A	1402	U
20	A	1404	G
20	A	1411	G
20	A	1414	A
20	A	1415	U
20	A	1420	A
20	A	1427	U
20	A	1428	G
20	A	1431	A
20	A	1432	U
20	A	1447	U
20	A	1448	U
20	A	1449	U

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Mol	Chain	Res	Type
20	A	1451	U
20	A	1452	G
20	A	1453	U
20	A	1454	U
20	A	1455	U
20	A	1456	G
20	A	1457	A
20	A	1461	A
20	A	1462	U
20	A	1463	G
20	A	1465	A
20	A	1469	A
20	A	1470	C
20	A	1475	U
20	A	1489	C
20	A	1490	A
20	A	1491	U
20	A	1492	G
20	A	1493	C
20	A	1494	G
20	A	1495	A
20	A	1497	U
20	A	1500	A
20	A	1501	A
20	A	1502	G
20	A	1503	U
20	A	1504	G
20	A	1510	C
20	A	1512	A
20	A	1519	G
20	A	1521	G
20	A	1525	U
20	A	1531	G
20	A	1532	A
20	A	1533	G
20	A	1535	U
20	A	1536	A
20	A	1539	U
20	A	1551	U
20	A	1552	A
20	A	1559	A
20	A	1560	G

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Mol	Chain	Res	Type
20	A	1568	G
20	A	1573	G
20	A	1584	G
20	A	1585	U
20	A	1586	A
20	A	1590	A
20	A	1593	U
20	A	1601	G
20	A	1605	C
20	A	1606	A
20	A	1612	A
20	A	1613	A
20	A	1615	A
20	A	1618	A
20	A	1623	C
20	A	1624	U
20	A	1627	U
20	A	1629	A
20	A	1630	G
20	A	1631	A
20	A	1632	A
20	A	1633	A
20	A	1634	A
20	A	1635	C
20	A	1640	G
20	A	1645	U
20	A	1650	U
20	A	1651	A
20	A	1653	A
20	A	1673	A
20	A	1674	G
20	A	1677	U
20	A	1685	G
20	A	1690	G
20	A	1691	C
20	A	1716	G
20	A	1717	G
20	A	1718	C
20	A	1738	G
20	A	1741	A
20	A	1742	G
20	A	1746	G

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Mol	Chain	Res	Type
20	A	1756	U
20	A	1757	U
20	A	1759	G
20	A	1770	G
20	A	1776	A
20	A	1777	G
20	A	1778	G
20	A	1787	A
20	A	1790	G
20	A	1793	U
20	A	1795	U
20	A	1798	A
20	A	1805	A
20	A	1814	C
20	A	1815	A
20	A	1823	A
20	A	1826	A
20	A	1830	A
20	A	1843	A
20	A	1868	A
20	A	1884	U
20	A	1886	G
20	A	1887	G
20	A	1896	A
20	A	1913	A
20	A	1919	C
20	A	1920	G
20	A	1923	C
20	A	1927	A
20	A	1928	C
20	A	1929	U
20	A	1930	A
20	A	1943	G
20	A	1944	G
20	A	1948	C
20	A	1952	A
20	A	1970	U
20	A	1976	C
20	A	1978	G
20	A	1979	C
20	A	1981	C
20	A	1984	A

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Mol	Chain	Res	Type
20	A	1985	A
20	A	1986	G
20	A	1989	G
20	A	1996	U
20	A	2005	U
20	A	2006	G
20	A	2007	U
20	A	2035	G
20	A	2037	A
20	A	2039	C
20	A	2044	A
20	A	2045	A
20	A	2046	G
20	A	2047	A
20	A	2057	C
20	A	2066	G
20	A	2069	C
20	A	2070	G
20	A	2074	A
20	A	2075	G
20	A	2076	A
20	A	2082	U
20	A	2083	G
20	A	2086	G
20	A	2107	G
20	A	2114	U
20	A	2115	G
20	A	2119	C
20	A	2123	U
20	A	2125	U
20	A	2126	A
20	A	2127	C
20	A	2129	G
20	A	2130	G
20	A	2131	A
20	A	2132	U
20	A	2133	A
20	A	2134	G
20	A	2139	G
20	A	2140	A
20	A	2143	C
20	A	2144	G

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Mol	Chain	Res	Type
20	A	2145	A
20	A	2146	U
20	A	2147	G
20	A	2148	A
20	A	2149	G
20	A	2154	G
20	A	2158	G
20	A	2159	C
20	A	2160	U
20	A	2162	G
20	A	2167	G
20	A	2172	A
20	A	2174	G
20	A	2178	U
20	A	2179	G
20	A	2182	G
20	A	2183	G
20	A	2184	G
20	A	2187	A
20	A	2194	U
20	A	2195	U
20	A	2204	A
20	A	2213	A
20	A	2217	G
20	A	2218	C
20	A	2239	A
20	A	2252	G
20	A	2253	G
20	A	2282	A
20	A	2283	A
20	A	2287	A
20	A	2293	G
20	A	2297	C
20	A	2298	C
20	A	2301	A
20	A	2302	A
20	A	2317	G
20	A	2318	G
20	A	2319	U
20	A	2334	A
20	A	2335	G
20	A	2336	A

