



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 01:28 pm GMT

PDB ID : 5MDW  
EMDB ID : EMD-3490  
Title : Structure of ArfA(A18T) and RF2 bound to the 70S ribosome (pre-accommodated state)  
Authors : James, N.R.; Brown, A.; Gordiyenko, Y.; Ramakrishnan, V.  
Deposited on : 2016-11-13  
Resolution : 3.06 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:

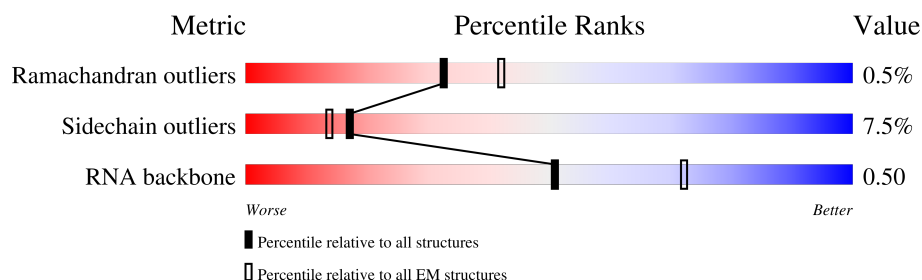
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et 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 3.06 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.



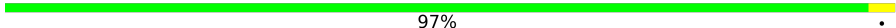


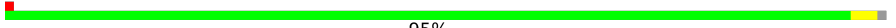









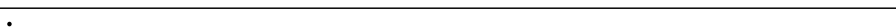

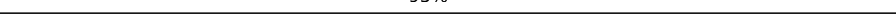

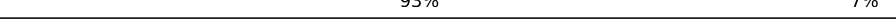

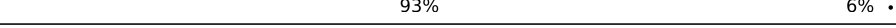
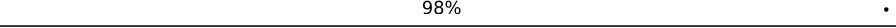




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	6	61	
7	7	365	
8	B	273	


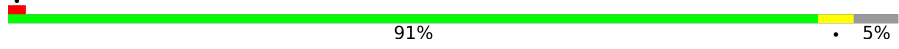

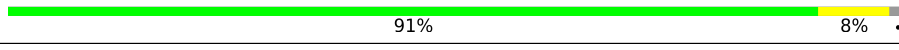

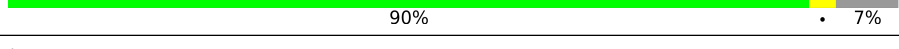
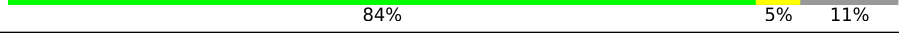
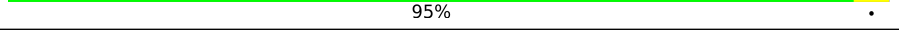
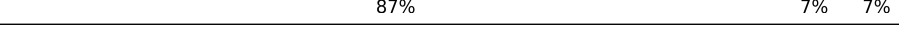
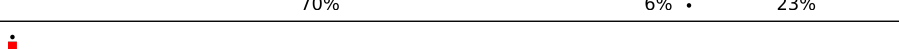
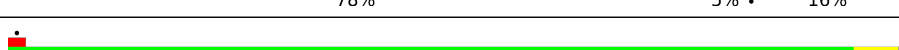
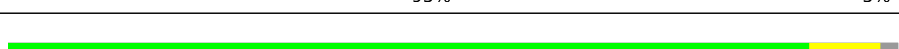
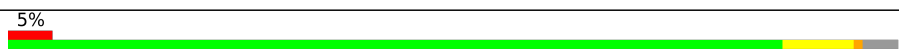

