



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 01:26 pm GMT

PDB ID : 5MDZ  
EMDB ID : EMD-3493  
Title : Structure of the 70S ribosome (empty A site)  
Authors : James, N.R.; Brown, A.; Gordiyenko, Y.; Ramakrishnan, V.  
Deposited on : 2016-11-13  
Resolution : 3.10 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](mailto: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>.

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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 : 1.8.4, 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

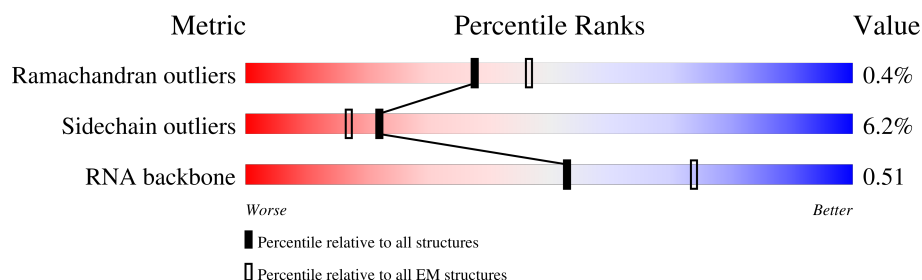
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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.



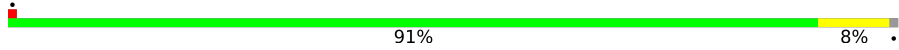
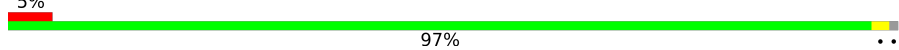
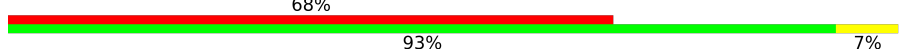


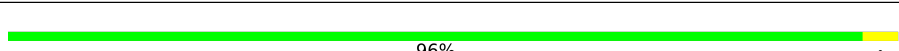
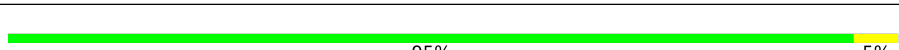
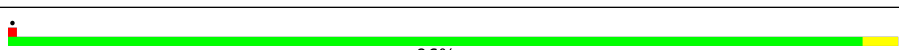
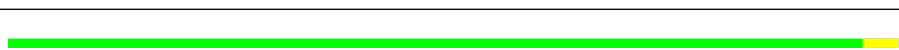
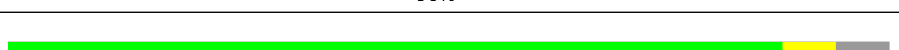
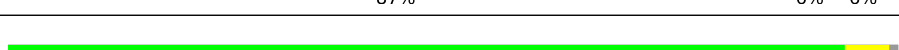
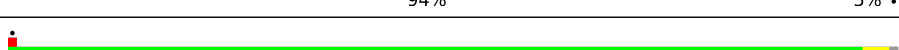
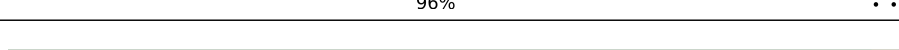
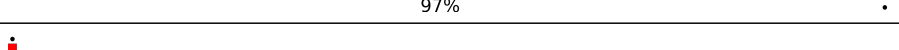
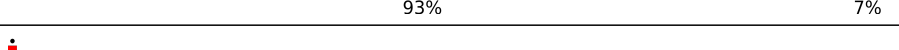
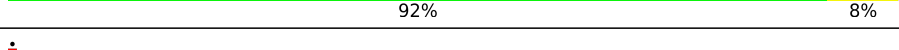

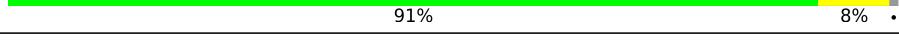
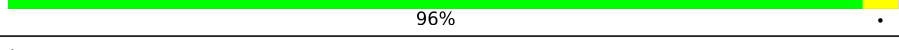

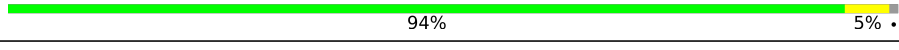
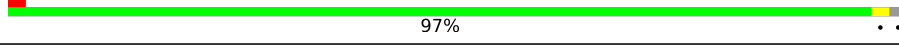
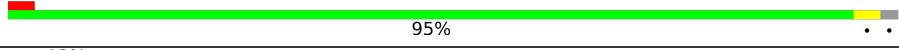


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	1	2904	
2	2	1534	
3	3	120	
4	4	18	
5	5	78	
6	B	273	
7	C	209	
8	D	201	

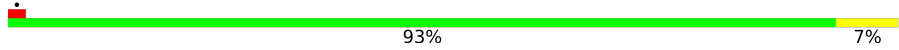
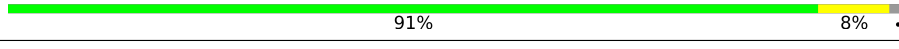
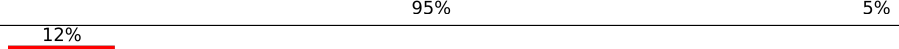
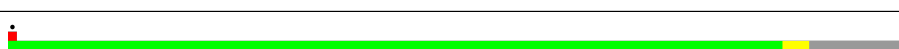
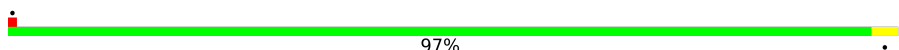


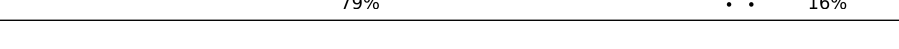



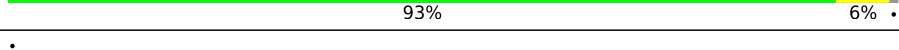
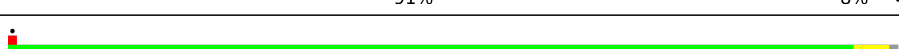
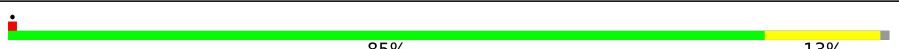
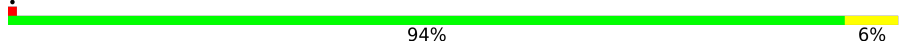
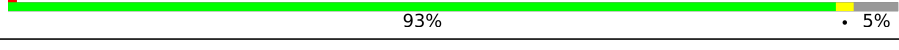
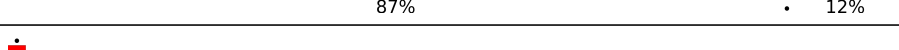

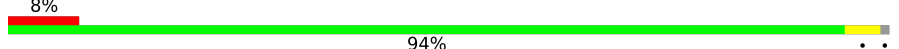




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Mol	Chain	Length	Quality of chain
9	E	179	
10	F	177	
11	G	149	
12	H	165	
13	I	142	
14	J	142	
15	K	123	
16	L	144	
17	M	136	
18	N	127	
19	O	117	
20	P	115	
21	Q	118	
22	R	103	
23	S	110	
24	T	100	
25	U	104	
26	V	94	
27	W	85	
28	X	78	
29	Y	63	
30	Z	59	
31	a	70	
32	b	57	
33	c	55	

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Mol	Chain	Length	Quality of chain
34	d	46	
35	e	65	
36	f	38	
37	g	241	
38	h	233	
39	i	206	
40	j	167	
41	k	135	
42	l	179	
43	m	130	
44	n	130	
45	o	103	
46	p	129	
47	q	124	
48	r	118	
49	s	101	
50	t	89	
51	u	82	
52	v	84	
53	w	75	
54	x	92	
55	y	87	
56	z	71	

## 2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 146639 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	887	A	U	conflict	GB 802133627

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	5	Total	C	N	O	P	0	0
			109	49	22	33	5		

- Molecule 5 is a RNA chain called fMet-NH-tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	5	76	Total	C	N	O	P	S	0	0
			1622	725	292	528	76	1		

- Molecule 6 is a protein called 50S ribosomal protein L2.

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

- Molecule 7 is a protein called 50S ribosomal protein L3.

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

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L5.

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

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 11 is a protein called 50S ribosomal protein L9.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	135	Total	C	N	O	S	0	0
			984	622	171	185	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	103	Total	C	N	O	S	0	0
			788	498	148	142			

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

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

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



Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
33	c	52	Total	C	N	O	0	0
			426	275	78	73		

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

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

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

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

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

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

- Molecule 37 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 38 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 39 is a protein called 30S ribosomal protein S4.

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

- Molecule 40 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 41 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 42 is a protein called 30S ribosomal protein S7.

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

- Molecule 43 is a protein called 30S ribosomal protein S8.

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

- Molecule 44 is a protein called 30S ribosomal protein S9.

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

- Molecule 45 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 46 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 47 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 48 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 49 is a protein called 30S ribosomal protein S14.

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

- Molecule 50 is a protein called 30S ribosomal protein S15.

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

- Molecule 51 is a protein called 30S ribosomal protein S16.

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

- Molecule 52 is a protein called 30S ribosomal protein S17.

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

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 54 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 55 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

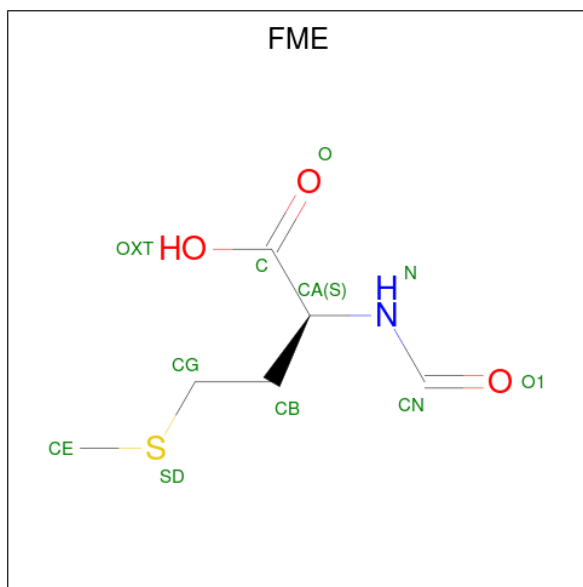
- Molecule 56 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	1	295	Total	Mg	0
			295	295	
57	2	128	Total	Mg	0
			128	128	
57	3	8	Total	Mg	0
			8	8	
57	5	2	Total	Mg	0
			2	2	
57	b	1	Total	Mg	0
			1	1	
57	f	1	Total	Mg	0
			1	1	
57	i	1	Total	Mg	0
			1	1	
57	n	1	Total	Mg	0
			1	1	

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



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

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	a	1	Total	Zn	0
			1	1	
59	f	1	Total	Zn	0
			1	1	

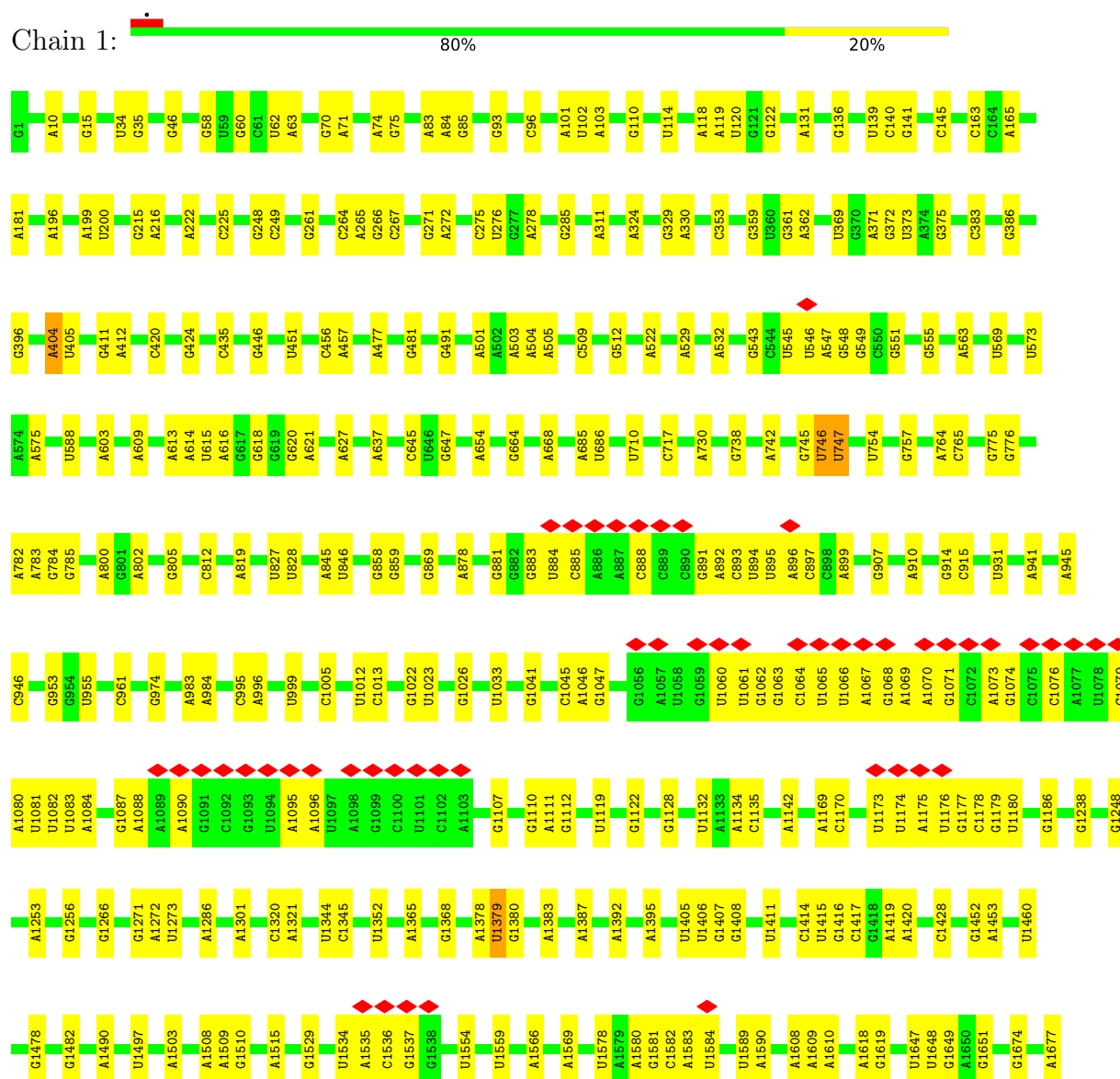
- Molecule 60 is water.

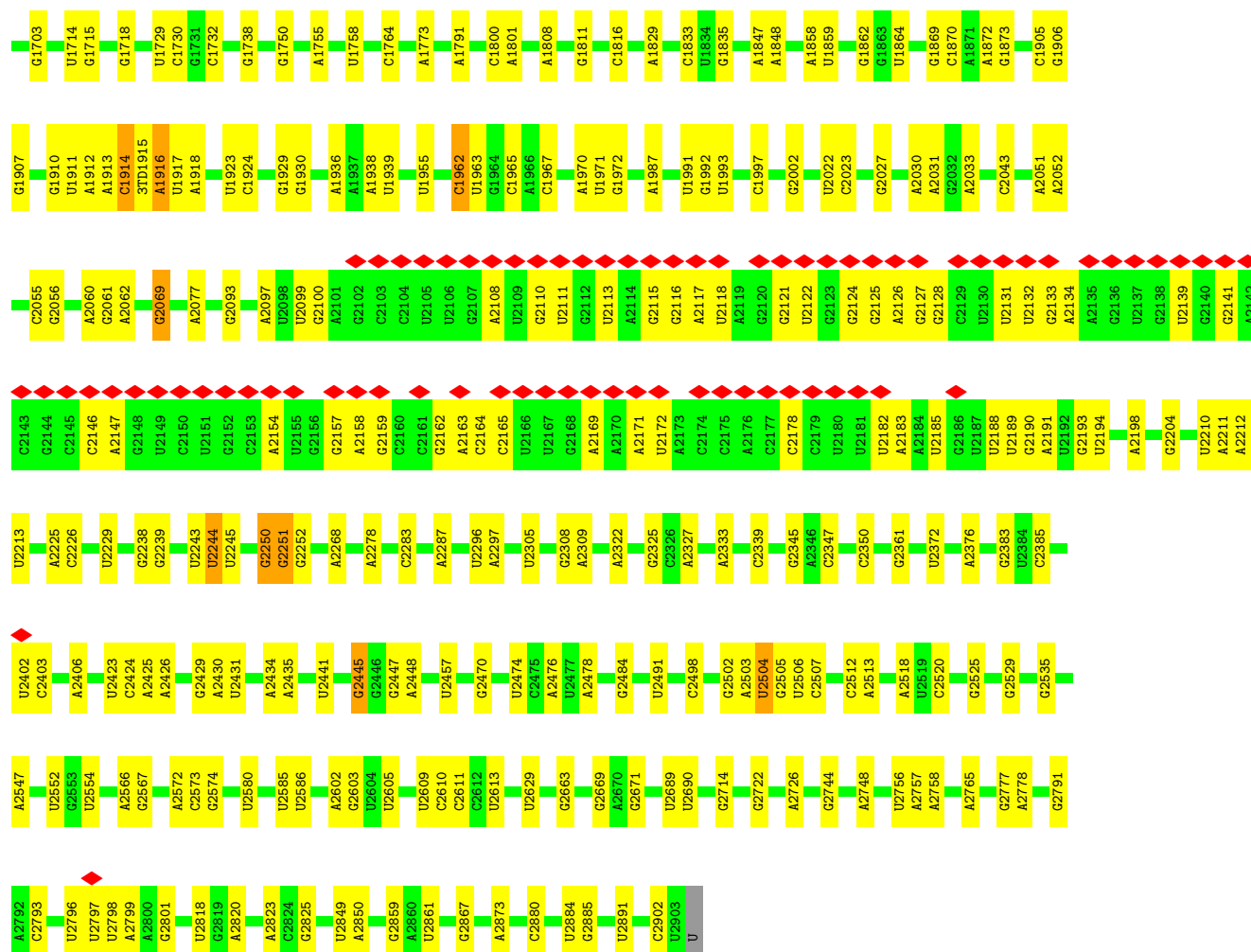
Mol	Chain	Residues	Atoms		AltConf
60	B	2	Total	O	0
			2	2	