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Mol	Chain	Res	Type
20	A	2339	G
20	A	2341	A
20	A	2348	G
20	A	2349	A
20	A	2351	G
20	A	2359	G
20	A	2364	C
20	A	2372	A
20	A	2393	G
20	A	2397	G
20	A	2399	C
20	A	2404	U
20	A	2406	A
20	A	2416	U
20	A	2417	C
20	A	2420	C
20	A	2427	G
20	A	2433	U
20	A	2436	C
20	A	2437	U
20	A	2439	A
20	A	2442	G
20	A	2443	G
20	A	2445	U
20	A	2455	C
20	A	2461	G
20	A	2462	A
20	A	2482	A
20	A	2488	C
20	A	2489	C
20	A	2492	A
20	A	2505	U
20	A	2512	C
20	A	2515	C
20	A	2517	A
20	A	2519	G
20	A	2532	A
20	A	2534	C
20	A	2548	C
20	A	2549	G
20	A	2566	U
20	A	2580	A

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Mol	Chain	Res	Type
20	A	2581	G
20	A	2587	C
20	A	2592	G
20	A	2596	G
20	A	2599	U
20	A	2600	C
20	A	2611	G
20	A	2616	A
20	A	2624	C
20	A	2625	C
20	A	2627	U
20	A	2628	A
20	A	2629	U
20	A	2650	U
20	A	2659	G
20	A	2660	C
20	A	2675	G
20	A	2677	G
20	A	2693	A
20	A	2696	G
20	A	2703	U
20	A	2704	A
20	A	2707	A
20	A	2719	A
20	A	2726	U
20	A	2727	U
20	A	2728	G
20	A	2747	A
20	A	2762	A
20	A	2766	C
20	A	2771	A
20	A	2779	A
20	A	2780	G
20	A	2791	G
20	A	2792	A
20	A	2793	U
20	A	2794	G
20	A	2795	A
20	A	2803	C
20	A	2804	A
20	A	2805	U
20	A	2808	C

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Mol	Chain	Res	Type
20	A	2810	U
20	A	2812	A
20	A	2813	A
20	A	2836	G
20	A	2843	U
20	A	2844	A
20	A	2846	A
20	A	2847	U
20	A	2858	U
20	A	2868	G
20	A	2872	U
20	A	2878	G
20	A	2883	G
20	A	2891	C
20	A	2897	G
20	A	2902	A
20	A	2904	G
20	A	2911	C
21	B	2	G
21	B	8	G
21	B	10	G
21	B	11	A
21	B	13	A
21	B	14	G
21	B	22	G
21	B	23	A
21	B	29	C
21	B	31	G
21	B	33	U
21	B	40	C
21	B	42	G
21	B	43	A
21	B	54	U
21	B	55	A
21	B	64	A
21	B	70	G
21	B	71	A
21	B	73	U
21	B	74	G
21	B	85	U
21	B	86	U
21	B	87	U

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Mol	Chain	Res	Type
21	B	92	U
21	B	94	G
21	B	95	U
21	B	97	A
21	B	102	A
21	B	107	G

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	A	13	U
20	A	29	A
20	A	179	A
20	A	182	U
20	A	312	U
20	A	427	A
20	A	519	A
20	A	693	U
20	A	755	A
20	A	890	A
20	A	949	U
20	A	974	A
20	A	1087	G
20	A	1100	U
20	A	1101	U
20	A	1147	G
20	A	1226	U
20	A	1584	G
20	A	1585	U
20	A	1600	C
20	A	1604	A
20	A	1605	C
20	A	1689	A
20	A	2132	U
20	A	2144	G
20	A	2317	G
20	A	2812	A
21	B	32	U
21	B	93	U
21	B	101	U

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)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

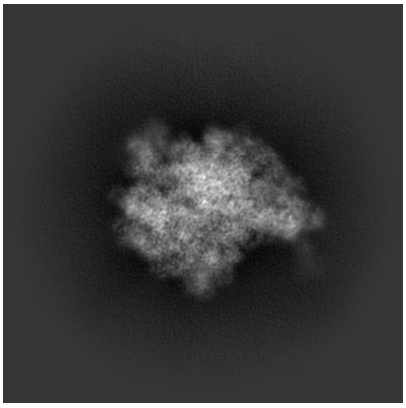
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0659. These allow visual inspection of the internal detail of the map and identification of artifacts.