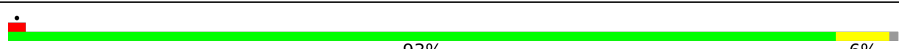

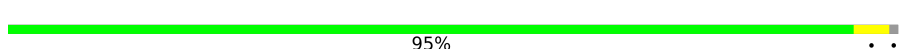

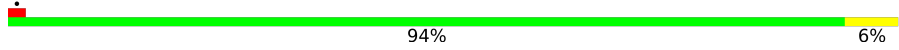
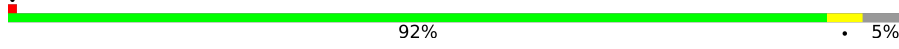
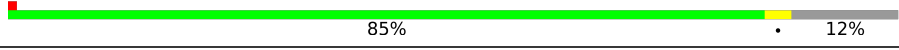
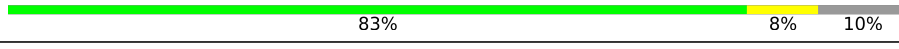
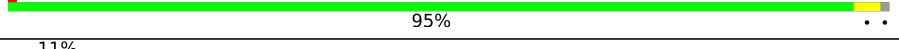


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Mol	Chain	Length	Quality of chain
9	C	209	 97% .
10	D	201	 93% 6% .
11	E	179	 92% 7% .
12	F	177	 95% . .
13	G	149	 48% 91% 9%
14	H	165	 67% 71% 8% 21%
15	I	142	 59% 87% 8% 5%
16	J	142	 96% .
17	K	123	 95% 5%
18	L	144	 96% .
19	M	136	 93% 7%
20	N	127	 87% 7% 6%
21	O	117	 93% 6% .
22	P	115	 92% 7% .
23	Q	118	 95% . .
24	R	103	 89% 11%
25	S	110	 93% 7%
26	T	100	 91% . 6%
27	U	104	 93% 6% .
28	V	94	 98% .
29	W	85	 84% 6% 11%
30	X	78	 91% 8% .
31	Y	63	 90% 8% .
32	Z	59	 88% 10% .
33	a	70	 9% 84% 10% 6%

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Mol	Chain	Length	Quality of chain
34	b	57	
35	c	55	
36	d	46	
37	e	65	
38	f	38	
39	g	241	
40	h	233	
41	i	206	
42	j	167	
43	k	135	
44	l	179	
45	m	130	
46	n	130	
47	o	103	
48	p	129	
49	q	124	
50	r	118	
51	s	101	
52	t	89	
53	u	82	
54	v	84	
55	w	75	
56	x	92	
57	y	87	
58	z	71	

## 2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 149607 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 Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	32	Total	C	N	O	S	0	0
			261	164	53	43	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	0	HIS	-	expression tag	UNP P36675
6	18	THR	ALA	engineered mutation	UNP P36675

- Molecule 7 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	341	Total	C	N	O	S	0	0
			2706	1669	470	558	9		

- Molecule 8 is a protein called 50S ribosomal protein L2.

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

- Molecule 9 is a protein called 50S ribosomal protein L3.

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

- Molecule 10 is a protein called 50S ribosomal protein L4.

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

- Molecule 11 is a protein called 50S ribosomal protein L5.

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

- Molecule 12 is a protein called 50S ribosomal protein L6.

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

- Molecule 13 is a protein called 50S ribosomal protein L9.

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

- Molecule 14 is a protein called 50S ribosomal protein L10.

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

- Molecule 15 is a protein called 50S ribosomal protein L11.

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

- Molecule 16 is a protein called 50S ribosomal protein L13.

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

- Molecule 17 is a protein called 50S ribosomal protein L14.

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

- Molecule 18 is a protein called 50S ribosomal protein L15.

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

- Molecule 19 is a protein called 50S ribosomal protein L16.

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

- Molecule 20 is a protein called 50S ribosomal protein L17.

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

- Molecule 21 is a protein called 50S ribosomal protein L18.

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

- Molecule 22 is a protein called 50S ribosomal protein L19.

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

- Molecule 23 is a protein called 50S ribosomal protein L20.

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

- Molecule 24 is a protein called 50S ribosomal protein L21.