### 3 Residue-property plots

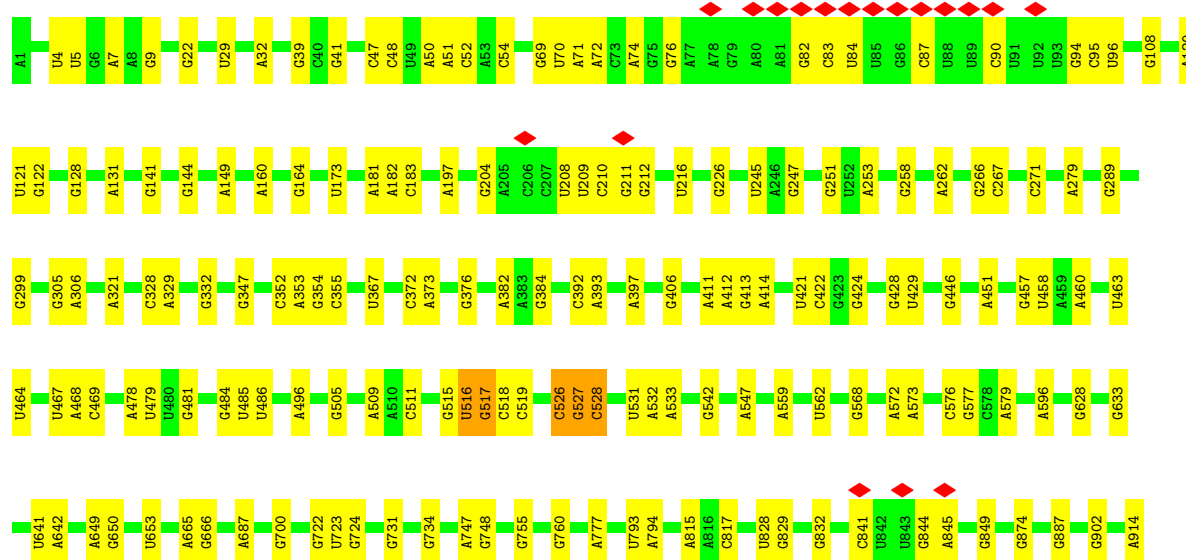
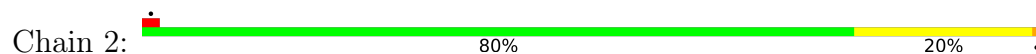
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 23S ribosomal RNA

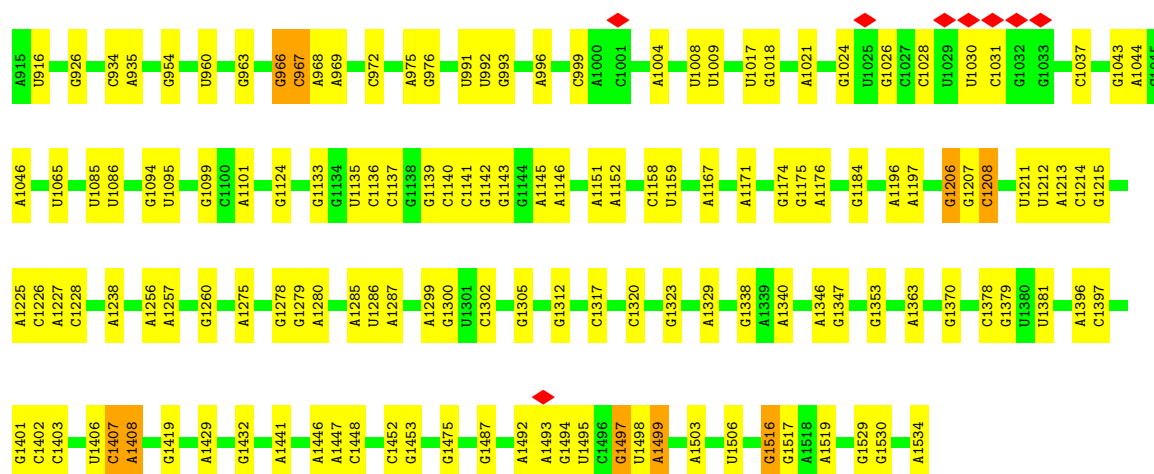




• Molecule 2: 16S ribosomal RNA







• Molecule 3: 5S ribosomal RNA



• Molecule 4: mRNA



• Molecule 5: fMet-NH-tRNA(fMet)



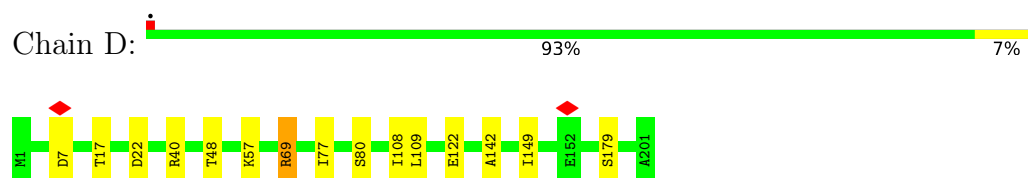
• Molecule 6: 50S ribosomal protein L2



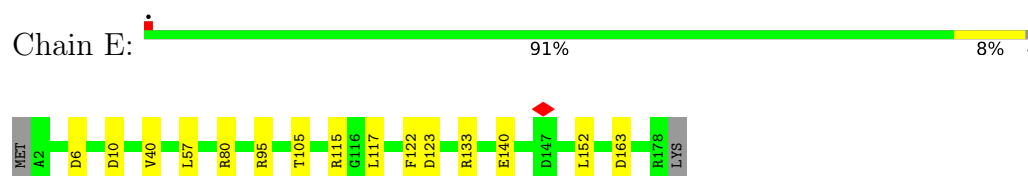
• Molecule 7: 50S ribosomal protein L3



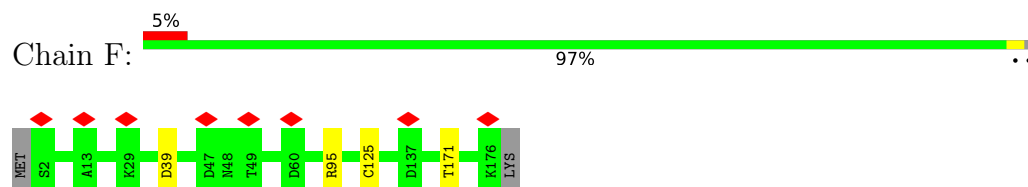
- Molecule 8: 50S ribosomal protein L4



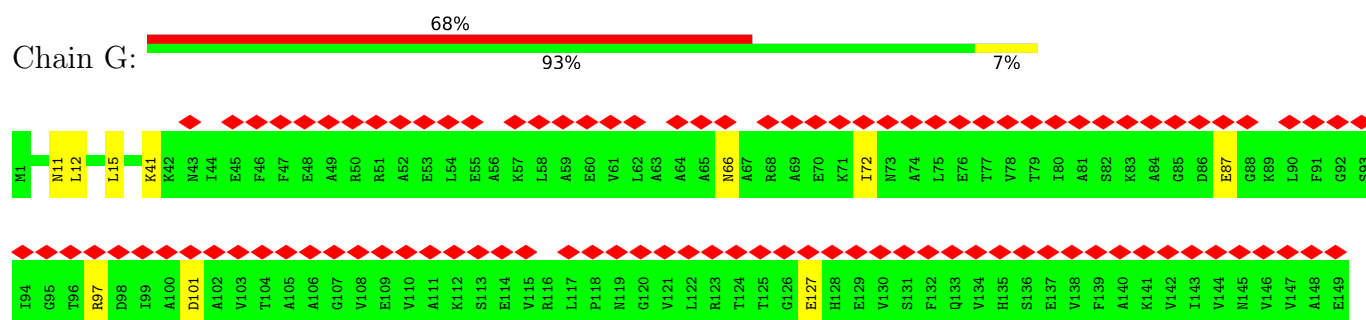
- Molecule 9: 50S ribosomal protein L5



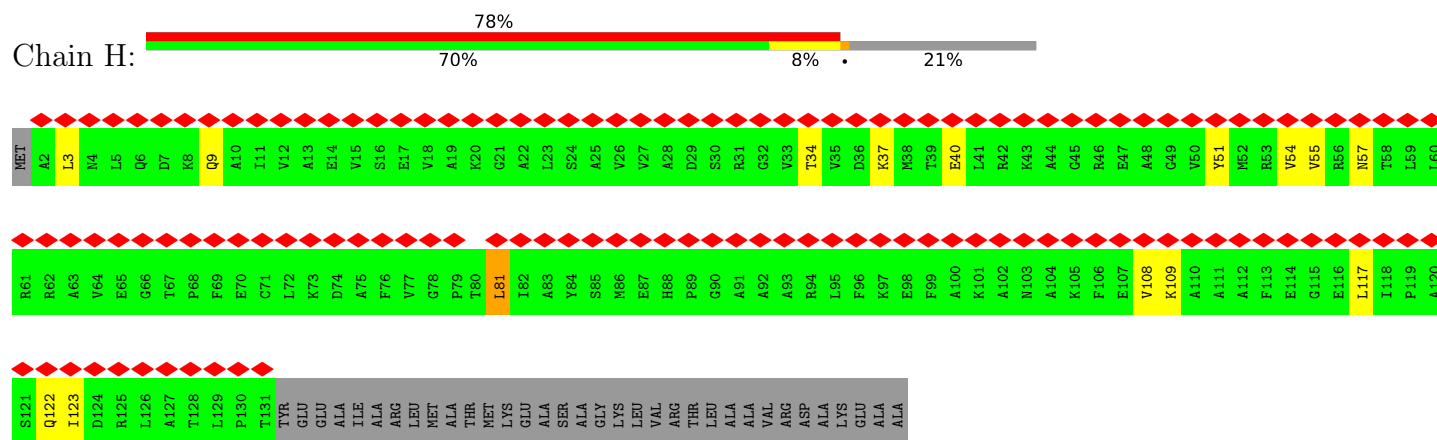
- Molecule 10: 50S ribosomal protein L6



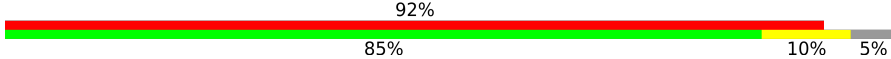
- Molecule 11: 50S ribosomal protein L9



- Molecule 12: 50S ribosomal protein L10



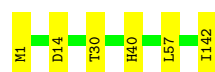
- Molecule 13: 50S ribosomal protein L11

Chain I: 



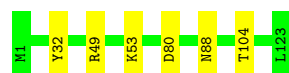
- Molecule 14: 50S ribosomal protein L13

Chain J: 



- Molecule 15: 50S ribosomal protein L14

Chain K: 



- Molecule 16: 50S ribosomal protein L15

Chain L: 




- Molecule 17: 50S ribosomal protein L16

Chain M: 



- Molecule 18: 50S ribosomal protein L17

Chain N: 



- Molecule 19: 50S ribosomal protein L18

Chain O:  94% 5%



- Molecule 20: 50S ribosomal protein L19

Chain P:  96% ..




- Molecule 21: 50S ribosomal protein L20

Chain Q:  97% ..




- Molecule 22: 50S ribosomal protein L21

Chain R:  93% 7%



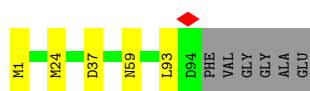
- Molecule 23: 50S ribosomal protein L22

Chain S:  92% 8%




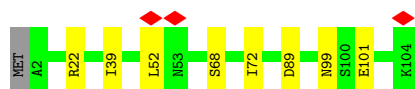
- Molecule 24: 50S ribosomal protein L23

Chain T:  89% 5% 6%



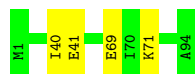
- Molecule 25: 50S ribosomal protein L24

Chain U:  91% 8%




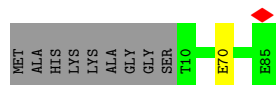
- Molecule 26: 50S ribosomal protein L25

Chain V:  96% .



- Molecule 27: 50S ribosomal protein L27

Chain W:  88% . 11%



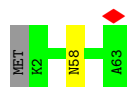
- Molecule 28: 50S ribosomal protein L28

Chain X:  94% 5% .



- Molecule 29: 50S ribosomal protein L29

Chain Y:  97% . .




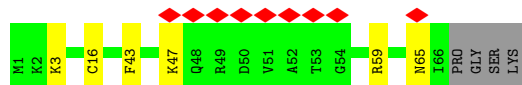
- Molecule 30: 50S ribosomal protein L30

Chain Z:  95% . .




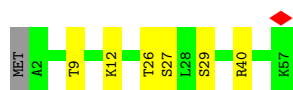
- Molecule 31: 50S ribosomal protein L31

Chain a:  13% 86% 9% 6%

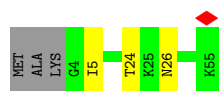
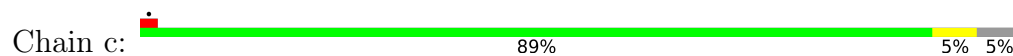


- Molecule 32: 50S ribosomal protein L32

Chain b:  88% 11% .



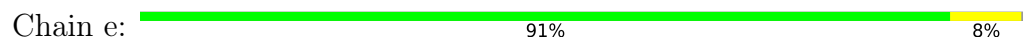
- Molecule 33: 50S ribosomal protein L33



- Molecule 34: 50S ribosomal protein L34



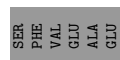
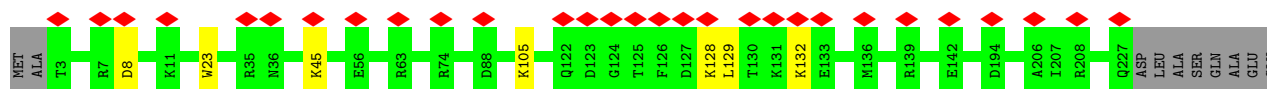
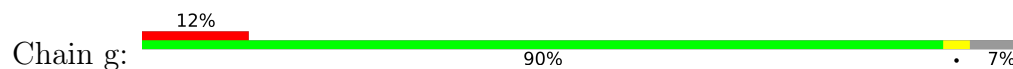
- Molecule 35: 50S ribosomal protein L35



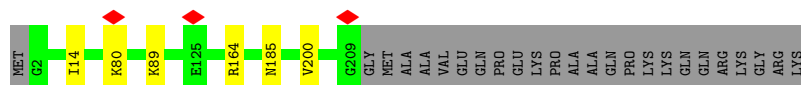
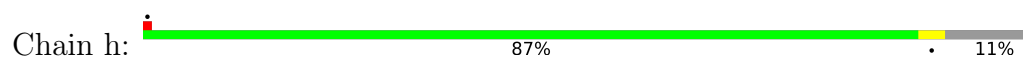
- Molecule 36: 50S ribosomal protein L36



- Molecule 37: 30S ribosomal protein S2



- Molecule 38: 30S ribosomal protein S3




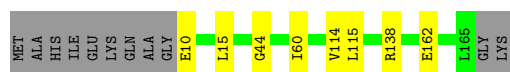
- Molecule 39: 30S ribosomal protein S4

Chain i:  97%



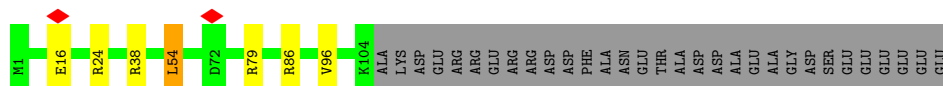
- Molecule 40: 30S ribosomal protein S5

Chain j:  89% 5% 7%




- Molecule 41: 30S ribosomal protein S6

Chain k:  72% 23%



- Molecule 42: 30S ribosomal protein S7

Chain l:  79% 16%



- Molecule 43: 30S ribosomal protein S8

Chain m:  97%




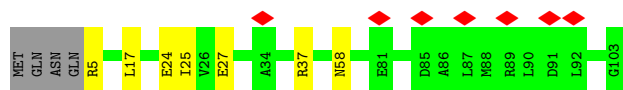
- Molecule 44: 30S ribosomal protein S9

Chain n:  93% 5%

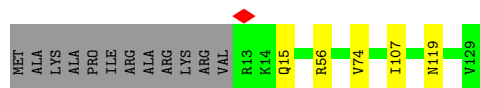
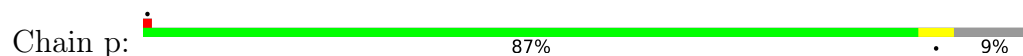