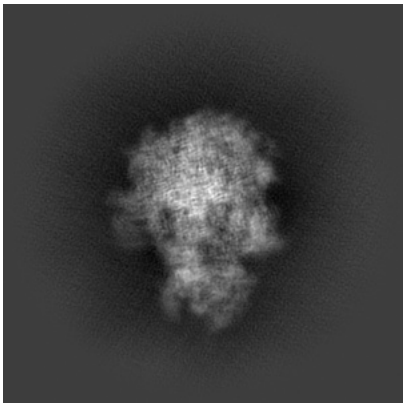
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

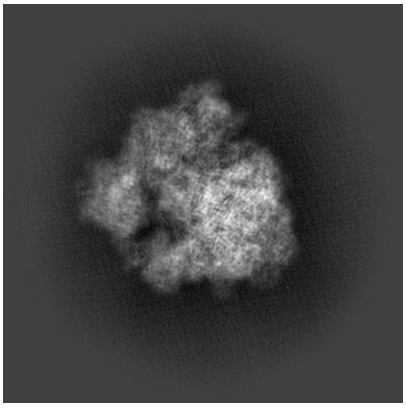
6.1.1 Primary map



X



Y

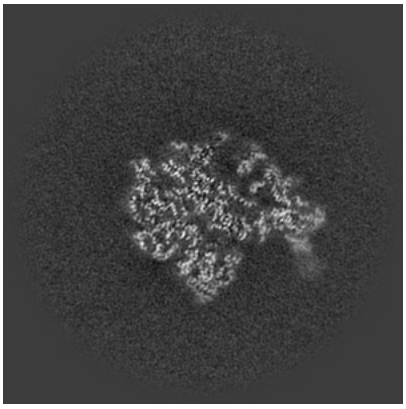


Z

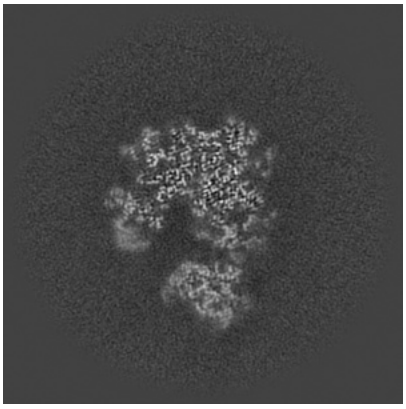
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

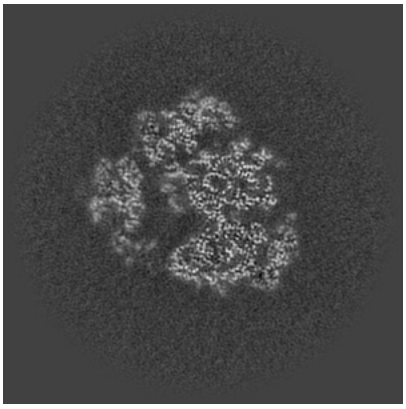
6.2.1 Primary map



X Index: 220



Y Index: 220

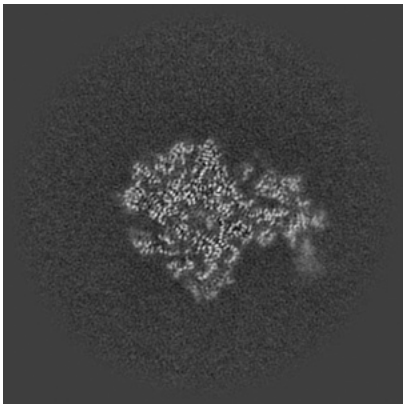


Z Index: 220

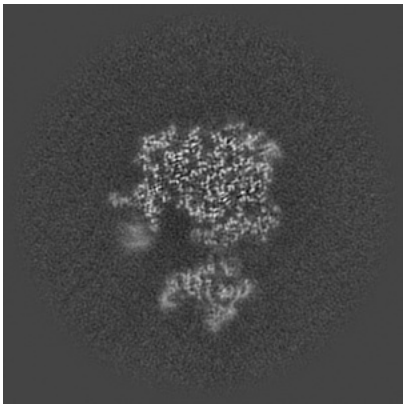
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