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

- Molecule 25 is a protein called 50S ribosomal protein L22.

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

- Molecule 26 is a protein called 50S ribosomal protein L23.



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

- Molecule 27 is a protein called 50S ribosomal protein L24.

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

- Molecule 28 is a protein called 50S ribosomal protein L25.

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

- Molecule 29 is a protein called 50S ribosomal protein L27.

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

- Molecule 30 is a protein called 50S ribosomal protein L28.

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

- Molecule 31 is a protein called 50S ribosomal protein L29.

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

- Molecule 32 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 34 is a protein called 50S ribosomal protein L32.

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

- Molecule 35 is a protein called 50S ribosomal protein L33.

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

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L35.

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

- Molecule 38 is a protein called 50S ribosomal protein L36.

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

- Molecule 39 is a protein called 30S ribosomal protein S2.

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

- Molecule 40 is a protein called 30S ribosomal protein S3.

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

- Molecule 41 is a protein called 30S ribosomal protein S4.

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

- Molecule 42 is a protein called 30S ribosomal protein S5.

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

- Molecule 43 is a protein called 30S ribosomal protein S6.

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

- Molecule 44 is a protein called 30S ribosomal protein S7.

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

- Molecule 45 is a protein called 30S ribosomal protein S8.

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

- Molecule 46 is a protein called 30S ribosomal protein S9.

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

- Molecule 47 is a protein called 30S ribosomal protein S10.

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

- Molecule 48 is a protein called 30S ribosomal protein S11.

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

- Molecule 49 is a protein called 30S ribosomal protein S12.

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

- Molecule 50 is a protein called 30S ribosomal protein S13.

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

- Molecule 51 is a protein called 30S ribosomal protein S14.

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

- Molecule 52 is a protein called 30S ribosomal protein S15.

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

- Molecule 53 is a protein called 30S ribosomal protein S16.

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

- Molecule 54 is a protein called 30S ribosomal protein S17.

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

- Molecule 55 is a protein called 30S ribosomal protein S18.

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

- Molecule 56 is a protein called 30S ribosomal protein S19.

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

- Molecule 57 is a protein called 30S ribosomal protein S20.

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

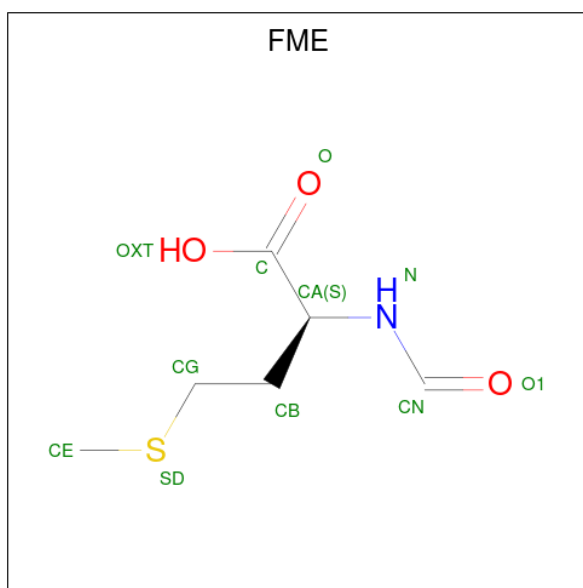
- Molecule 58 is a protein called 30S ribosomal protein S21.

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

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	1	295	Total	Mg	0
			295	295	
59	2	133	Total	Mg	0
			133	133	
59	3	6	Total	Mg	0
			6	6	
59	5	2	Total	Mg	0
			2	2	
59	b	1	Total	Mg	0
			1	1	
59	i	1	Total	Mg	0
			1	1	

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula:  $C_6H_{11}NO_3S$ ).