- Molecule 45: 30S ribosomal protein S10

Chain o:  7% 89% 7%



- Molecule 46: 30S ribosomal protein S11



- Molecule 47: 30S ribosomal protein S12



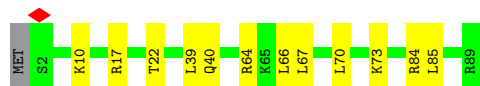
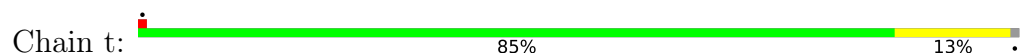
- Molecule 48: 30S ribosomal protein S13



- Molecule 49: 30S ribosomal protein S14



- Molecule 50: 30S ribosomal protein S15




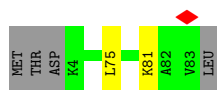
- Molecule 51: 30S ribosomal protein S16




- Molecule 52: 30S ribosomal protein S17



Chain v:  93% 5%




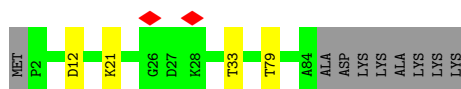
- Molecule 53: 30S ribosomal protein S18

Chain w:  87% 12%




- Molecule 54: 30S ribosomal protein S19

Chain x:  86% 10%



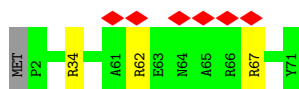
- Molecule 55: 30S ribosomal protein S20

Chain y:  93% 6%



- Molecule 56: 30S ribosomal protein S21

Chain z:  8% 94% 2%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140027	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 ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	134615	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.942	Depositor
Minimum map value	-0.531	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0TD, FME, UR3, 7MG, 6MZ, ZN, OMC, 1MG, PSU, H2U, 5MU, 2MG, 3TD, 5MC, MA6, OMG, G7M, MG, 4SU, OMU, 4OC, 2MA, 8AN

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	1	0.36	0/69284	0.72	18/108079 (0.0%)
2	2	0.28	0/36583	0.71	15/57046 (0.0%)
3	3	0.26	0/2872	0.69	0/4478
4	4	0.35	0/122	0.59	0/188
5	5	0.27	0/1672	0.77	2/2603 (0.1%)
6	B	0.39	0/2121	0.77	0/2852
7	C	0.43	0/1586	0.70	0/2134
8	D	0.45	0/1571	0.77	2/2113 (0.1%)
9	E	0.44	0/1434	0.77	0/1926
10	F	0.39	0/1333	0.67	0/1805
11	G	0.43	0/1122	0.69	0/1515
12	H	0.49	0/993	0.80	1/1340 (0.1%)
13	I	0.45	0/998	0.69	0/1348
14	J	0.49	0/1152	0.75	0/1551
15	K	0.41	0/955	0.77	0/1279
16	L	0.40	0/1062	0.76	0/1413
17	M	0.46	0/1093	0.81	0/1460
18	N	0.51	0/964	0.87	0/1289
19	O	0.46	0/902	0.81	0/1209
20	P	0.41	0/929	0.72	0/1242
21	Q	0.59	0/960	0.91	0/1278
22	R	0.37	0/829	0.66	0/1107
23	S	0.48	0/864	0.82	0/1156
24	T	0.41	0/752	0.71	0/1005
25	U	0.34	0/796	0.67	2/1062 (0.2%)
26	V	0.40	0/766	0.67	0/1025
27	W	0.38	0/589	0.71	0/779
28	X	0.48	0/635	0.81	1/848 (0.1%)
29	Y	0.53	0/502	0.82	0/667
30	Z	0.44	0/452	0.77	0/605
31	a	0.42	0/531	0.68	0/709

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	b	0.40	0/450	0.79	0/599
33	c	0.34	0/433	0.64	0/576
34	d	0.52	0/380	0.98	0/498
35	e	0.45	0/513	0.82	0/676
36	f	0.37	0/303	0.78	0/397
37	g	0.47	0/1791	0.71	0/2413
38	h	0.43	0/1663	0.71	0/2241
39	i	0.46	0/1665	0.73	0/2227
40	j	0.45	0/1165	0.75	0/1568
41	k	0.43	0/867	0.75	1/1171 (0.1%)
42	l	0.50	0/1195	0.81	0/1602
43	m	0.41	0/989	0.69	0/1326
44	n	0.42	0/1034	0.75	0/1375
45	o	0.39	0/800	0.75	0/1082
46	p	0.40	0/893	0.69	0/1205
47	q	0.35	0/960	0.74	0/1286
48	r	0.47	0/909	0.82	0/1215
49	s	0.49	0/817	0.78	0/1088
50	t	0.53	0/722	0.85	0/964
51	u	0.44	0/659	0.77	0/884
52	v	0.33	0/657	0.62	0/881
53	w	0.45	0/553	0.77	0/743
54	x	0.38	0/680	0.62	0/915
55	y	0.57	0/675	0.85	0/895
56	z	0.55	0/597	0.88	0/792
All	All	0.37	0/157794	0.73	42/235730 (0.0%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	516	PSU	P-O3'-C3'	14.64	137.27	119.70
1	1	2252	G	N9-C1'-C2'	-10.99	99.72	114.00
2	2	1401	G	N9-C1'-C2'	-10.73	100.05	114.00
5	5	20	H2U	P-O3'-C3'	10.49	132.29	119.70
2	2	528	C	N1-C1'-C2'	-10.28	100.64	114.00
2	2	1499	A	N9-C1'-C2'	-10.26	100.66	114.00
2	2	526	C	N1-C1'-C2'	-8.77	102.35	112.00
2	2	1208	C	N1-C1'-C2'	-8.58	102.56	112.00
2	2	1206	G	N9-C1'-C2'	-8.43	102.73	112.00
2	2	1406	U	N1-C1'-C2'	-7.83	103.38	112.00
5	5	20	H2U	O3'-P-O5'	7.39	118.03	104.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1206	G	C4'-C3'-O3'	7.17	127.35	113.00
1	1	2245	U	N1-C1'-C2'	-7.11	104.17	112.00
1	1	1910	G	N9-C1'-C2'	-6.73	104.59	112.00
2	2	1403	C	N1-C1'-C2'	-6.67	104.66	112.00
2	2	1401	G	C4'-C3'-O3'	6.61	126.22	113.00
1	1	1914	C	C4'-C3'-O3'	6.60	126.21	113.00
1	1	2250	G	C4'-C3'-O3'	-6.60	95.54	109.40
1	1	1379	U	C2'-C3'-O3'	6.57	124.21	113.70
1	1	2243	U	N1-C1'-C2'	-6.57	104.78	112.00
2	2	1408	A	N9-C1'-C2'	-6.49	104.86	112.00
2	2	515	G	N9-C1'-C2'	-6.44	104.92	112.00
2	2	1497	G	N9-C1'-C2'	-6.31	105.06	112.00
12	H	81	LEU	CA-CB-CG	6.10	129.33	115.30
1	1	754	U	N1-C1'-C2'	5.88	121.65	114.00
2	2	517	G	C5'-C4'-C3'	5.67	125.07	116.00
1	1	2244	U	C1'-C2'-O2'	-5.60	93.81	110.60
41	k	54	LEU	CA-CB-CG	5.58	128.14	115.30
25	U	22	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	1	783	A	C4'-C3'-O3'	5.50	123.99	113.00
25	U	22	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	1	1914	C	C3'-C2'-C1'	5.30	105.74	101.50
28	X	28	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	1	742	A	C8-N9-C1'	-5.19	118.36	127.70
1	1	404	A	C2'-C3'-O3'	5.18	121.98	113.70
8	D	69	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	1	2244	U	C4'-C3'-O3'	5.17	123.34	113.00
1	1	2252	G	C4'-C3'-O3'	5.12	123.23	113.00
1	1	1916	A	N9-C1'-C2'	-5.09	106.40	112.00
8	D	69	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	1	742	A	C4-N9-C1'	5.08	135.45	126.30
1	1	2243	U	C4'-C3'-O3'	5.08	123.15	113.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	
6	B	269/273 (98%)	259 (96%)	9 (3%)	1 (0%)	34	69
7	C	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
8	D	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	29	64
9	E	175/179 (98%)	164 (94%)	10 (6%)	1 (1%)	25	59
10	F	173/177 (98%)	161 (93%)	12 (7%)	0	100	100
11	G	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
12	H	128/165 (78%)	106 (83%)	18 (14%)	4 (3%)	4	23
13	I	133/142 (94%)	119 (90%)	13 (10%)	1 (1%)	19	54
14	J	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
15	K	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
16	L	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
17	M	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
18	N	117/127 (92%)	107 (92%)	10 (8%)	0	100	100
19	O	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
20	P	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
21	Q	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17	52
22	R	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	15	49
23	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
24	T	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
25	U	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	15	49
26	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
27	W	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
28	X	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
29	Y	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
30	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	a	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
32	b	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
33	c	50/55 (91%)	50 (100%)	0	0	100	100
34	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
35	e	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
36	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
37	g	223/241 (92%)	210 (94%)	13 (6%)	0	100	100
38	h	206/233 (88%)	196 (95%)	9 (4%)	1 (0%)	29	64
39	i	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
40	j	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	25	59
41	k	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	15	49
42	l	149/179 (83%)	144 (97%)	4 (3%)	1 (1%)	22	57
43	m	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	19	54
44	n	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	19	54
45	o	97/103 (94%)	89 (92%)	7 (7%)	1 (1%)	15	49
46	p	115/129 (89%)	104 (90%)	9 (8%)	2 (2%)	9	36
47	q	120/124 (97%)	119 (99%)	1 (1%)	0	100	100
48	r	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
49	s	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
50	t	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
51	u	80/82 (98%)	75 (94%)	4 (5%)	1 (1%)	12	42
52	v	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
53	w	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
54	x	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
55	y	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
56	z	68/71 (96%)	68 (100%)	0	0	100	100
All	All	5869/6220 (94%)	5572 (95%)	276 (5%)	21 (0%)	38	69

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	n	56	ASP
6	B	158	ALA

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Mol	Chain	Res	Type
8	D	142	ALA
12	H	51	TYR
12	H	117	LEU
21	Q	3	ARG
42	l	130	ASN
45	o	58	ASN
46	p	119	ASN
9	E	40	VAL
38	h	80	LYS
25	U	39	ILE
12	H	108	VAL
41	k	96	VAL
22	R	44	GLY
40	j	44	GLY
13	I	136	GLY
46	p	74	VAL
51	u	64	GLY
12	H	55	VAL
43	m	75	ILE

### 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	
6	B	216/218 (99%)	199 (92%)	17 (8%)	12	40
7	C	164/164 (100%)	157 (96%)	7 (4%)	29	62
8	D	165/165 (100%)	151 (92%)	14 (8%)	10	37
9	E	148/150 (99%)	134 (90%)	14 (10%)	8	31
10	F	136/138 (99%)	132 (97%)	4 (3%)	42	72
11	G	114/114 (100%)	104 (91%)	10 (9%)	10	36
12	H	99/123 (80%)	88 (89%)	11 (11%)	6	24
13	I	104/110 (94%)	91 (88%)	13 (12%)	4	18
14	J	116/116 (100%)	110 (95%)	6 (5%)	23	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	K	104/104 (100%)	98 (94%)	6 (6%)	20	51
16	L	103/103 (100%)	97 (94%)	6 (6%)	20	51
17	M	109/109 (100%)	104 (95%)	5 (5%)	27	59
18	N	99/103 (96%)	91 (92%)	8 (8%)	11	39
19	O	86/87 (99%)	80 (93%)	6 (7%)	15	45
20	P	99/100 (99%)	95 (96%)	4 (4%)	31	65
21	Q	89/90 (99%)	87 (98%)	2 (2%)	52	78
22	R	84/84 (100%)	78 (93%)	6 (7%)	14	44
23	S	93/93 (100%)	84 (90%)	9 (10%)	8	30
24	T	81/84 (96%)	76 (94%)	5 (6%)	18	49
25	U	84/85 (99%)	78 (93%)	6 (7%)	14	44
26	V	78/78 (100%)	74 (95%)	4 (5%)	24	56
27	W	58/63 (92%)	57 (98%)	1 (2%)	60	83
28	X	67/68 (98%)	64 (96%)	3 (4%)	27	60
29	Y	54/55 (98%)	53 (98%)	1 (2%)	57	81
30	Z	48/49 (98%)	46 (96%)	2 (4%)	30	62
31	a	59/62 (95%)	53 (90%)	6 (10%)	7	27
32	b	47/48 (98%)	41 (87%)	6 (13%)	4	18
33	c	47/49 (96%)	44 (94%)	3 (6%)	17	48
34	d	38/38 (100%)	35 (92%)	3 (8%)	12	40
35	e	51/52 (98%)	46 (90%)	5 (10%)	8	29
36	f	34/34 (100%)	32 (94%)	2 (6%)	19	50
37	g	187/199 (94%)	180 (96%)	7 (4%)	34	66
38	h	171/190 (90%)	166 (97%)	5 (3%)	42	72
39	i	172/173 (99%)	166 (96%)	6 (4%)	36	68
40	j	119/126 (94%)	112 (94%)	7 (6%)	19	50
41	k	91/116 (78%)	85 (93%)	6 (7%)	16	47
42	l	124/147 (84%)	115 (93%)	9 (7%)	14	43
43	m	104/105 (99%)	102 (98%)	2 (2%)	57	81
44	n	105/107 (98%)	100 (95%)	5 (5%)	25	58
45	o	86/90 (96%)	80 (93%)	6 (7%)	15	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	p	90/99 (91%)	87 (97%)	3 (3%)	38	69
47	q	102/103 (99%)	95 (93%)	7 (7%)	15	45
48	r	94/96 (98%)	85 (90%)	9 (10%)	8	31
49	s	83/84 (99%)	79 (95%)	4 (5%)	25	58
50	t	76/77 (99%)	64 (84%)	12 (16%)	2	11
51	u	65/65 (100%)	61 (94%)	4 (6%)	18	49
52	v	74/78 (95%)	72 (97%)	2 (3%)	44	74
53	w	57/65 (88%)	56 (98%)	1 (2%)	59	82
54	x	72/79 (91%)	68 (94%)	4 (6%)	21	52
55	y	65/66 (98%)	60 (92%)	5 (8%)	13	41
56	z	60/61 (98%)	57 (95%)	3 (5%)	24	57
All	All	4871/5062 (96%)	4569 (94%)	302 (6%)	22	49

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	51	THR
6	B	52	ARG
6	B	118	SER
6	B	125	LYS
6	B	130	LEU
6	B	141	VAL
6	B	156	ARG
6	B	187	ASP
6	B	189	ARG
6	B	195	VAL
6	B	202	LEU
6	B	203	ARG
6	B	204	VAL
6	B	205	LEU
6	B	242	LYS
6	B	258	ARG
6	B	271	ARG
7	C	13	ARG
7	C	18	ASP
7	C	32	ASN
7	C	46	ARG
7	C	91	THR

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Mol	Chain	Res	Type
7	C	103	ASP
7	C	131	ASP
8	D	7	ASP
8	D	17	THR
8	D	22	ASP
8	D	40	ARG
8	D	48	THR
8	D	57	LYS
8	D	69	ARG
8	D	77	ILE
8	D	80	SER
8	D	108	ILE
8	D	109	LEU
8	D	122	GLU
8	D	149	ILE
8	D	179	SER
9	E	6	ASP
9	E	10	ASP
9	E	57	LEU
9	E	80	ARG
9	E	95	ARG
9	E	105	THR
9	E	115	ARG
9	E	117	LEU
9	E	122	PHE
9	E	123	ASP
9	E	133	ARG
9	E	140	GLU
9	E	152	LEU
9	E	163	ASP
10	F	39	ASP
10	F	95	ARG
10	F	125	CYS
10	F	171	THR
11	G	11	ASN
11	G	12	LEU
11	G	15	LEU
11	G	41	LYS
11	G	66	ASN
11	G	72	ILE
11	G	87	GLU
11	G	97	ARG

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Mol	Chain	Res	Type
11	G	101	ASP
11	G	127	GLU
12	H	3	LEU
12	H	9	GLN
12	H	34	THR
12	H	37	LYS
12	H	40	GLU
12	H	54	VAL
12	H	57	ASN
12	H	81	LEU
12	H	109	LYS
12	H	122	GLN
12	H	123	ILE
13	I	10	LEU
13	I	11	GLN
13	I	38	CYS
13	I	42	ASN
13	I	46	ASP
13	I	48	ILE
13	I	67	THR
13	I	78	LEU
13	I	79	LEU
13	I	81	LYS
13	I	91	LYS
13	I	95	ASP
13	I	111	THR
14	J	1	MET
14	J	14	ASP
14	J	30	THR
14	J	40	HIS
14	J	57	LEU
14	J	142	ILE
15	K	32	TYR
15	K	49	ARG
15	K	53	LYS
15	K	80	ASP
15	K	88	ASN
15	K	104	THR
16	L	5	THR
16	L	27	LEU
16	L	48	ARG
16	L	59	ARG