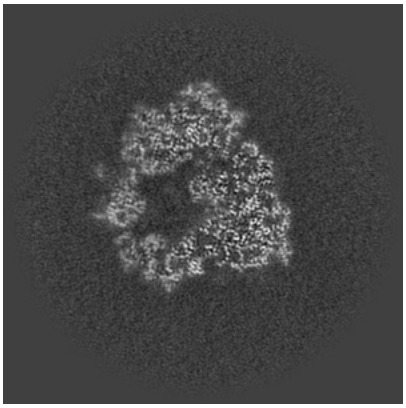
6.3.1 Primary map



X Index: 227



Y Index: 231

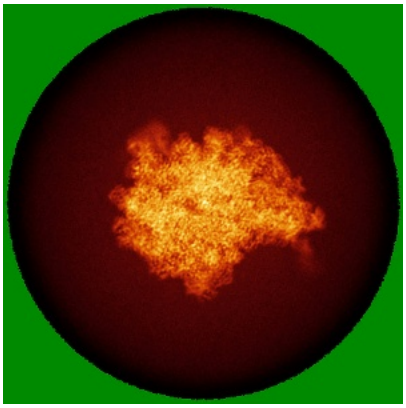


Z Index: 205

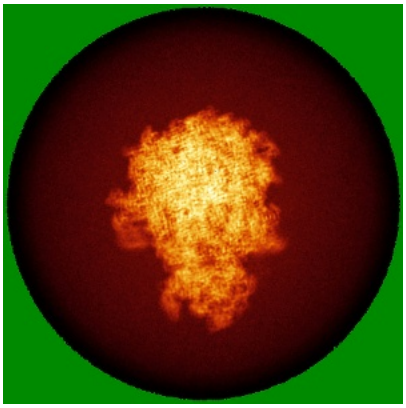
The images above show the largest variance slices of the map in three orthogonal directions.

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

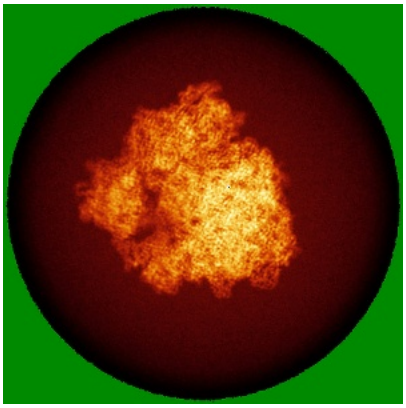
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.238. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

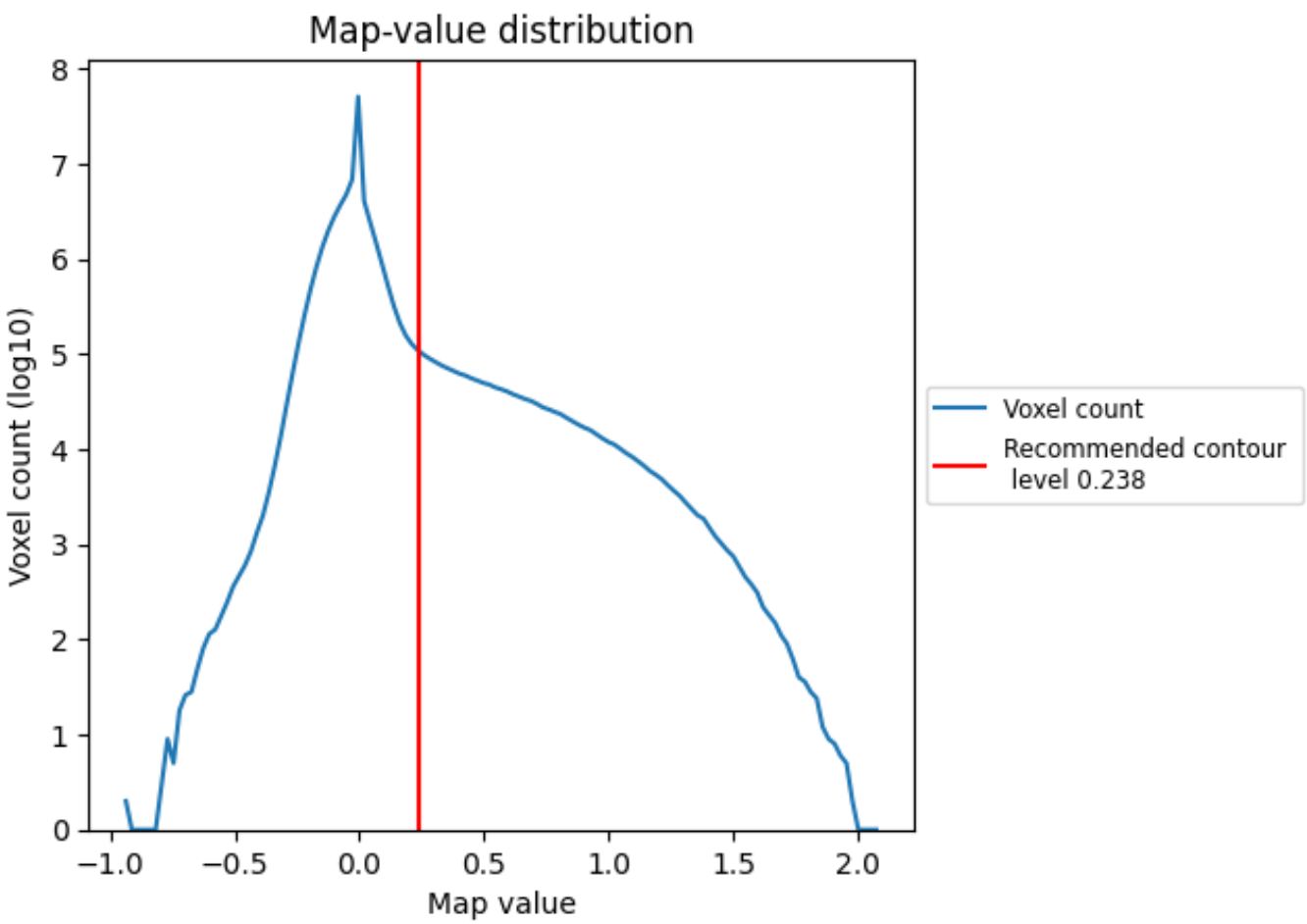
6.6 Mask visualisation (i)