Mol	Chain	Residues	Atoms					AltConf
60	5	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

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

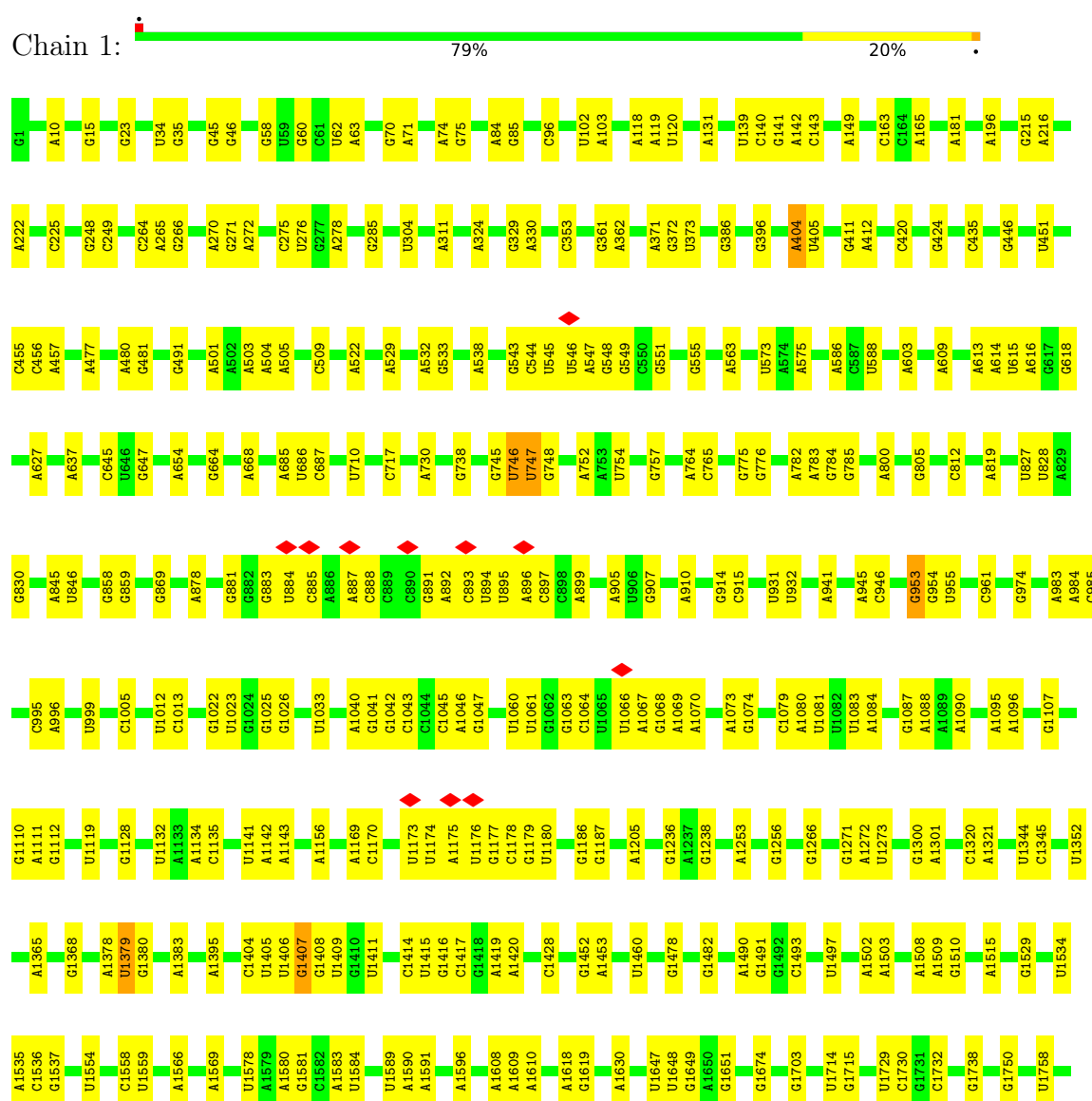
- Molecule 62 is water.