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Mol	Chain	Res	Type
16	L	76	GLU
16	L	78	ARG
17	M	18	ARG
17	M	84	LYS
17	M	110	GLU
17	M	126	ILE
17	M	128	THR
18	N	2	ARG
18	N	20	MET
18	N	24	MET
18	N	51	LEU
18	N	63	ARG
18	N	65	LEU
18	N	69	ARG
18	N	95	THR
19	O	13	ARG
19	O	19	GLN
19	O	31	THR
19	O	47	VAL
19	O	48	LEU
19	O	91	SER
20	P	10	GLN
20	P	27	GLU
20	P	85	SER
20	P	114	LEU
21	Q	18	LEU
21	Q	51	ARG
22	R	10	LYS
22	R	13	ARG
22	R	48	LYS
22	R	51	VAL
22	R	68	ARG
22	R	86	GLN
23	S	7	HIS
23	S	19	LEU
23	S	30	SER
23	S	41	LYS
23	S	69	LEU
23	S	97	LEU
23	S	107	VAL
23	S	109	ASP
23	S	110	ARG

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Mol	Chain	Res	Type
24	T	1	MET
24	T	24	MET
24	T	37	ASP
24	T	59	ASN
24	T	93	LEU
25	U	52	LEU
25	U	68	SER
25	U	72	ILE
25	U	89	ASP
25	U	99	ASN
25	U	101	GLU
26	V	40	ILE
26	V	41	GLU
26	V	69	GLU
26	V	71	LYS
27	W	70	GLU
28	X	48	THR
28	X	54	LYS
28	X	71	LEU
29	Y	58	ASN
30	Z	3	LYS
30	Z	45	ARG
31	a	3	LYS
31	a	16	CYS
31	a	43	PHE
31	a	47	LYS
31	a	59	ARG
31	a	65	ASN
32	b	9	THR
32	b	12	LYS
32	b	26	THR
32	b	27	SER
32	b	29	SER
32	b	40	ARG
33	c	5	ILE
33	c	24	THR
33	c	26	ASN
34	d	22	MET
34	d	41	ARG
34	d	42	LEU
35	e	8	ARG
35	e	30	ARG

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Mol	Chain	Res	Type
35	e	31	HIS
35	e	54	ASP
35	e	55	LEU
36	f	3	VAL
36	f	26	ILE
37	g	8	ASP
37	g	23	TRP
37	g	45	LYS
37	g	105	LYS
37	g	128	LYS
37	g	129	LEU
37	g	132	LYS
38	h	14	ILE
38	h	89	LYS
38	h	164	ARG
38	h	185	ASN
38	h	200	VAL
39	i	47	ARG
39	i	95	GLU
39	i	104	ARG
39	i	116	GLN
39	i	138	SER
39	i	143	VAL
40	j	10	GLU
40	j	15	LEU
40	j	60	ILE
40	j	114	VAL
40	j	115	LEU
40	j	138	ARG
40	j	162	GLU
41	k	16	GLU
41	k	24	ARG
41	k	38	ARG
41	k	54	LEU
41	k	79	ARG
41	k	86	ARG
42	l	7	ILE
42	l	17	LYS
42	l	21	GLU
42	l	23	LEU
42	l	79	ARG
42	l	97	ASN

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Mol	Chain	Res	Type
42	l	109	ARG
42	l	130	ASN
42	l	146	GLU
43	m	96	MET
43	m	121	LEU
44	n	12	ARG
44	n	27	LYS
44	n	60	LYS
44	n	63	LEU
44	n	118	LEU
45	o	5	ARG
45	o	17	LEU
45	o	24	GLU
45	o	25	ILE
45	o	27	GLU
45	o	37	ARG
46	p	15	GLN
46	p	56	ARG
46	p	107	ILE
47	q	5	ASN
47	q	12	ARG
47	q	24	LEU
47	q	56	ARG
47	q	62	GLU
47	q	74	LEU
47	q	102	LEU
48	r	11	ASP
48	r	16	VAL
48	r	25	VAL
48	r	29	ARG
48	r	59	GLU
48	r	92	ARG
48	r	93	ARG
48	r	104	THR
48	r	117	LYS
49	s	45	VAL
49	s	46	LEU
49	s	89	MET
49	s	92	GLU
50	t	10	LYS
50	t	17	ARG
50	t	22	THR

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Mol	Chain	Res	Type
50	t	39	LEU
50	t	40	GLN
50	t	64	ARG
50	t	66	LEU
50	t	67	LEU
50	t	70	LEU
50	t	73	LYS
50	t	84	ARG
50	t	85	LEU
51	u	1	MET
51	u	2	VAL
51	u	6	LEU
51	u	19	VAL
52	v	75	LEU
52	v	81	LYS
53	w	74	HIS
54	x	12	ASP
54	x	21	LYS
54	x	33	THR
54	x	79	THR
55	y	6	SER
55	y	10	ARG
55	y	48	GLN
55	y	54	MET
55	y	64	LYS
56	z	34	ARG
56	z	62	ARG
56	z	67	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2896/2904 (99%)	538 (18%)	81 (2%)
2	2	1522/1534 (99%)	292 (19%)	38 (2%)
3	3	119/120 (99%)	17 (14%)	0
4	4	4/18 (22%)	1 (25%)	0
5	5	73/78 (93%)	23 (31%)	8 (10%)
All	All	4614/4654 (99%)	871 (18%)	127 (2%)

All (871) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	34	U
1	1	35	G
1	1	46	G
1	1	58	G
1	1	60	G
1	1	63	A
1	1	71	A
1	1	74	A
1	1	75	G
1	1	83	A
1	1	84	A
1	1	85	G
1	1	93	G
1	1	96	C
1	1	102	U
1	1	103	A
1	1	110	G
1	1	114	U
1	1	118	A
1	1	119	A
1	1	120	U
1	1	122	G
1	1	131	A
1	1	136	G
1	1	139	U
1	1	140	C
1	1	141	G
1	1	145	C
1	1	163	C
1	1	165	A
1	1	181	A
1	1	196	A
1	1	200	U
1	1	215	G
1	1	216	A
1	1	222	A
1	1	225	C
1	1	248	G
1	1	249	C
1	1	261	G

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Mol	Chain	Res	Type
1	1	264	C
1	1	265	A
1	1	266	G
1	1	267	C
1	1	271	G
1	1	272	A
1	1	275	C
1	1	276	U
1	1	278	A
1	1	285	G
1	1	311	A
1	1	324	A
1	1	329	G
1	1	330	A
1	1	353	C
1	1	359	G
1	1	361	G
1	1	362	A
1	1	371	A
1	1	372	G
1	1	373	U
1	1	375	G
1	1	383	C
1	1	386	G
1	1	396	G
1	1	405	U
1	1	411	G
1	1	412	A
1	1	420	C
1	1	424	G
1	1	435	C
1	1	451	U
1	1	456	C
1	1	457	A
1	1	477	A
1	1	481	G
1	1	491	G
1	1	501	A
1	1	503	A
1	1	504	A
1	1	505	A
1	1	509	C

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Mol	Chain	Res	Type
1	1	522	A
1	1	529	A
1	1	532	A
1	1	543	G
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	551	G
1	1	563	A
1	1	569	U
1	1	573	U
1	1	575	A
1	1	588	U
1	1	603	A
1	1	609	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	618	G
1	1	621	A
1	1	627	A
1	1	637	A
1	1	645	C
1	1	647	G
1	1	654	A
1	1	664	G
1	1	668	A
1	1	685	A
1	1	686	U
1	1	710	U
1	1	717	C
1	1	730	A
1	1	738	G
1	1	746	PSU
1	1	747	5MU
1	1	757	G
1	1	764	A
1	1	765	C
1	1	775	G
1	1	776	G

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Mol	Chain	Res	Type
1	1	782	A
1	1	784	G
1	1	785	G
1	1	800	A
1	1	802	A
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	845	A
1	1	846	U
1	1	858	G
1	1	859	G
1	1	869	G
1	1	878	A
1	1	881	G
1	1	884	U
1	1	885	C
1	1	888	C
1	1	891	G
1	1	892	A
1	1	893	C
1	1	895	U
1	1	896	A
1	1	897	C
1	1	899	A
1	1	907	G
1	1	910	A
1	1	914	G
1	1	915	C
1	1	931	U
1	1	941	A
1	1	945	A
1	1	946	C
1	1	953	G
1	1	961	C
1	1	974	G
1	1	983	A
1	1	995	C
1	1	996	A
1	1	999	U

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Mol	Chain	Res	Type
1	1	1005	C
1	1	1012	U
1	1	1013	C
1	1	1022	G
1	1	1023	U
1	1	1026	G
1	1	1033	U
1	1	1041	G
1	1	1045	C
1	1	1046	A
1	1	1047	G
1	1	1060	U
1	1	1061	U
1	1	1062	G
1	1	1063	G
1	1	1064	C
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1069	A
1	1	1070	A
1	1	1071	G
1	1	1073	A
1	1	1074	G
1	1	1076	C
1	1	1079	C
1	1	1080	A
1	1	1081	U
1	1	1082	U
1	1	1083	U
1	1	1084	A
1	1	1087	G
1	1	1088	A
1	1	1090	A
1	1	1095	A
1	1	1096	A
1	1	1107	G
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1119	U

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Mol	Chain	Res	Type
1	1	1122	G
1	1	1132	U
1	1	1134	A
1	1	1135	C
1	1	1142	A
1	1	1169	A
1	1	1170	C
1	1	1173	U
1	1	1174	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1179	G
1	1	1180	U
1	1	1186	G
1	1	1238	G
1	1	1248	G
1	1	1253	A
1	1	1256	G
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1273	U
1	1	1301	A
1	1	1321	A
1	1	1345	C
1	1	1352	U
1	1	1365	A
1	1	1368	G
1	1	1378	A
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1387	A
1	1	1392	A
1	1	1395	A
1	1	1406	U
1	1	1407	G
1	1	1408	G
1	1	1411	U
1	1	1414	C

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Mol	Chain	Res	Type
1	1	1415	U
1	1	1416	G
1	1	1417	C
1	1	1419	A
1	1	1420	A
1	1	1428	C
1	1	1452	G
1	1	1453	A
1	1	1460	U
1	1	1478	G
1	1	1482	G
1	1	1490	A
1	1	1497	U
1	1	1503	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1529	G
1	1	1534	U
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1554	U
1	1	1559	U
1	1	1566	A
1	1	1569	A
1	1	1578	U
1	1	1580	A
1	1	1581	G
1	1	1582	C
1	1	1583	A
1	1	1584	U
1	1	1589	U
1	1	1590	A
1	1	1608	A
1	1	1609	A
1	1	1610	A
1	1	1619	G
1	1	1647	U
1	1	1648	U
1	1	1649	G

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Mol	Chain	Res	Type
1	1	1651	G
1	1	1674	G
1	1	1677	A
1	1	1703	G
1	1	1714	U
1	1	1715	G
1	1	1718	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1750	G
1	1	1755	A
1	1	1758	U
1	1	1764	C
1	1	1773	A
1	1	1791	A
1	1	1800	C
1	1	1801	A
1	1	1808	A
1	1	1811	G
1	1	1816	C
1	1	1829	A
1	1	1833	C
1	1	1847	A
1	1	1848	A
1	1	1858	A
1	1	1859	U
1	1	1862	G
1	1	1864	U
1	1	1869	G
1	1	1870	C
1	1	1872	A
1	1	1873	G
1	1	1905	C
1	1	1906	G
1	1	1907	G
1	1	1912	A
1	1	1913	A
1	1	1914	C
1	1	1916	A
1	1	1923	U

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Mol	Chain	Res	Type
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1938	A
1	1	1955	U
1	1	1963	U
1	1	1965	C
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1987	A
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2022	U
1	1	2023	C
1	1	2027	G
1	1	2031	A
1	1	2033	A
1	1	2043	C
1	1	2051	A
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2077	A
1	1	2093	G
1	1	2097	A
1	1	2099	U
1	1	2100	G
1	1	2108	A
1	1	2110	G
1	1	2111	U
1	1	2113	U
1	1	2115	G

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Mol	Chain	Res	Type
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2121	G
1	1	2122	U
1	1	2124	G
1	1	2125	G
1	1	2126	A
1	1	2127	G
1	1	2128	G
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2139	U
1	1	2141	G
1	1	2146	C
1	1	2147	A
1	1	2154	A
1	1	2157	G
1	1	2158	A
1	1	2159	G
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2169	A
1	1	2171	A
1	1	2172	U
1	1	2178	C
1	1	2182	U
1	1	2183	A
1	1	2185	U
1	1	2188	U
1	1	2189	U
1	1	2190	G
1	1	2191	A
1	1	2193	G
1	1	2194	U
1	1	2198	A
1	1	2204	G
1	1	2210	U

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Mol	Chain	Res	Type
1	1	2211	A
1	1	2212	A
1	1	2213	U
1	1	2225	A
1	1	2226	C
1	1	2229	U
1	1	2238	G
1	1	2239	G
1	1	2244	U
1	1	2250	G
1	1	2251	OMG
1	1	2268	A
1	1	2278	A
1	1	2283	C
1	1	2287	A
1	1	2297	A
1	1	2305	U
1	1	2308	G
1	1	2309	A
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2339	C
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2361	G
1	1	2372	U
1	1	2376	A
1	1	2383	G
1	1	2385	C
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2426	A
1	1	2429	G
1	1	2430	A
1	1	2431	U

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Mol	Chain	Res	Type
1	1	2434	A
1	1	2435	A
1	1	2441	U
1	1	2445	2MG
1	1	2447	G
1	1	2448	A
1	1	2470	G
1	1	2474	U
1	1	2476	A
1	1	2478	A
1	1	2484	G
1	1	2491	U
1	1	2502	G
1	1	2504	PSU
1	1	2505	G
1	1	2506	U
1	1	2507	C
1	1	2512	C
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2525	G
1	1	2529	G
1	1	2535	G
1	1	2547	A
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2574	G
1	1	2585	U
1	1	2586	U
1	1	2602	A
1	1	2603	G
1	1	2609	U
1	1	2610	C
1	1	2611	C
1	1	2613	U
1	1	2629	U
1	1	2663	G
1	1	2669	G

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Mol	Chain	Res	Type
1	1	2671	G
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2722	G
1	1	2726	A
1	1	2744	G
1	1	2748	A
1	1	2757	A
1	1	2758	A
1	1	2765	A
1	1	2777	G
1	1	2778	A
1	1	2791	G
1	1	2793	C
1	1	2796	U
1	1	2797	U
1	1	2798	U
1	1	2799	A
1	1	2801	G
1	1	2818	U
1	1	2820	A
1	1	2823	A
1	1	2825	G
1	1	2849	U
1	1	2850	A
1	1	2859	G
1	1	2861	U
1	1	2867	G
1	1	2880	C
1	1	2884	U
1	1	2885	G
1	1	2891	U
1	1	2902	C
2	2	4	U
2	2	5	U
2	2	9	G
2	2	22	G
2	2	29	U
2	2	32	A
2	2	39	G
2	2	41	G

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Mol	Chain	Res	Type
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	54	C
2	2	69	G
2	2	70	U
2	2	71	A
2	2	72	A
2	2	74	A
2	2	76	G
2	2	82	G
2	2	83	C
2	2	84	U
2	2	87	C
2	2	90	C
2	2	94	G
2	2	95	C
2	2	96	U
2	2	108	G
2	2	120	A
2	2	122	G
2	2	128	G
2	2	131	A
2	2	141	G
2	2	144	G
2	2	149	A
2	2	160	A
2	2	164	G
2	2	173	U
2	2	181	A
2	2	182	A
2	2	197	A
2	2	204	G
2	2	208	U
2	2	209	U
2	2	210	C
2	2	211	G
2	2	212	G
2	2	216	U
2	2	226	G

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Mol	Chain	Res	Type
2	2	245	U
2	2	247	G
2	2	251	G
2	2	253	A
2	2	258	G
2	2	262	A
2	2	266	G
2	2	267	C
2	2	271	C
2	2	279	A
2	2	289	G
2	2	299	G
2	2	306	A
2	2	321	A
2	2	328	C
2	2	329	A
2	2	332	G
2	2	347	G
2	2	352	C
2	2	353	A
2	2	354	G
2	2	355	C
2	2	367	U
2	2	372	C
2	2	373	A
2	2	376	G
2	2	382	A
2	2	384	G
2	2	392	C
2	2	393	A
2	2	397	A
2	2	406	G
2	2	411	A
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	429	U
2	2	446	G
2	2	451	A

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Mol	Chain	Res	Type
2	2	457	G
2	2	458	U
2	2	460	A
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	469	C
2	2	478	A
2	2	479	U
2	2	484	G
2	2	485	U
2	2	486	U
2	2	505	G
2	2	509	A
2	2	511	C
2	2	517	G
2	2	518	C
2	2	519	C
2	2	526	C
2	2	527	7MG
2	2	528	C
2	2	531	U
2	2	532	A
2	2	533	A
2	2	542	G
2	2	547	A
2	2	559	A
2	2	562	U
2	2	568	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	579	A
2	2	596	A
2	2	628	G
2	2	633	G
2	2	642	A
2	2	649	A
2	2	650	G
2	2	653	U