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

7 Map analysis (i)

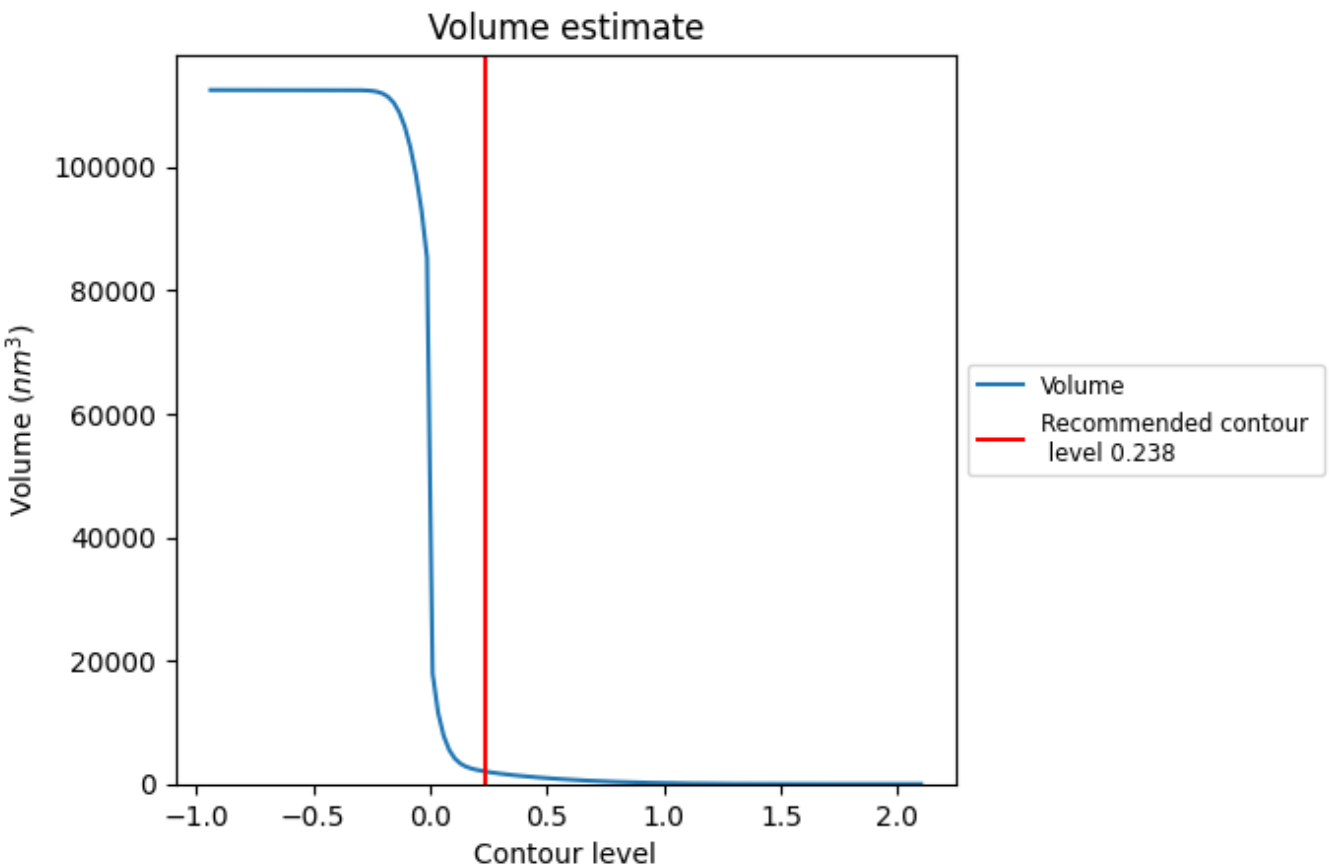
This section contains the results of statistical analysis of the map.

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.