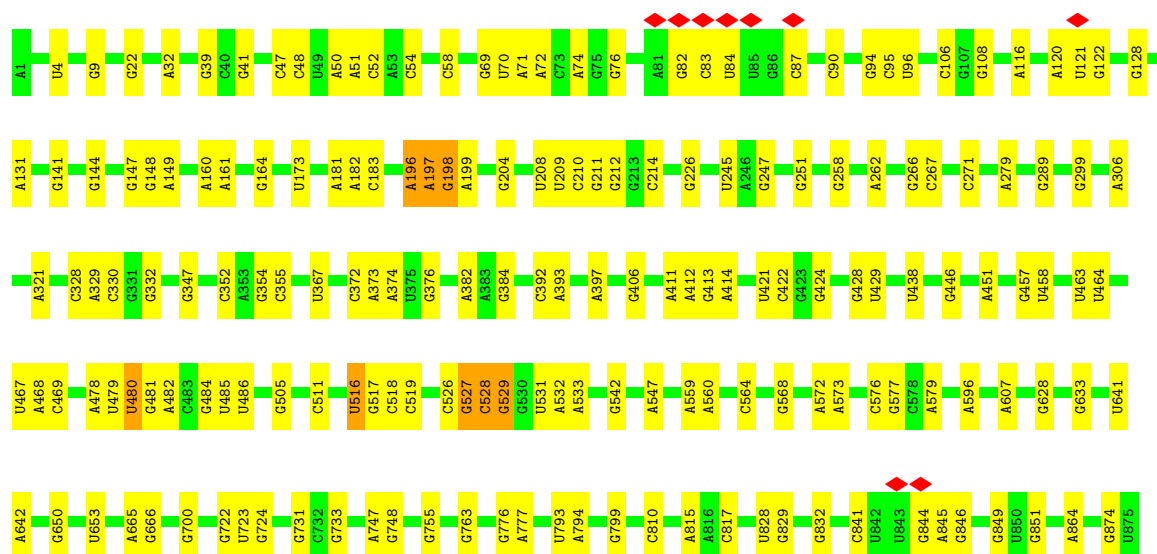
Mol	Chain	Residues	Atoms		AltConf
62	B	2	Total	O	0
			2	2	

### 3 Residue-property plots

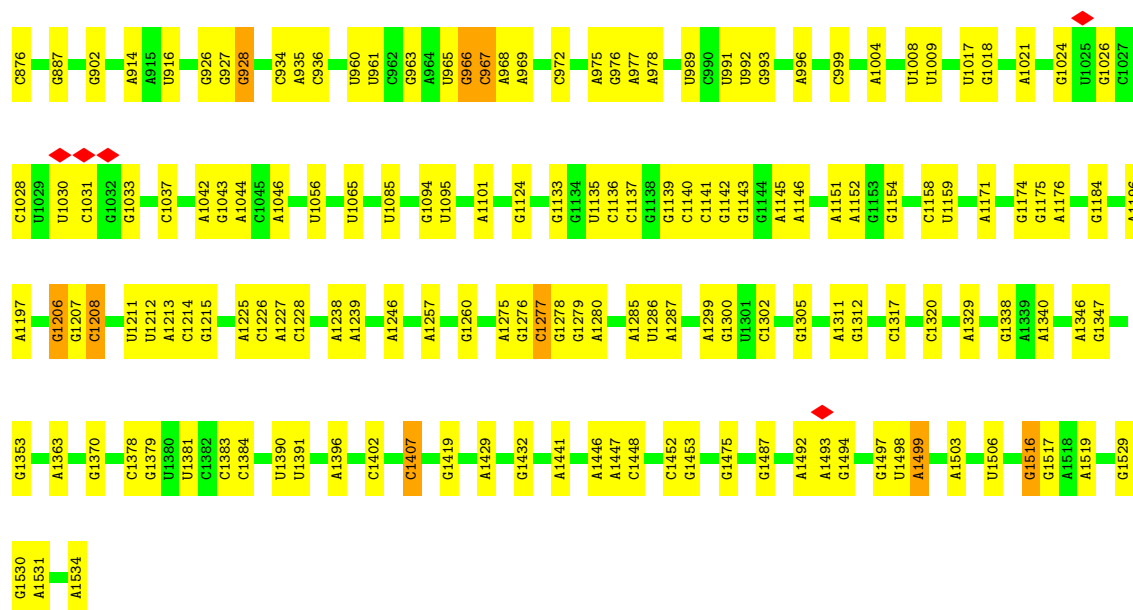
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 3: 5S ribosomal RNA