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Mol	Chain	Res	Type
2	2	665	A
2	2	666	G
2	2	687	A
2	2	700	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	747	A
2	2	748	G
2	2	755	G
2	2	760	G
2	2	777	A
2	2	793	U
2	2	794	A
2	2	815	A
2	2	817	C
2	2	828	U
2	2	829	G
2	2	832	G
2	2	841	C
2	2	844	G
2	2	845	A
2	2	849	G
2	2	874	G
2	2	887	G
2	2	902	G
2	2	914	A
2	2	916	U
2	2	926	G
2	2	934	C
2	2	935	A
2	2	954	G
2	2	960	U
2	2	963	G
2	2	966	2MG
2	2	967	5MC
2	2	968	A
2	2	969	A
2	2	972	C
2	2	975	A
2	2	976	G

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Mol	Chain	Res	Type
2	2	991	U
2	2	992	U
2	2	993	G
2	2	996	A
2	2	999	C
2	2	1004	A
2	2	1008	U
2	2	1009	U
2	2	1017	U
2	2	1018	G
2	2	1021	A
2	2	1024	G
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1037	C
2	2	1043	G
2	2	1044	A
2	2	1046	A
2	2	1065	U
2	2	1085	U
2	2	1086	U
2	2	1094	G
2	2	1095	U
2	2	1099	G
2	2	1101	A
2	2	1124	G
2	2	1133	G
2	2	1135	U
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1142	G
2	2	1143	G
2	2	1145	A
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1158	C

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Mol	Chain	Res	Type
2	2	1159	U
2	2	1167	A
2	2	1171	A
2	2	1174	G
2	2	1175	G
2	2	1176	A
2	2	1184	G
2	2	1196	A
2	2	1197	A
2	2	1206	G
2	2	1208	C
2	2	1211	U
2	2	1212	U
2	2	1213	A
2	2	1214	C
2	2	1215	G
2	2	1226	C
2	2	1227	A
2	2	1228	C
2	2	1238	A
2	2	1256	A
2	2	1257	A
2	2	1260	G
2	2	1275	A
2	2	1278	G
2	2	1279	G
2	2	1280	A
2	2	1285	A
2	2	1286	U
2	2	1287	A
2	2	1299	A
2	2	1300	G
2	2	1302	C
2	2	1305	G
2	2	1312	G
2	2	1317	C
2	2	1320	C
2	2	1323	G
2	2	1329	A
2	2	1338	G
2	2	1340	A
2	2	1346	A

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Mol	Chain	Res	Type
2	2	1347	G
2	2	1353	G
2	2	1363	A
2	2	1370	G
2	2	1378	C
2	2	1379	G
2	2	1381	U
2	2	1396	A
2	2	1397	C
2	2	1407	5MC
2	2	1408	A
2	2	1419	G
2	2	1429	A
2	2	1441	A
2	2	1446	A
2	2	1447	A
2	2	1448	C
2	2	1452	C
2	2	1453	G
2	2	1475	G
2	2	1487	G
2	2	1492	A
2	2	1494	G
2	2	1495	U
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1529	G
2	2	1530	G
2	2	1534	A
3	3	2	G
3	3	9	G
3	3	13	G
3	3	16	G
3	3	17	C
3	3	35	C
3	3	36	C
3	3	45	A
3	3	51	G
3	3	56	G

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Mol	Chain	Res	Type
3	3	64	G
3	3	66	A
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	109	A
4	4	15	A
5	5	5	G
5	5	8	4SU
5	5	13	A
5	5	15	C
5	5	16	C
5	5	17	U
5	5	18	G
5	5	19	G
5	5	20	H2U
5	5	21	A
5	5	22	G
5	5	25	C
5	5	37	A
5	5	47	U
5	5	48	C
5	5	49	G
5	5	55	PSU
5	5	58	A
5	5	59	A
5	5	60	U
5	5	64	G
5	5	69	C
5	5	74	C

All (127) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	62	U
1	1	70	G
1	1	101	A
1	1	140	C
1	1	196	A
1	1	199	A
1	1	271	G

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Mol	Chain	Res	Type
1	1	369	U
1	1	404	A
1	1	446	G
1	1	503	A
1	1	512	G
1	1	545	U
1	1	546	U
1	1	548	G
1	1	555	G
1	1	614	A
1	1	620	G
1	1	685	A
1	1	764	A
1	1	784	G
1	1	883	G
1	1	892	A
1	1	894	U
1	1	896	A
1	1	984	A
1	1	995	C
1	1	1041	G
1	1	1045	C
1	1	1061	U
1	1	1063	G
1	1	1064	C
1	1	1069	A
1	1	1070	A
1	1	1110	G
1	1	1128	G
1	1	1142	A
1	1	1173	U
1	1	1174	U
1	1	1177	G
1	1	1286	A
1	1	1320	C
1	1	1344	U
1	1	1379	U
1	1	1405	U
1	1	1406	U
1	1	1415	U
1	1	1420	A
1	1	1490	A

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Mol	Chain	Res	Type
1	1	1509	A
1	1	1582	C
1	1	1583	A
1	1	1584	U
1	1	1608	A
1	1	1847	A
1	1	1913	A
1	1	1918	A
1	1	1962	5MC
1	1	2062	A
1	1	2146	C
1	1	2162	G
1	1	2189	U
1	1	2193	G
1	1	2210	U
1	1	2211	A
1	1	2212	A
1	1	2225	A
1	1	2250	G
1	1	2296	U
1	1	2425	A
1	1	2447	G
1	1	2506	U
1	1	2572	A
1	1	2602	A
1	1	2610	C
1	1	2756	U
1	1	2796	U
1	1	2797	U
1	1	2798	U
1	1	2849	U
1	1	2873	A
2	2	7	A
2	2	70	U
2	2	121	U
2	2	181	A
2	2	183	C
2	2	209	U
2	2	305	G
2	2	328	C
2	2	428	G
2	2	481	G

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Mol	Chain	Res	Type
2	2	496	A
2	2	516	PSU
2	2	517	G
2	2	531	U
2	2	532	A
2	2	559	A
2	2	562	U
2	2	641	U
2	2	722	G
2	2	793	U
2	2	966	2MG
2	2	967	5MC
2	2	991	U
2	2	992	U
2	2	1145	A
2	2	1196	A
2	2	1211	U
2	2	1212	U
2	2	1213	A
2	2	1214	C
2	2	1225	A
2	2	1299	A
2	2	1396	A
2	2	1407	5MC
2	2	1432	G
2	2	1447	A
2	2	1493	A
2	2	1516	2MG
5	5	16	C
5	5	17	U
5	5	18	G
5	5	19	G
5	5	20	H2U
5	5	47	U
5	5	58	A
5	5	60	U

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

40 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
47	0TD	q	89	47	7,9,10	6.74	5 (71%)	6,11,13	4.11	2 (33%)
1	6MZ	1	2030	1	18,25,26	0.96	1 (5%)	16,36,39	1.98	4 (25%)
1	PSU	1	1911	1	18,21,22	0.85	1 (5%)	22,30,33	1.02	1 (4%)
2	5MC	2	967	2	18,22,23	0.82	1 (5%)	26,32,35	1.46	2 (7%)
1	PSU	1	2457	1	18,21,22	2.20	1 (5%)	22,30,33	1.51	3 (13%)
1	2MG	1	1835	1	18,26,27	1.19	3 (16%)	16,38,41	1.67	3 (18%)
5	5MU	5	54	5	19,22,23	0.65	0	28,32,35	1.00	2 (7%)
1	G7M	1	2069	1	20,26,27	1.53	1 (5%)	17,39,42	2.38	5 (29%)
1	5MU	1	747	1	19,22,23	0.75	1 (5%)	28,32,35	0.98	3 (10%)
5	PSU	5	55	5	18,21,22	1.85	1 (5%)	22,30,33	1.54	2 (9%)
1	PSU	1	955	1	18,21,22	1.97	1 (5%)	22,30,33	1.65	3 (13%)
1	PSU	1	2580	1,57	18,21,22	1.76	1 (5%)	22,30,33	1.52	3 (13%)
5	4SU	5	8	5	18,21,22	1.57	4 (22%)	26,30,33	2.37	6 (23%)
1	1MG	1	745	1	18,26,27	1.62	2 (11%)	19,39,42	1.94	4 (21%)
1	OMC	1	2498	1,57	19,22,23	1.08	2 (10%)	26,31,34	1.77	4 (15%)
2	7MG	2	527	2	22,26,27	1.54	4 (18%)	29,39,42	2.69	10 (34%)
2	PSU	2	516	57,2	18,21,22	0.90	1 (5%)	22,30,33	1.04	1 (4%)
2	2MG	2	966	2	18,26,27	1.20	3 (16%)	16,38,41	2.29	3 (18%)
1	PSU	1	746	1,57	18,21,22	2.12	1 (5%)	22,30,33	2.10	3 (13%)
2	2MG	2	1516	2	18,26,27	1.22	3 (16%)	16,38,41	1.58	2 (12%)
1	PSU	1	1917	1	18,21,22	0.75	1 (5%)	22,30,33	0.99	1 (4%)
5	8AN	5	76	57,58,5	19,24,25	0.71	0	13,35,38	0.91	0
1	OMG	1	2251	1,5	18,26,27	1.12	1 (5%)	19,38,41	0.90	1 (5%)
2	2MG	2	1207	2	18,26,27	1.63	4 (22%)	16,38,41	1.11	1 (6%)
2	UR3	2	1498	2	19,22,23	0.81	0	26,32,35	0.98	2 (7%)
1	PSU	1	2605	1	18,21,22	1.97	1 (5%)	22,30,33	1.62	3 (13%)
2	MA6	2	1519	2	19,26,27	0.58	0	18,38,41	0.83	1 (5%)
5	4OC	5	32	5	20,23,24	0.47	0	26,32,35	1.28	2 (7%)
1	5MC	1	1962	1	18,22,23	0.81	1 (5%)	26,32,35	1.62	3 (11%)
1	5MU	1	1939	1	19,22,23	0.80	1 (5%)	28,32,35	0.96	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2MG	1	2445	1	18,26,27	1.29	3 (16%)	16,38,41	1.43	2 (12%)
1	6MZ	1	1618	1	18,25,26	0.93	1 (5%)	16,36,39	1.66	3 (18%)
1	2MA	1	2503	1,57	17,25,26	1.16	2 (11%)	17,37,40	2.94	6 (35%)
5	H2U	5	20	5	18,21,22	0.65	0	21,30,33	1.88	4 (19%)
1	OMU	1	2552	1	19,22,23	0.46	0	26,31,34	0.83	1 (3%)
2	4OC	2	1402	2	20,23,24	0.66	0	26,32,35	0.79	1 (3%)
2	MA6	2	1518	2	19,26,27	0.59	0	18,38,41	0.75	0
1	3TD	1	1915	1	18,22,23	0.67	0	22,32,35	1.35	4 (18%)
1	PSU	1	2504	1	18,21,22	1.94	1 (5%)	22,30,33	1.60	3 (13%)
2	5MC	2	1407	2	18,22,23	0.61	0	26,32,35	1.31	3 (11%)

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
47	0TD	q	89	47	-	2/7/12/14	-
1	6MZ	1	2030	1	-	1/5/27/28	0/3/3/3
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
2	5MC	2	967	2	-	5/7/25/26	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	0/5/27/28	0/3/3/3
5	5MU	5	54	5	-	0/7/25/26	0/2/2/2
1	G7M	1	2069	1	-	2/3/25/26	0/3/3/3
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
5	PSU	5	55	5	-	2/7/25/26	0/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2580	1,57	-	0/7/25/26	0/2/2/2
5	4SU	5	8	5	-	4/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
1	OMC	1	2498	1,57	-	0/9/27/28	0/2/2/2
2	7MG	2	527	2	-	2/7/37/38	0/3/3/3
2	PSU	2	516	57,2	-	2/7/25/26	0/2/2/2
2	2MG	2	966	2	-	2/5/27/28	0/3/3/3
1	PSU	1	746	1,57	-	2/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	8AN	5	76	57,58,5	-	3/3/25/26	0/3/3/3
1	OMG	1	2251	1,5	-	0/5/27/28	0/3/3/3
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	5/7/29/30	0/3/3/3
5	4OC	5	32	5	-	0/9/29/30	0/2/2/2
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
1	5MU	1	1939	1	-	0/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	3/5/27/28	0/3/3/3
1	6MZ	1	1618	1	-	4/5/27/28	0/3/3/3
1	2MA	1	2503	1,57	-	1/3/25/26	0/3/3/3
5	H2U	5	20	5	-	4/7/38/39	0/2/2/2
1	OMU	1	2552	1	-	2/9/27/28	0/2/2/2
2	4OC	2	1402	2	-	1/9/29/30	0/2/2/2
2	MA6	2	1518	2	-	0/7/29/30	0/3/3/3
1	3TD	1	1915	1	-	4/7/25/26	0/2/2/2
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	q	89	0TD	CB-SB	-16.93	1.65	1.82
1	1	2457	PSU	C2'-C1'	-8.97	1.42	1.53
1	1	746	PSU	C2'-C1'	-8.77	1.42	1.53
1	1	2605	PSU	C2'-C1'	-8.05	1.43	1.53
1	1	2504	PSU	C2'-C1'	-7.91	1.43	1.53
1	1	955	PSU	C2'-C1'	-7.89	1.43	1.53
5	5	55	PSU	C2'-C1'	-7.65	1.43	1.53
1	1	2580	PSU	C2'-C1'	-7.06	1.44	1.53
1	1	2069	G7M	C2'-C1'	-5.62	1.45	1.53
1	1	745	1MG	C2'-C1'	-4.50	1.46	1.53
5	5	8	4SU	C4-S4	-4.22	1.60	1.68
2	2	527	7MG	C4-N9	-4.07	1.33	1.37
2	2	1207	2MG	C2'-C1'	-3.61	1.48	1.53
1	1	2498	OMC	C3'-C2'	-3.42	1.45	1.52
47	q	89	0TD	CA-N	-3.17	1.37	1.47
1	1	2251	OMG	C5-C4	-3.09	1.35	1.43
1	1	745	1MG	C5-C6	-3.05	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2445	2MG	C5-C6	-3.03	1.41	1.47
2	2	1207	2MG	C6-N1	2.88	1.42	1.37
2	2	1516	2MG	C5-C6	-2.88	1.41	1.47
1	1	2030	6MZ	C2'-C1'	-2.85	1.49	1.53
1	1	1835	2MG	C5-C6	-2.82	1.41	1.47
2	2	966	2MG	C6-N1	2.81	1.42	1.37
2	2	527	7MG	C6-N1	-2.76	1.33	1.38
5	5	8	4SU	C2-N1	2.75	1.42	1.38
47	q	89	0TD	OD2-CG	-2.70	1.21	1.30
1	1	1911	PSU	C2'-C1'	-2.68	1.50	1.53
47	q	89	0TD	CB-CG	-2.68	1.47	1.52
2	2	516	PSU	C2'-C1'	-2.67	1.50	1.53
2	2	1207	2MG	C5-C6	-2.64	1.42	1.47
2	2	966	2MG	C5-C6	-2.63	1.42	1.47
1	1	1962	5MC	C2'-C1'	-2.61	1.45	1.53
1	1	1618	6MZ	C2'-C1'	-2.57	1.49	1.53
1	1	1939	5MU	C2'-C1'	-2.56	1.45	1.53
2	2	527	7MG	C5-C4	2.54	1.46	1.38
47	q	89	0TD	CSB-SB	-2.53	1.74	1.79
1	1	2445	2MG	C5-C4	-2.48	1.36	1.43
2	2	1516	2MG	C6-N1	2.44	1.41	1.37
1	1	1835	2MG	C6-N1	2.43	1.41	1.37
2	2	527	7MG	C5-N7	-2.43	1.32	1.35
1	1	2503	2MA	C2'-C3'	-2.38	1.46	1.53
1	1	2498	OMC	C2'-C1'	-2.35	1.47	1.53
2	2	1516	2MG	C5-C4	-2.29	1.37	1.43
2	2	967	5MC	C2'-C1'	-2.27	1.46	1.53
1	1	1835	2MG	C5-C4	-2.26	1.37	1.43
1	1	747	5MU	C2'-C1'	-2.25	1.46	1.53
2	2	966	2MG	C5-C4	-2.21	1.37	1.43
1	1	1917	PSU	C2'-C1'	-2.18	1.50	1.53
5	5	8	4SU	C5-C4	-2.11	1.39	1.42
2	2	1207	2MG	C5-C4	-2.11	1.37	1.43
1	1	2445	2MG	C6-N1	2.07	1.41	1.37
1	1	2503	2MA	C5-C4	-2.03	1.37	1.43
5	5	8	4SU	C4-N3	-2.01	1.35	1.37