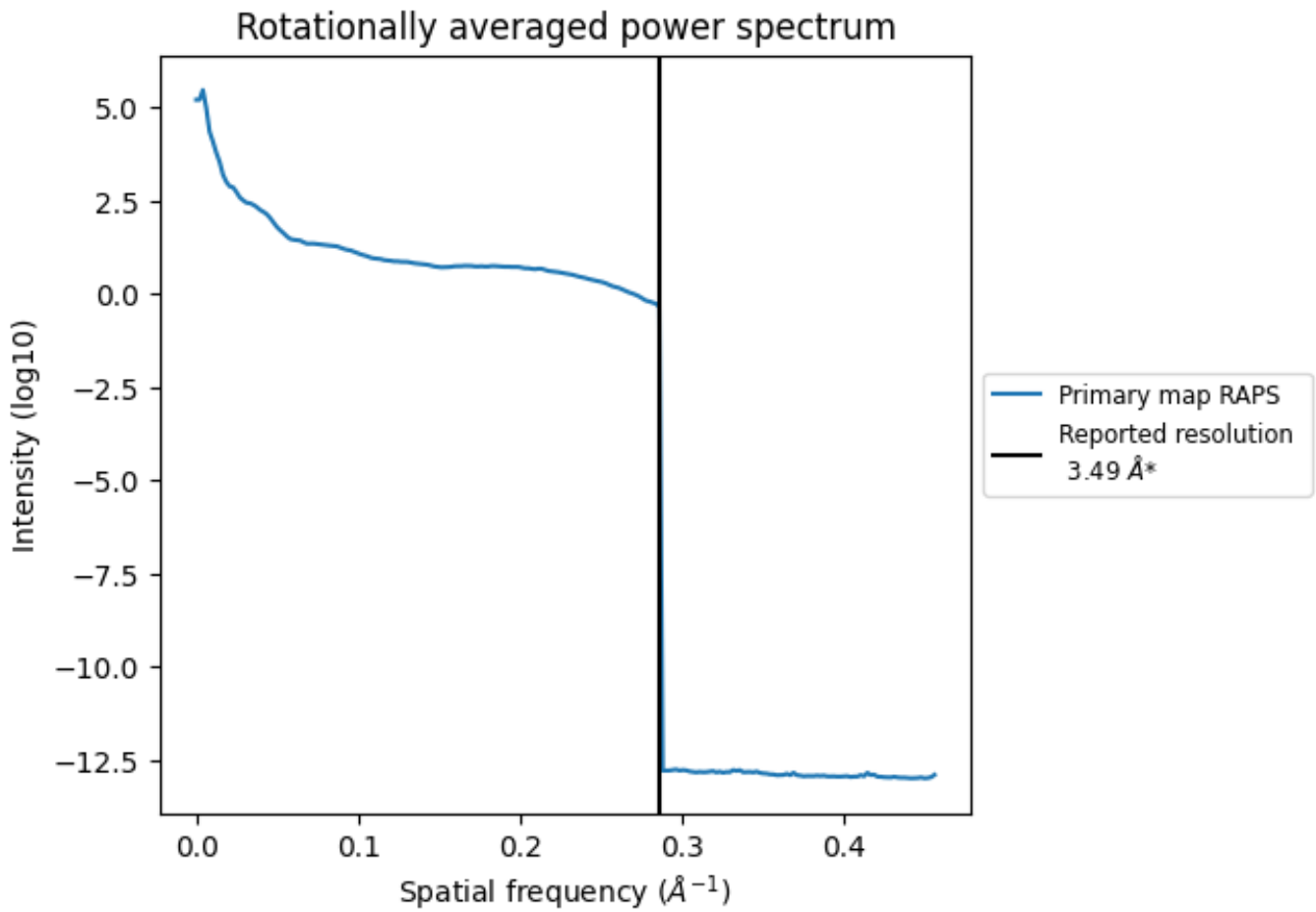
7.2 Volume estimate (i)



The volume at the recommended contour level is 2013 nm^3; this corresponds to an approximate mass of 1818 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 0.287 Å^{-1}

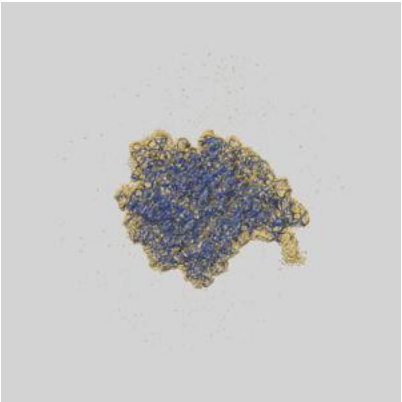
8 Fourier-Shell correlation (i)

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

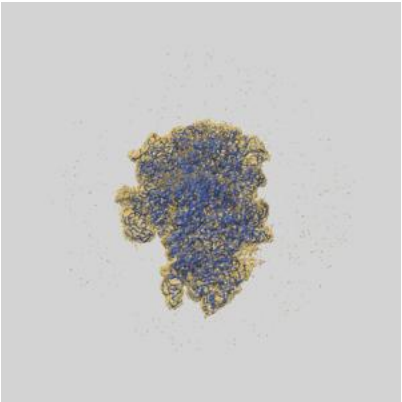
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0659 and PDB model 6O8Z. Per-residue inclusion information can be found in section 3 on page 13.