Chain 3: 85% 15%



- Molecule 4: mRNA

Chain 4: 22% 6% 72%



- Molecule 5: fMet-NH-tRNA(fMet)

Chain 5: 68% 26% 6%



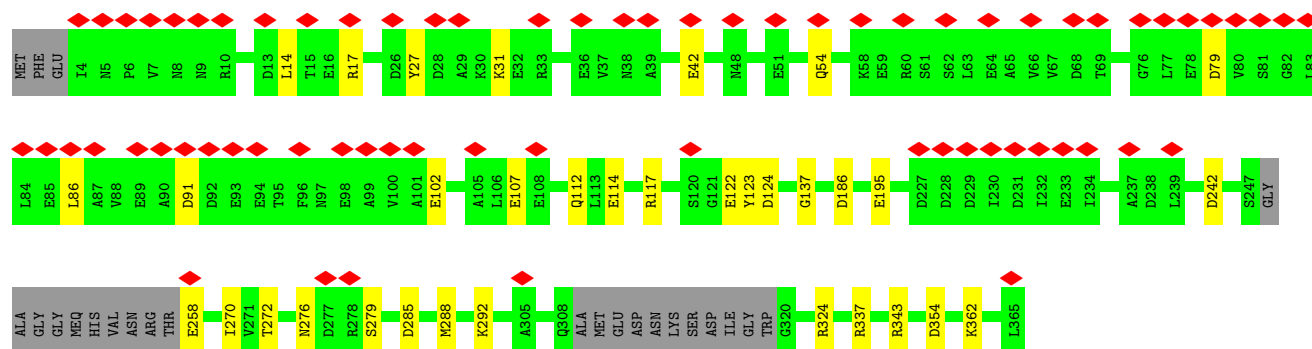
- Molecule 6: Alternative ribosome-rescue factor A