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	527	7MG	N9-C4-N3	8.71	138.49	125.47
1	1	746	PSU	C3'-C2'-C1'	7.77	110.69	101.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2503	2MA	C3'-C2'-C1'	-7.73	89.34	100.98
47	q	89	0TD	CB-CA-N	-7.52	93.08	109.10
2	2	966	2MG	O3'-C3'-C4'	7.46	132.61	111.05
1	1	1962	5MC	O3'-C3'-C4'	6.32	129.33	111.05
5	5	8	4SU	C4-N3-C2	-6.25	121.27	127.34
47	q	89	0TD	CSB-SB-CB	6.19	113.63	102.44
5	5	8	4SU	C5-C4-N3	6.15	120.39	114.69
1	1	2498	OMC	O2'-C2'-C1'	5.93	120.64	109.08
2	2	967	5MC	O3'-C3'-C4'	5.71	127.55	111.05
2	2	527	7MG	N9-C8-N7	-5.59	95.38	103.38
1	1	2498	OMC	O3'-C3'-C2'	5.52	126.84	111.17
5	5	55	PSU	O2'-C2'-C3'	5.22	128.70	111.82
1	1	2069	G7M	O2'-C2'-C3'	5.21	128.67	111.82
1	1	955	PSU	O2'-C2'-C3'	5.14	128.45	111.82
2	2	527	7MG	C5-C4-N3	-5.06	118.48	128.13
1	1	1618	6MZ	O3'-C3'-C4'	4.97	125.41	111.05
1	1	2069	G7M	C3'-C2'-C1'	-4.91	93.58	100.98
1	1	745	1MG	C3'-C2'-C1'	4.83	108.26	100.98
5	5	32	4OC	O3'-C3'-C2'	4.83	124.89	111.17
5	5	20	H2U	O2'-C2'-C3'	4.73	127.13	111.82
1	1	2069	G7M	O2'-C2'-C1'	4.72	128.27	110.85
1	1	2504	PSU	O2'-C2'-C3'	4.71	127.06	111.82
2	2	1407	5MC	O3'-C3'-C2'	4.68	126.96	111.82
1	1	2457	PSU	O2'-C2'-C3'	4.65	126.85	111.82
1	1	2605	PSU	O2'-C2'-C3'	4.63	126.80	111.82
1	1	2503	2MA	O3'-C3'-C4'	4.47	123.97	111.05
1	1	2503	2MA	O3'-C3'-C2'	4.45	126.21	111.82
2	2	1516	2MG	O3'-C3'-C2'	4.43	126.16	111.82
1	1	745	1MG	O3'-C3'-C2'	4.39	126.03	111.82
1	1	2605	PSU	O2'-C2'-C1'	4.31	121.52	111.23
1	1	2580	PSU	O2'-C2'-C1'	4.31	121.51	111.23
1	1	746	PSU	O2'-C2'-C3'	4.30	125.73	111.82
1	1	2580	PSU	O2'-C2'-C3'	4.30	125.72	111.82
5	5	20	H2U	O3'-C3'-C2'	4.29	125.71	111.82
1	1	2504	PSU	O2'-C2'-C1'	4.29	121.46	111.23
1	1	1915	3TD	C5'-C4'-C3'	-4.25	99.24	115.18
1	1	955	PSU	O2'-C2'-C1'	4.25	121.36	111.23
1	1	2030	6MZ	C3'-C2'-C1'	-4.20	94.65	100.98
5	5	20	H2U	O3'-C3'-C4'	4.15	123.06	111.05
1	1	2503	2MA	O2'-C2'-C1'	4.12	126.07	110.85
5	5	55	PSU	O2'-C2'-C1'	4.12	121.06	111.23
5	5	8	4SU	C5-C4-S4	-4.07	119.22	124.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1835	2MG	O3'-C3'-C2'	4.07	125.00	111.82
1	1	2503	2MA	O4'-C1'-C2'	4.01	112.79	106.93
2	2	527	7MG	C2-N3-C4	4.00	119.42	112.30
1	1	2030	6MZ	O3'-C3'-C2'	3.89	124.39	111.82
5	5	8	4SU	N3-C2-N1	3.85	120.00	114.89
2	2	966	2MG	C2'-C3'-C4'	-3.77	95.31	102.64
1	1	2030	6MZ	O3'-C3'-C4'	3.76	121.92	111.05
1	1	2445	2MG	O3'-C3'-C2'	3.73	123.89	111.82
1	1	745	1MG	O3'-C3'-C4'	3.73	121.82	111.05
1	1	2457	PSU	O2'-C2'-C1'	3.72	120.11	111.23
1	1	1835	2MG	O3'-C3'-C4'	3.57	121.36	111.05
5	5	20	H2U	O2'-C2'-C1'	3.35	121.23	110.02
2	2	1516	2MG	O3'-C3'-C4'	3.31	120.62	111.05
5	5	8	4SU	C1'-N1-C2	3.27	123.48	117.57
1	1	1917	PSU	C3'-C2'-C1'	3.19	105.35	101.64
1	1	2030	6MZ	C2-N1-C6	3.18	119.31	116.59
1	1	2503	2MA	O2'-C2'-C3'	3.14	121.98	111.82
1	1	746	PSU	O2'-C2'-C1'	2.98	118.34	111.23
1	1	1618	6MZ	C2-N1-C6	2.97	119.14	116.59
2	2	1498	UR3	O4'-C1'-C2'	-2.97	100.17	106.64
2	2	527	7MG	O4'-C4'-C3'	-2.89	99.39	105.11
1	1	1835	2MG	C3'-C2'-C1'	2.87	105.30	100.98
2	2	516	PSU	C3'-C2'-C1'	2.86	104.97	101.64
5	5	32	4OC	O3'-C3'-C4'	2.85	119.28	111.05
1	1	1911	PSU	C3'-C2'-C1'	2.84	104.95	101.64
1	1	745	1MG	O2'-C2'-C3'	2.79	120.86	111.82
1	1	2504	PSU	C2'-C3'-C4'	-2.75	97.30	102.64
2	2	527	7MG	O4'-C1'-N9	2.74	113.03	109.30
2	2	527	7MG	C5-C6-N1	2.66	115.67	110.99
2	2	1407	5MC	C5'-C4'-C3'	2.65	125.13	115.18
1	1	1962	5MC	O3'-C3'-C2'	2.60	120.24	111.82
2	2	1402	4OC	O4'-C4'-C3'	-2.58	100.00	105.11
1	1	747	5MU	C2'-C1'-N1	2.58	120.53	113.22
1	1	1939	5MU	C2'-C1'-N1	2.58	120.53	113.22
5	5	54	5MU	C2'-C1'-N1	2.58	120.53	113.22
2	2	527	7MG	C5-C4-N9	-2.57	103.01	106.35
1	1	2498	OMC	O3'-C3'-C4'	2.55	118.43	111.05
1	1	2580	PSU	C3'-C2'-C1'	2.55	104.61	101.64
1	1	2605	PSU	C2'-C3'-C4'	-2.55	97.69	102.64
1	1	2069	G7M	C2'-C3'-C4'	-2.51	97.76	102.64
2	2	967	5MC	C2'-C1'-N1	2.48	120.24	113.22
2	2	1519	MA6	C2'-C3'-C4'	-2.47	97.84	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2445	2MG	O3'-C3'-C4'	2.47	118.19	111.05
1	1	2457	PSU	C2'-C3'-C4'	-2.43	97.91	102.64
1	1	955	PSU	C2'-C3'-C4'	-2.39	98.00	102.64
2	2	527	7MG	O6-C6-C5	-2.30	121.89	127.54
1	1	1962	5MC	C3'-C2'-C1'	2.30	105.79	101.43
1	1	2069	G7M	O3'-C3'-C2'	2.26	119.14	111.82
2	2	1207	2MG	O2'-C2'-C1'	-2.26	102.52	110.85
1	1	1939	5MU	C4-N3-C2	-2.22	124.47	127.35
1	1	2498	OMC	C3'-C2'-C1'	2.21	107.05	102.89
1	1	747	5MU	N3-C2-N1	2.20	117.81	114.89
1	1	1939	5MU	N3-C2-N1	2.19	117.79	114.89
5	5	54	5MU	N3-C2-N1	2.18	117.79	114.89
1	1	1915	3TD	O4'-C4'-C5'	-2.18	102.20	109.37
5	5	8	4SU	O4'-C1'-C2'	-2.18	101.89	106.64
1	1	1915	3TD	O5'-C5'-C4'	2.15	116.30	108.99
1	1	1915	3TD	C3'-C2'-C1'	2.14	104.13	101.64
1	1	747	5MU	C4-N3-C2	-2.08	124.65	127.35
2	2	1407	5MC	O4'-C4'-C5'	2.08	116.22	109.37
2	2	966	2MG	O3'-C3'-C2'	2.07	118.52	111.82
1	1	2552	OMU	N3-C2-N1	2.05	117.61	114.89
1	1	1618	6MZ	C3'-C2'-C1'	-2.03	97.92	100.98
2	2	1498	UR3	O3'-C3'-C4'	-2.03	105.18	111.05
1	1	2251	OMG	O2'-C2'-C1'	-2.01	105.10	109.09
2	2	527	7MG	O2'-C2'-C1'	-2.01	103.32	110.02

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	746	PSU	C2'-C1'-C5-C4
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2445	2MG	N3-C2-N2-CM2
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	966	2MG	O4'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
2	2	967	5MC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	2	1519	MA6	C5-C6-N6-C9
2	2	1519	MA6	C5-C6-N6-C10
5	5	20	H2U	O4'-C4'-C5'-O5'
5	5	20	H2U	O4'-C1'-N1-C6
5	5	55	PSU	C3'-C4'-C5'-O5'
47	q	89	0TD	SB-CB-CG-OD2
1	1	1915	3TD	O4'-C4'-C5'-O5'
2	2	967	5MC	C3'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'
1	1	2069	G7M	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
5	5	20	H2U	C3'-C4'-C5'-O5'
5	5	55	PSU	O4'-C4'-C5'-O5'
2	2	1519	MA6	N1-C6-N6-C10
5	5	76	8AN	C4'-C5'-O5'-P
5	5	20	H2U	O4'-C1'-N1-C2
2	2	527	7MG	C3'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
1	1	2504	PSU	O4'-C4'-C5'-O5'
2	2	527	7MG	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C5-C6-N6-C9
47	q	89	0TD	CG-CB-SB-CSB
1	1	2069	G7M	C4'-C5'-O5'-P
2	2	967	5MC	C4'-C5'-O5'-P
5	5	76	8AN	C3'-C4'-C5'-O5'
1	1	2552	OMU	O4'-C4'-C5'-O5'
5	5	8	4SU	O4'-C1'-N1-C6
1	1	2030	6MZ	O4'-C4'-C5'-O5'
2	2	967	5MC	C2'-C1'-N1-C6
5	5	8	4SU	O4'-C1'-N1-C2
5	5	8	4SU	C4'-C5'-O5'-P
1	1	2504	PSU	C3'-C4'-C5'-O5'
2	2	967	5MC	C2'-C1'-N1-C2
1	1	1915	3TD	C3'-C4'-C5'-O5'
1	1	2552	OMU	C3'-C4'-C5'-O5'
5	5	76	8AN	O4'-C4'-C5'-O5'
1	1	746	PSU	O4'-C1'-C5-C6
5	5	8	4SU	C2'-C1'-N1-C2
1	1	2503	2MA	O4'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 440 ligands modelled in this entry, 439 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
58	FME	5	101	5	8,9,10	0.54	0	7,9,11	1.15	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
58	FME	5	101	5	-	1/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	5	101	FME	O-C-CA	-2.93	117.10	124.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	7
1	1	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1276:G	O3'	1277:C	P	3.19
1	1	2314:A	O3'	2315:G	P	3.10
1	2	147:G	O3'	148:G	P	3.07
1	2	1383:C	O3'	1384:C	P	3.06
1	2	480:U	O3'	481:G	P	2.98
1	2	1390:U	O3'	1391:U	P	2.82
1	1	2196:C	O3'	2197:U	P	2.67
1	2	197:A	O3'	198:G	P	2.67
1	2	927:G	O3'	928:G	P	2.61

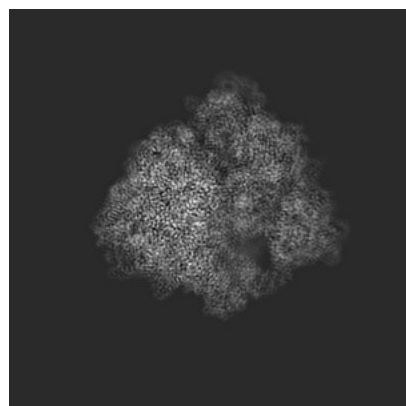
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3493. These allow visual inspection of the internal detail of the map and identification of artifacts.

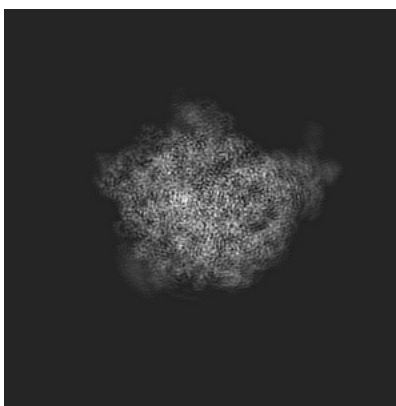
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

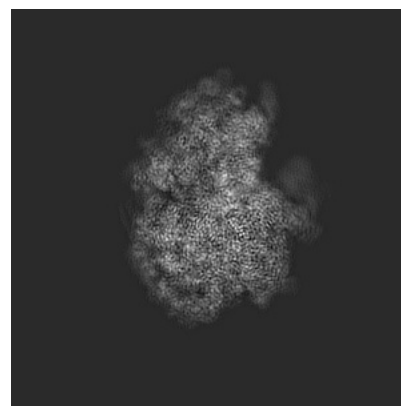
#### 6.1.1 Primary map



X

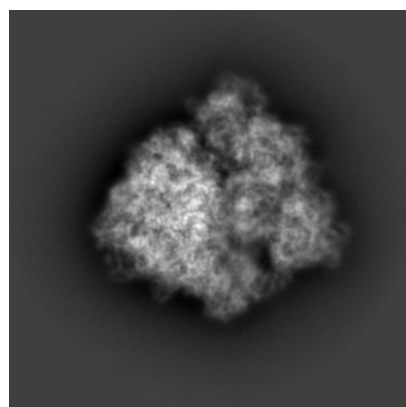


Y

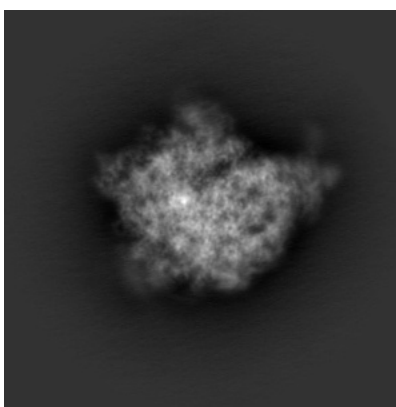


Z

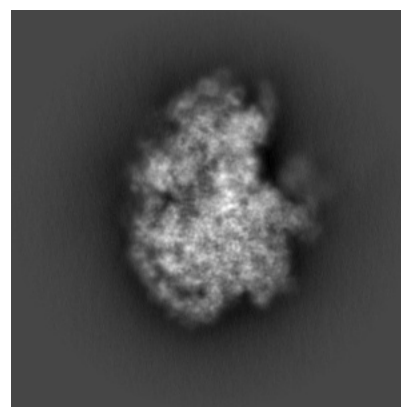
#### 6.1.2 Raw map



X



Y

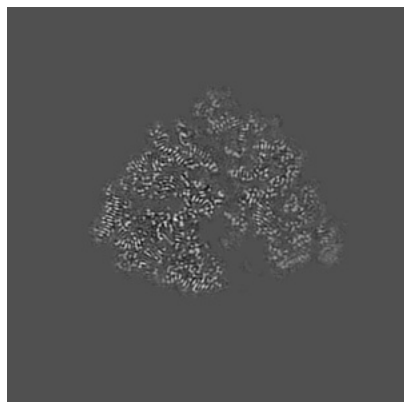


Z

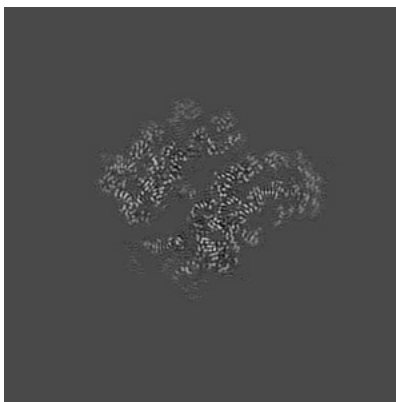
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