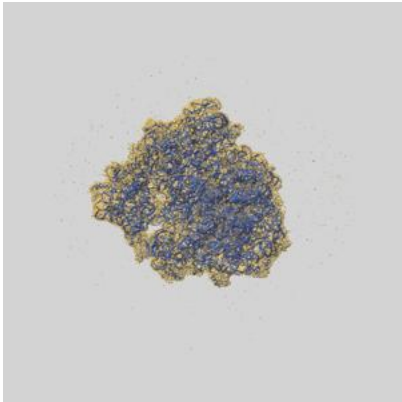
9.1 Map-model overlay (i)



X



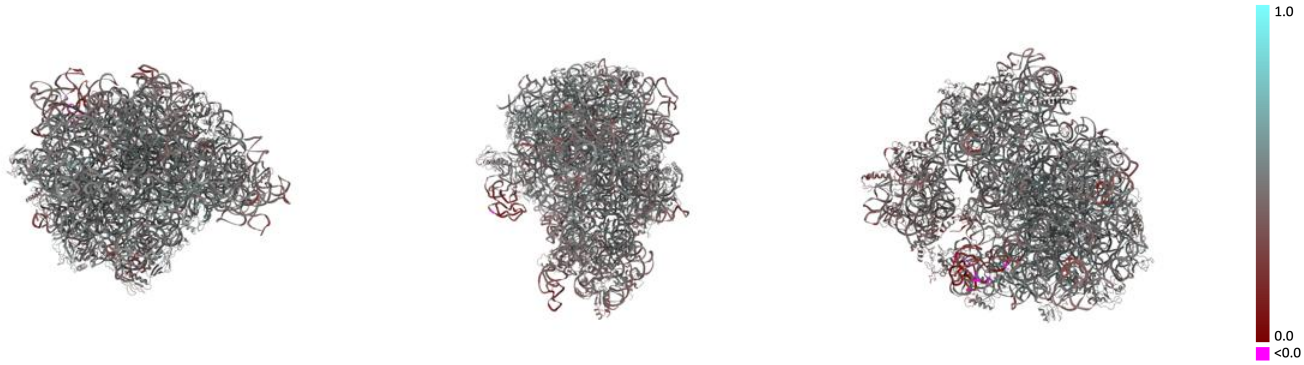
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.238 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

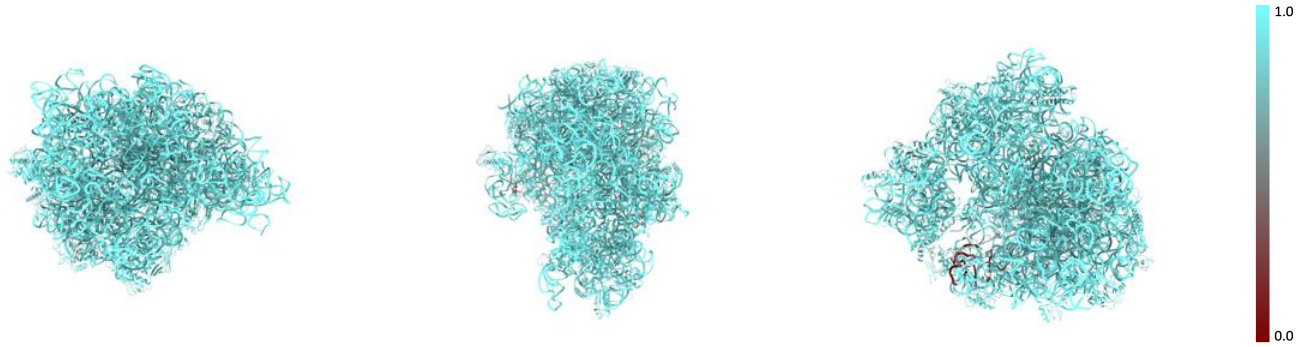
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