Chain 6: 48% 5% 48%



- Molecule 7: Peptide chain release factor 2

Chain 7: 19% 84% 9% 7%



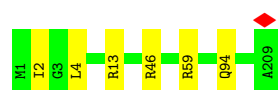
- Molecule 8: 50S ribosomal protein L2

Chain B: 93% 6%



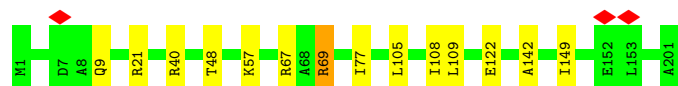
- Molecule 9: 50S ribosomal protein L3

Chain C: 97%



- Molecule 10: 50S ribosomal protein L4

Chain D: 93% 6%



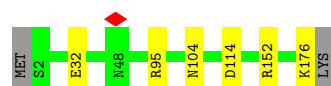
- Molecule 11: 50S ribosomal protein L5

Chain E: 92% 7%

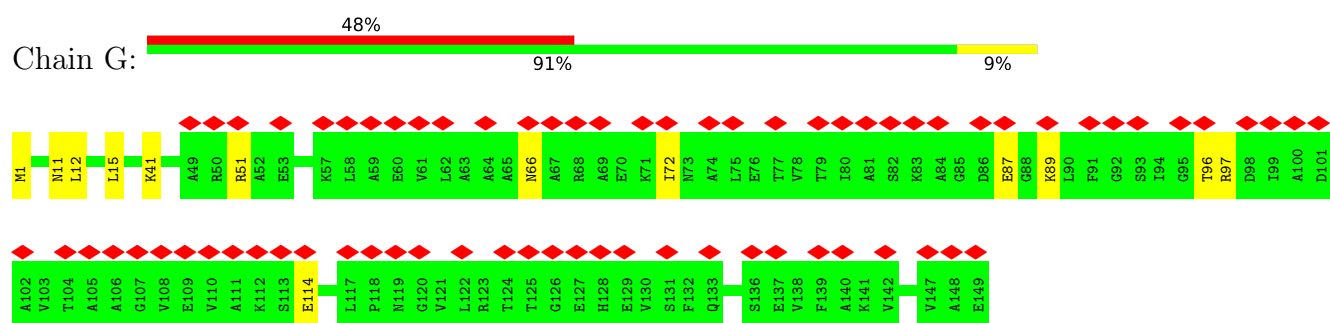


- Molecule 12: 50S ribosomal protein L6

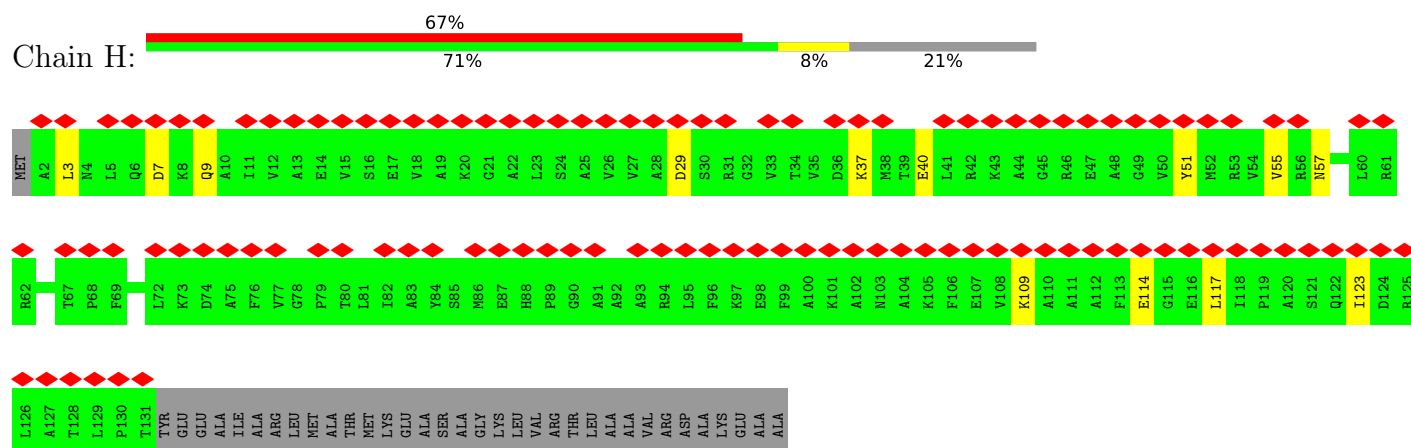
Chain F: 95%



- Molecule 13: 50S ribosomal protein L9



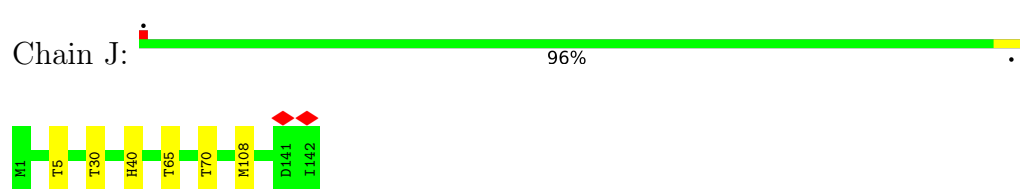
- Molecule 14: 50S ribosomal protein L10