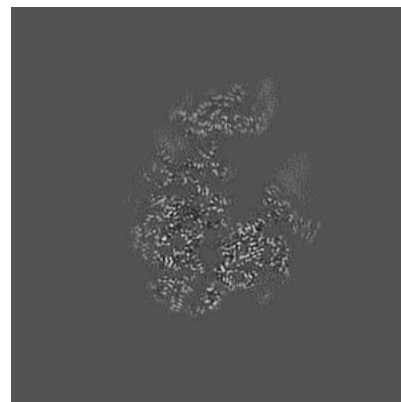
### 6.2.1 Primary map



X Index: 200

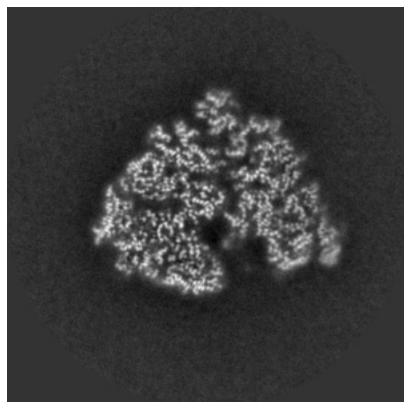


Y Index: 200

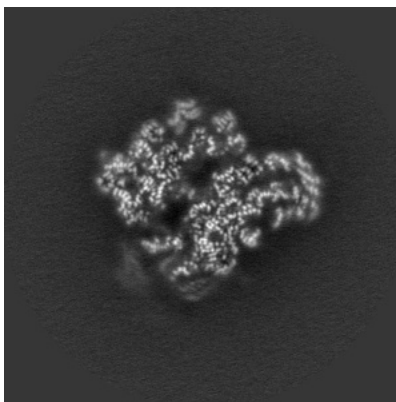


Z Index: 200

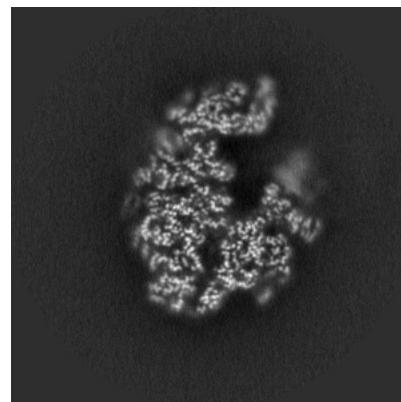
### 6.2.2 Raw map



X Index: 200



Y Index: 200

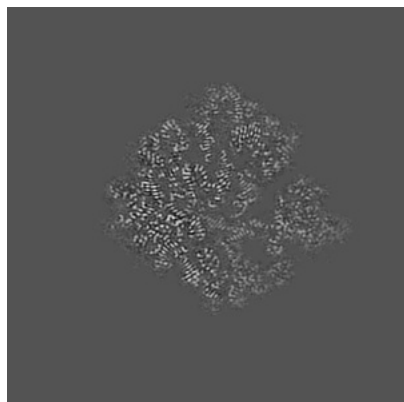


Z Index: 200

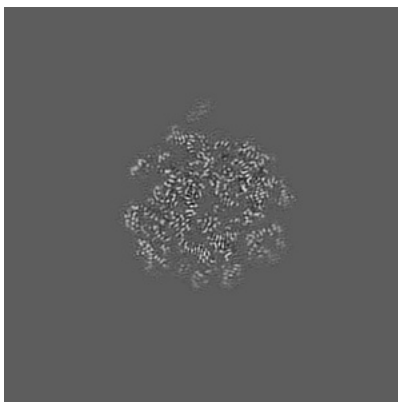
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

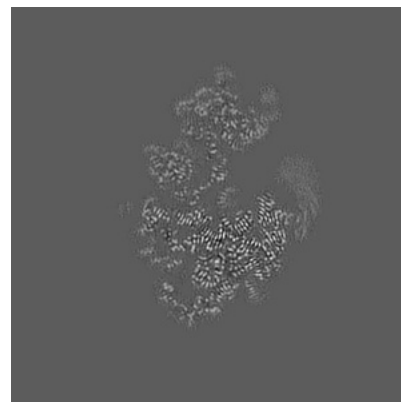
### 6.3.1 Primary map



X Index: 213

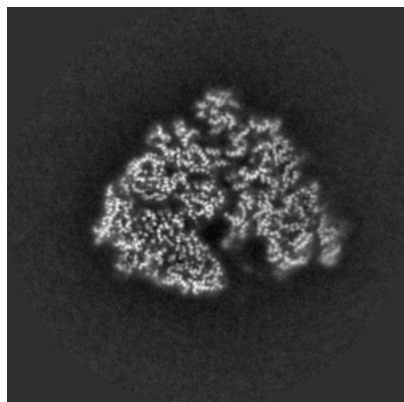


Y Index: 168

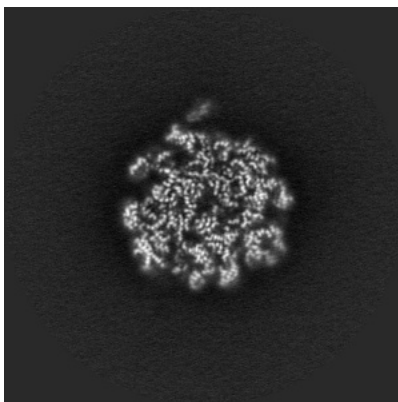


Z Index: 185

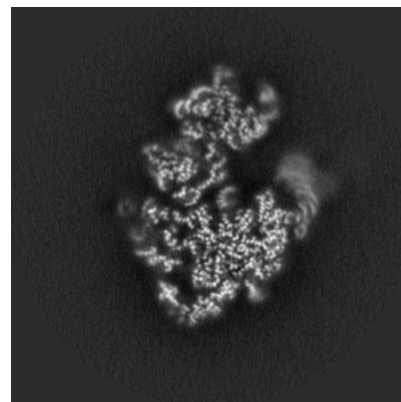
### 6.3.2 Raw map



X Index: 201



Y Index: 169

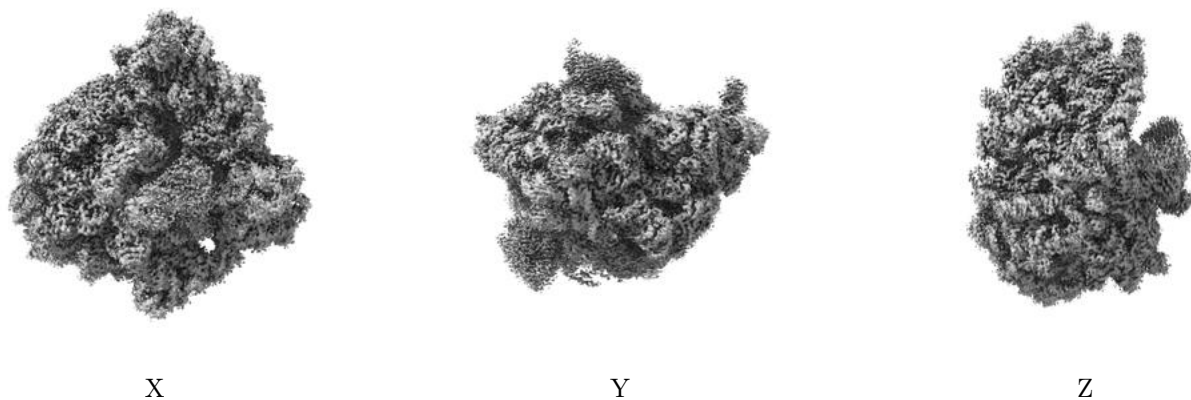


Z Index: 185

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

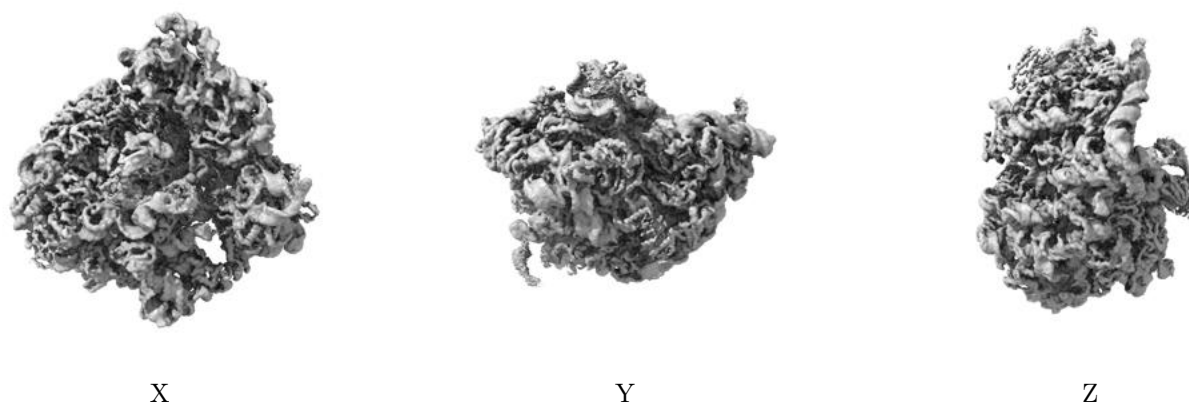
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

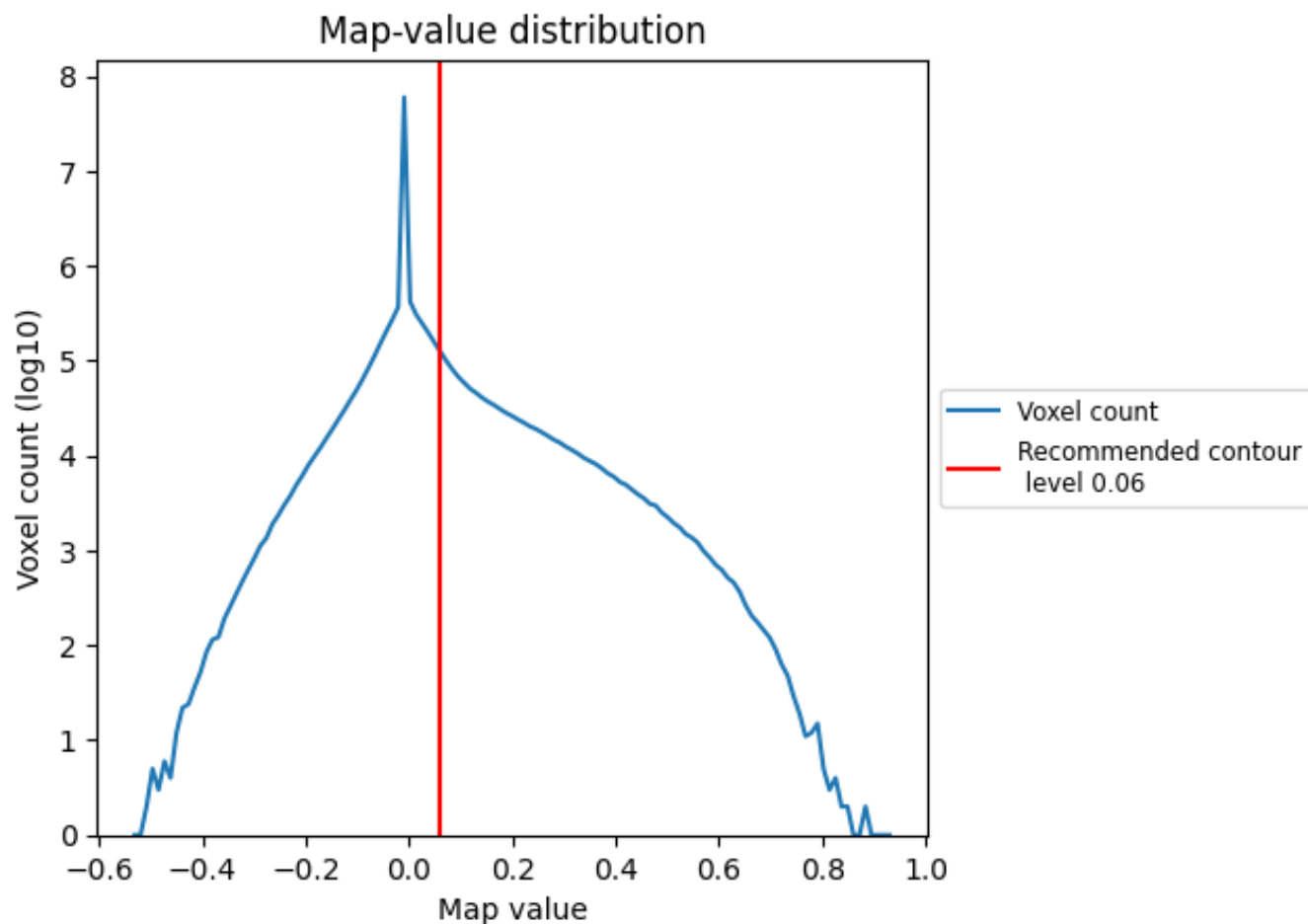
## 6.5 Mask visualisation [i](#)

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.

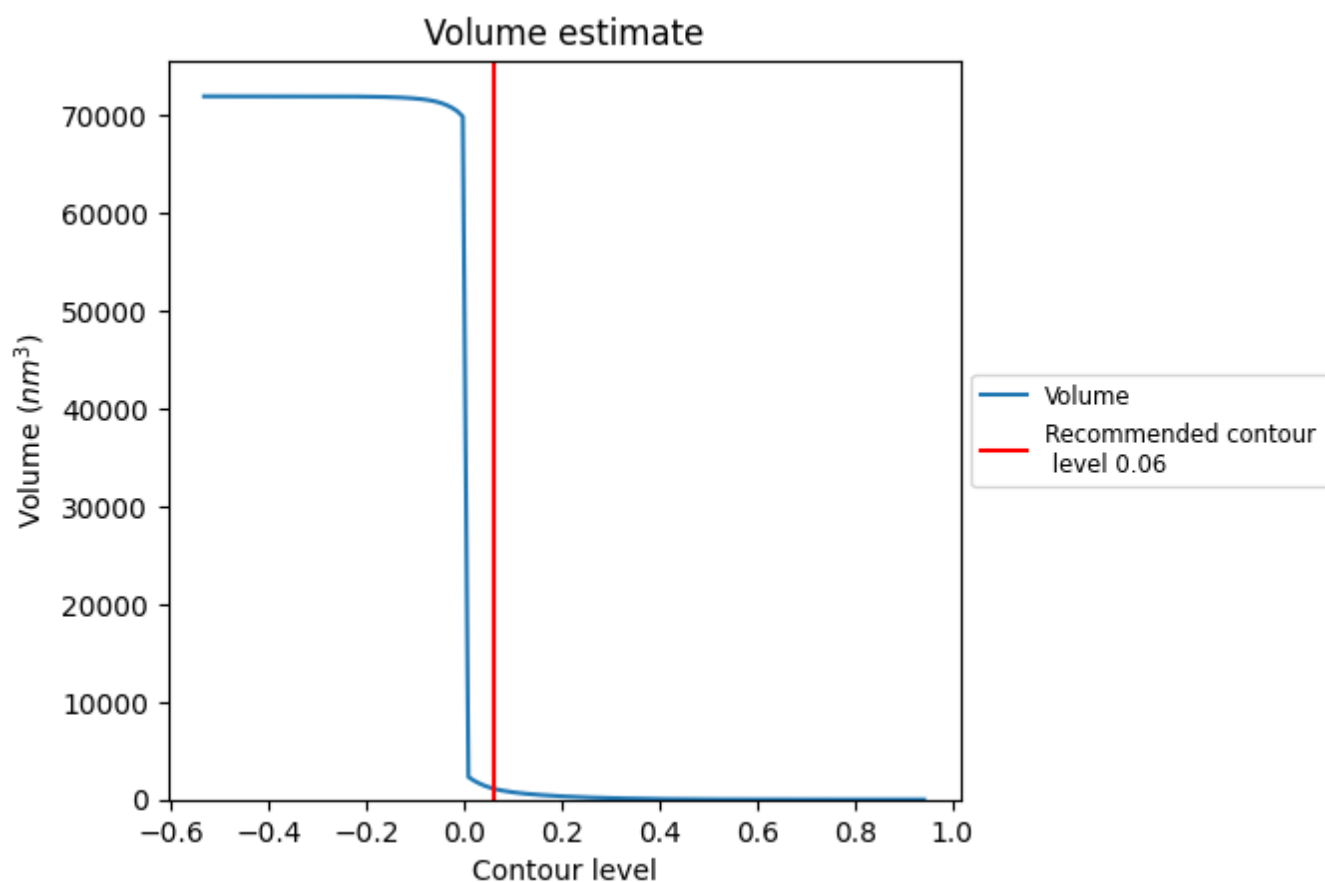
### 7.1 Map-value distribution [i](#)



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.