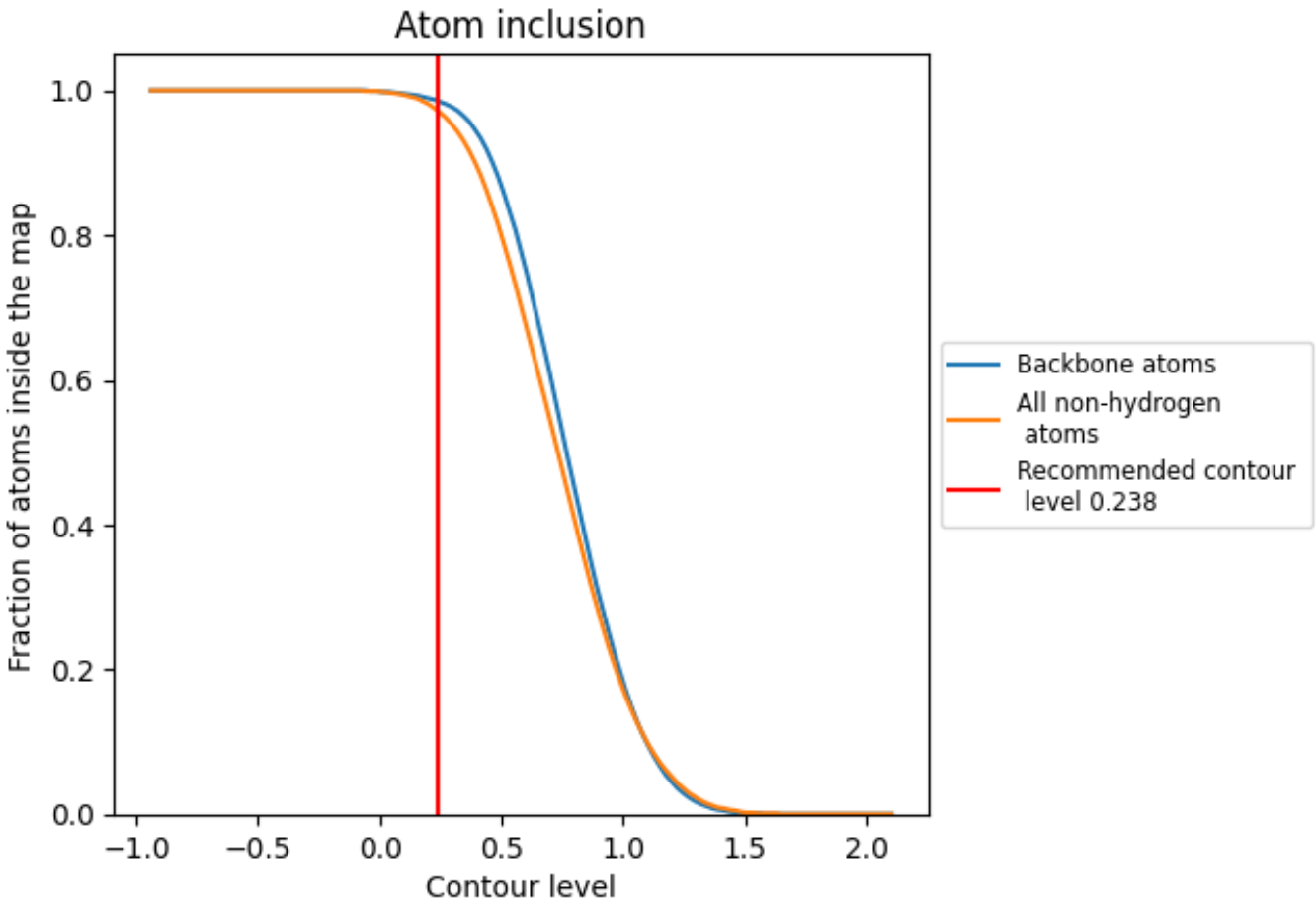
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.238).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.238) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9720	0.4600
0	0.9530	0.5030
1	0.9230	0.3680
2	0.9790	0.5270
3	0.9380	0.5030
4	0.9520	0.5090
5	0.9600	0.5370
6	0.9760	0.5230
A	0.9810	0.4600
B	0.9960	0.4360
C	0.9640	0.5140
D	0.9630	0.5210
E	0.9700	0.4940
F	0.9360	0.4430
G	0.9270	0.4420
K	0.9670	0.5100
L	0.9510	0.5260
M	0.9680	0.5020
N	0.8910	0.4780
O	0.9640	0.5020
P	0.9440	0.4500
Q	0.9680	0.5210
R	0.9470	0.4850
S	0.9340	0.5040
T	0.9680	0.5110
U	0.9570	0.4850
V	0.9250	0.4600
W	0.4090	0.3400
X	0.9530	0.5130
Y	0.9440	0.5060
Z	0.9450	0.4550
a	0.9970	0.4490
c	0.9270	0.4390
d	0.9510	0.4530
e	0.9470	0.4780

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Chain	Atom inclusion	Q-score
f	0.9420	0.4790
g	0.9230	0.4170
h	0.9670	0.4840
i	0.9620	0.4250
j	0.9240	0.4220
k	0.9260	0.4530
l	0.9260	0.4840
m	0.9020	0.3860
n	0.9750	0.4660
o	0.9430	0.4710
p	0.9700	0.4780
q	0.9350	0.4860
r	0.9230	0.4630
s	0.9570	0.4100
t	0.9530	0.4440