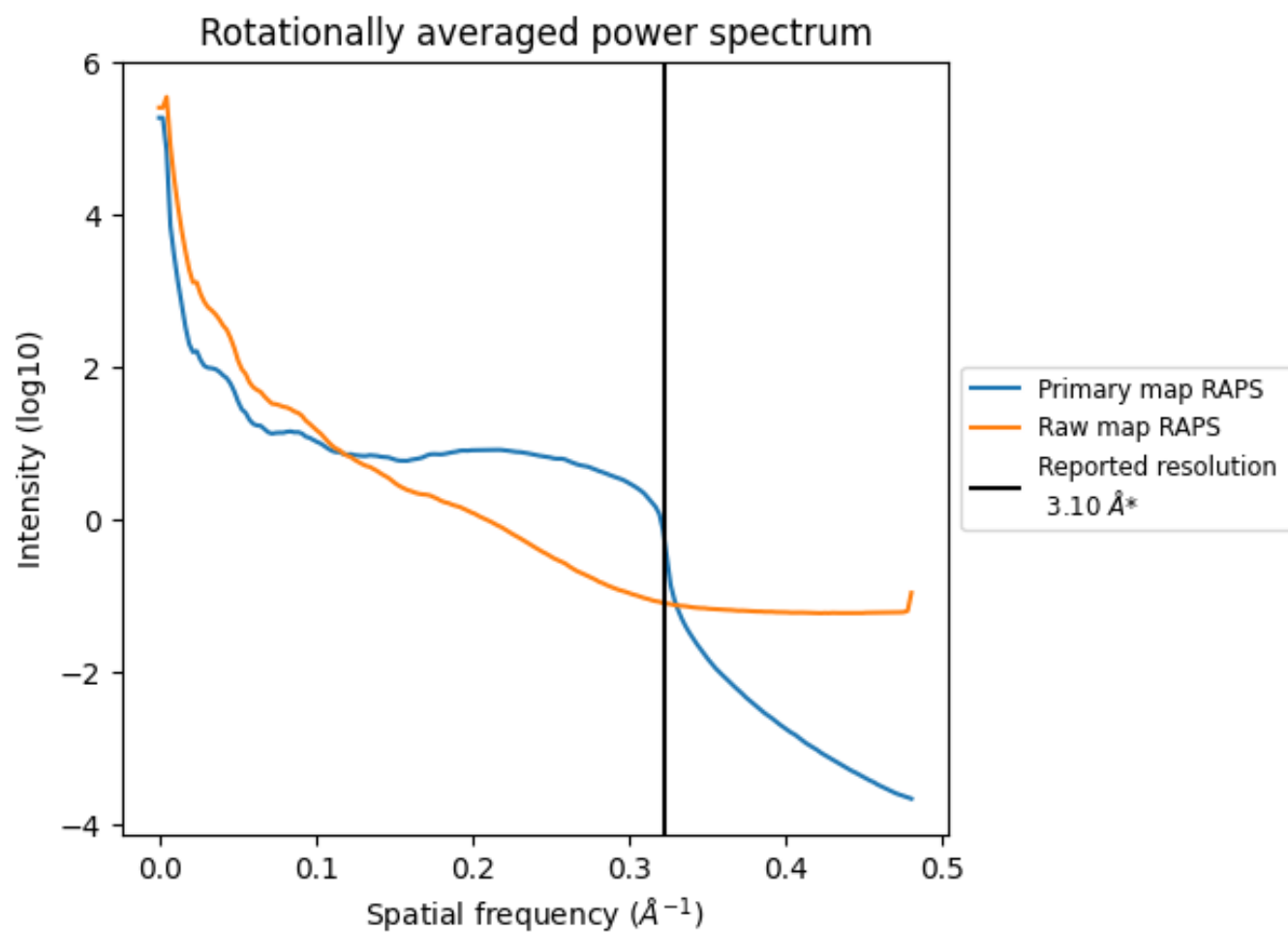
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $1142 \text{ nm}^3$ ; this corresponds to an approximate mass of 1031 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 ⓘ

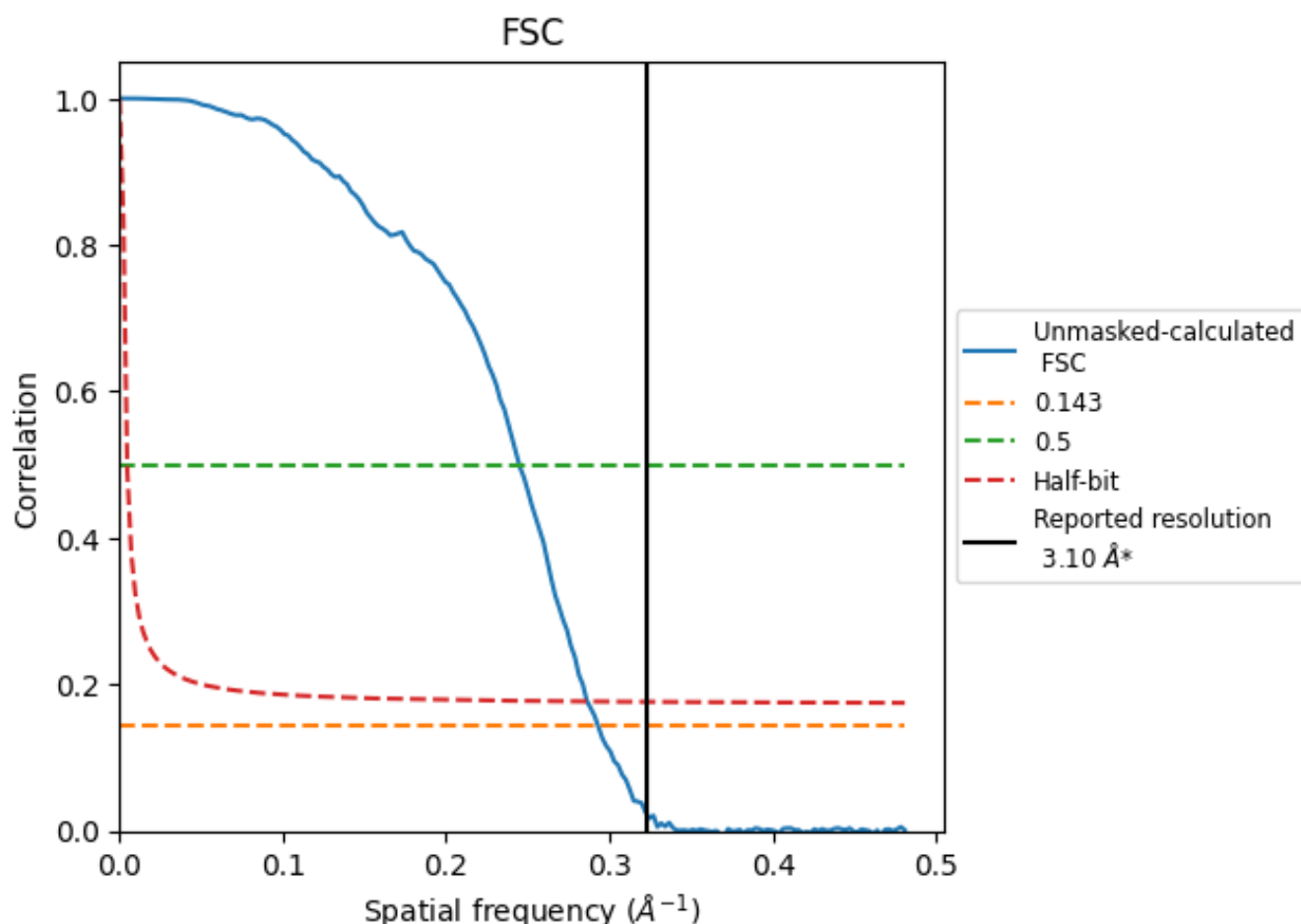


\*Reported resolution corresponds to spatial frequency of  $0.323 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

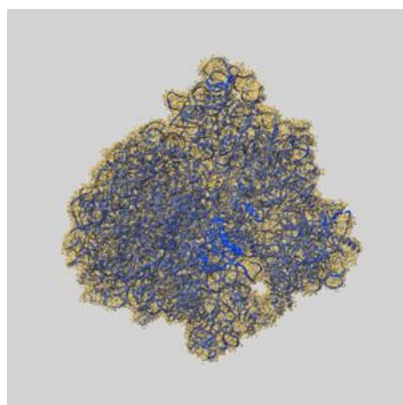
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.41	4.08	3.49

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.41 differs from the reported value 3.1 by more than 10 %

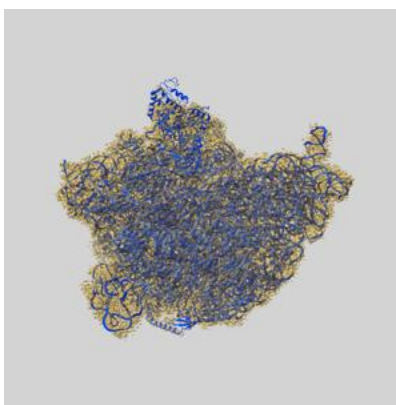
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3493 and PDB model 5MDZ. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

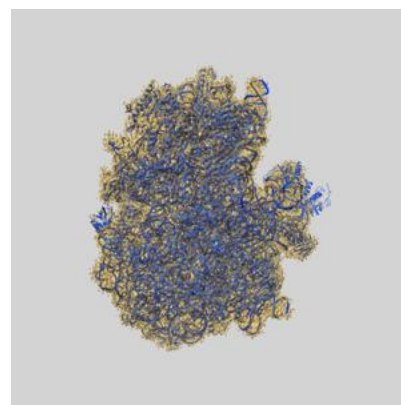
### 9.1 Map-model overlay [i](#)



X



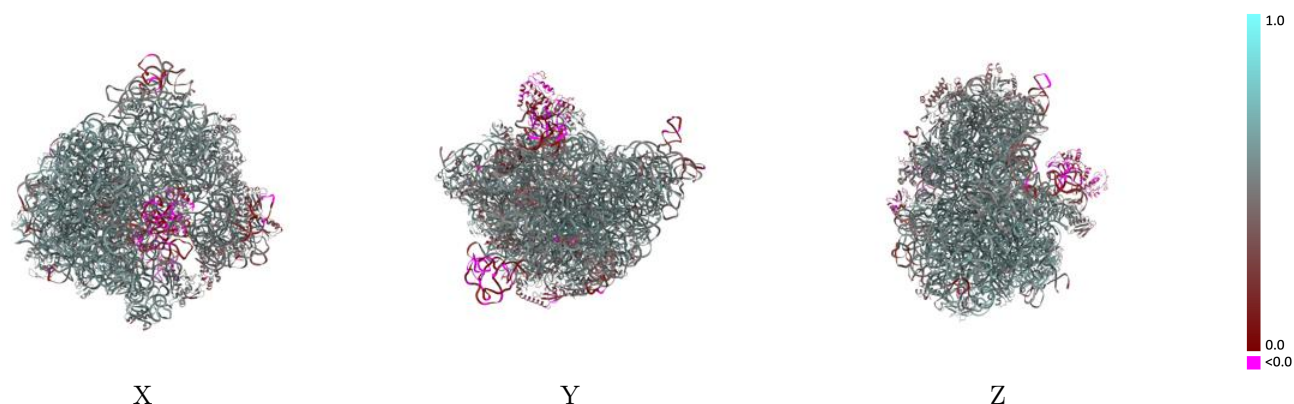
Y



Z

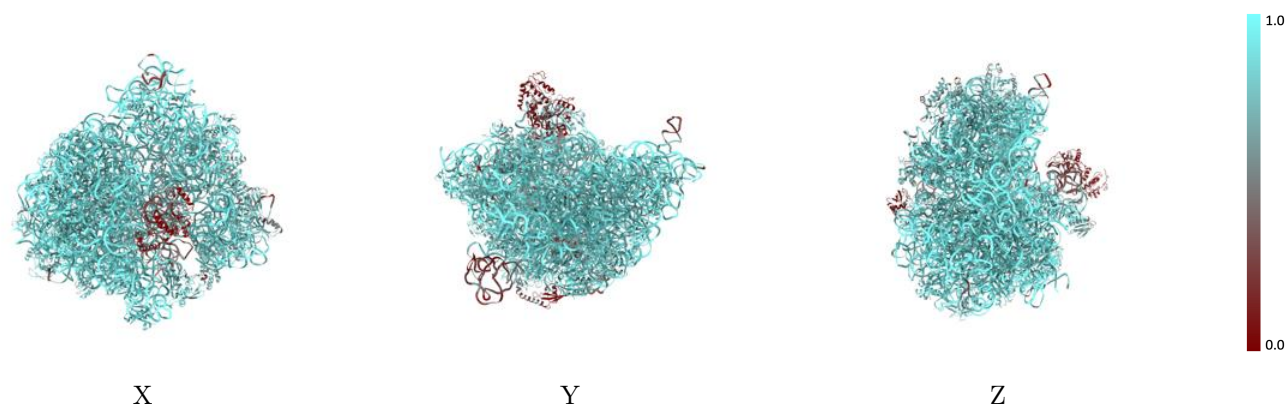
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



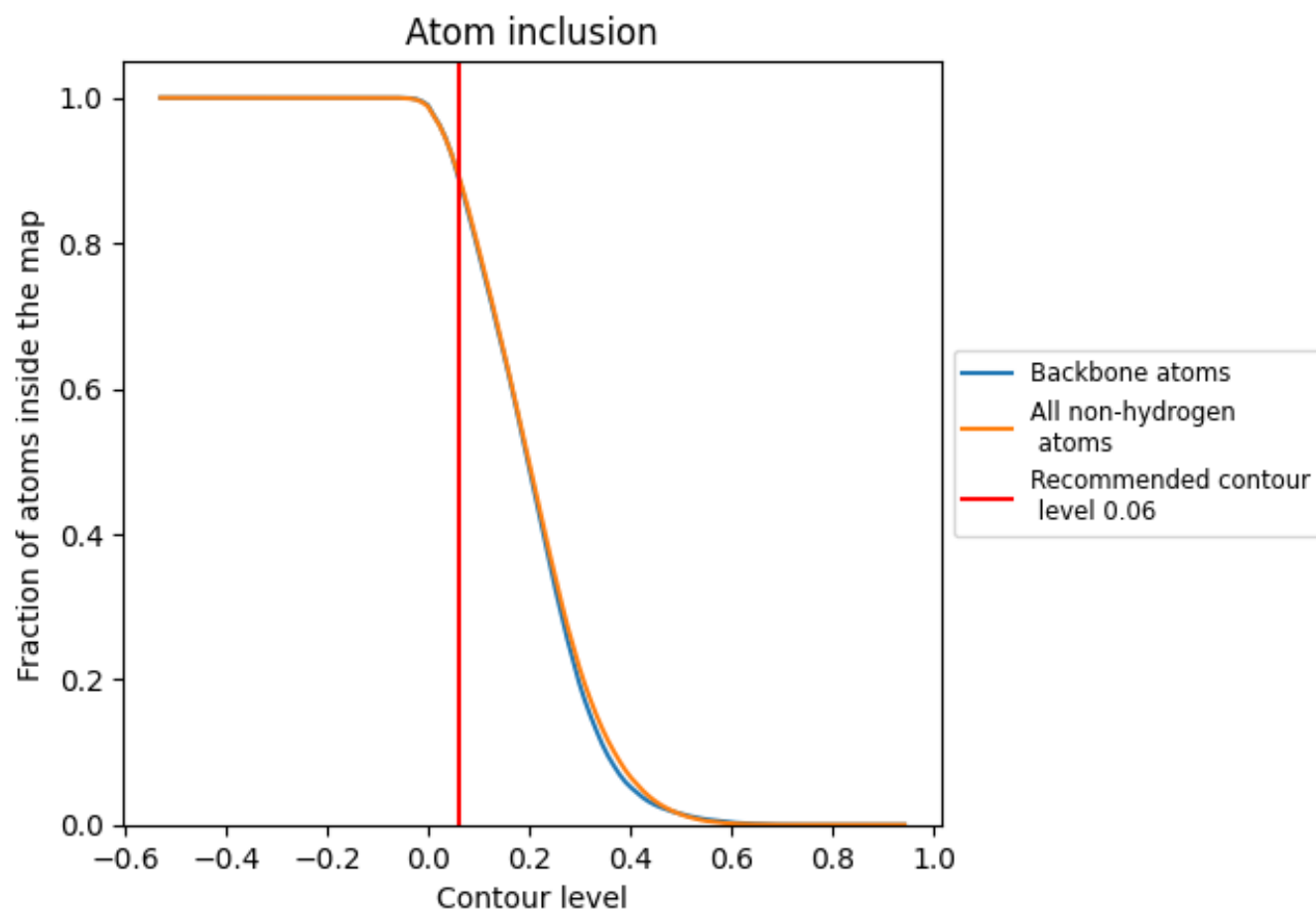
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.06) and Q-score for the entire model and for each chain.













































Chain	Atom inclusion	Q-score
All	 0.8909	 0.5180
1	 0.9311	 0.5360
2	 0.9406	 0.5250
3	 0.9659	 0.5510
4	 0.9633	 0.5670
5	 0.9168	 0.5110
B	 0.9127	 0.5740
C	 0.9200	 0.5680
D	 0.8638	 0.5290
E	 0.8369	 0.4850
F	 0.7739	 0.4460
G	 0.3057	 0.2440
H	 0.0448	 0.0430
I	 0.1027	 0.0510
J	 0.9118	 0.5660
K	 0.8903	 0.5570
L	 0.9072	 0.5580
M	 0.9088	 0.5600
N	 0.9102	 0.5710
O	 0.8725	 0.5250
P	 0.8885	 0.5570
Q	 0.9196	 0.5730
R	 0.8934	 0.5510
S	 0.8852	 0.5570
T	 0.8466	 0.5280
U	 0.8557	 0.5150
V	 0.8550	 0.5210
W	 0.9205	 0.5780
X	 0.9002	 0.5590
Y	 0.8344	 0.4930
Z	 0.8830	 0.5520
a	 0.7188	 0.3780
b	 0.9068	 0.5750
c	 0.8206	 0.5350
d	 0.9014	 0.5740



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Chain	Atom inclusion	Q-score
e	 0.9226	 0.5820
f	 0.8980	 0.5680
g	 0.6484	 0.4010
h	 0.8226	 0.4880
i	 0.8202	 0.4890
j	 0.8735	 0.5290
k	 0.8017	 0.4640
l	 0.7692	 0.4290
m	 0.8635	 0.5330
n	 0.8316	 0.4630
o	 0.7359	 0.4150
p	 0.8429	 0.5090
q	 0.8732	 0.5260
r	 0.8145	 0.4740
s	 0.8346	 0.4860
t	 0.8609	 0.5120
u	 0.8517	 0.5240
v	 0.8354	 0.5090
w	 0.8489	 0.5200
x	 0.8315	 0.4690
y	 0.8807	 0.5190
z	 0.7066	 0.4200