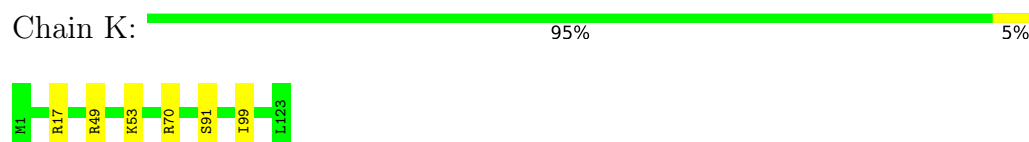
- Molecule 15: 50S ribosomal protein L11



- Molecule 16: 50S ribosomal protein L13

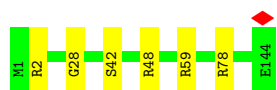


- Molecule 17: 50S ribosomal protein L14



- Molecule 18: 50S ribosomal protein L15

Chain L:  96%




- Molecule 19: 50S ribosomal protein L16

Chain M:  93% 7%



- Molecule 20: 50S ribosomal protein L17

Chain N:  87% 7% 6%



- Molecule 21: 50S ribosomal protein L18

Chain O:  93% 6%



- Molecule 22: 50S ribosomal protein L19

Chain P:  92% 7%




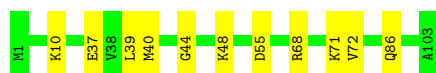
- Molecule 23: 50S ribosomal protein L20

Chain Q:  95%




- Molecule 24: 50S ribosomal protein L21

Chain R:  89% 11%



- Molecule 25: 50S ribosomal protein L22

Chain S:  93% 7%



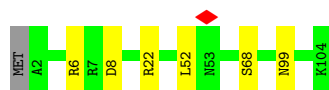
- Molecule 26: 50S ribosomal protein L23

Chain T:  91% 6%



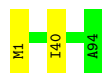
- Molecule 27: 50S ribosomal protein L24

Chain U:  93% 6%




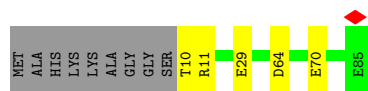
- Molecule 28: 50S ribosomal protein L25

Chain V:  98%



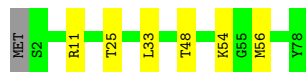
- Molecule 29: 50S ribosomal protein L27

Chain W:  84% 6% 11%




- Molecule 30: 50S ribosomal protein L28

Chain X:  91% 8%



- Molecule 31: 50S ribosomal protein L29

Chain Y:  90% 8%



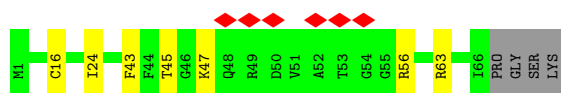
- Molecule 32: 50S ribosomal protein L30

Chain Z: 88% 10%



- Molecule 33: 50S ribosomal protein L31

Chain a: 9% 84% 10% 6%



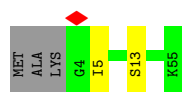
- Molecule 34: 50S ribosomal protein L32

Chain b: 9% 89% 9%



- Molecule 35: 50S ribosomal protein L33

Chain c: 91% 5%



- Molecule 36: 50S ribosomal protein L34

Chain d: 85% 15%

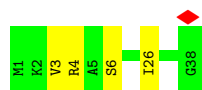
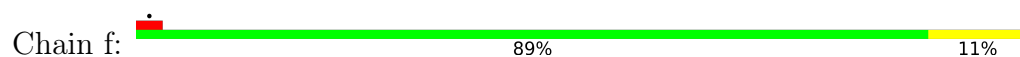


- Molecule 37: 50S ribosomal protein L35

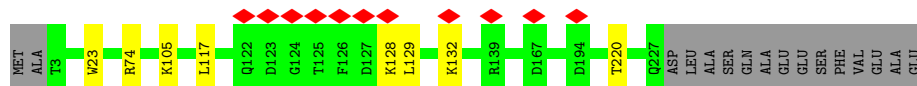
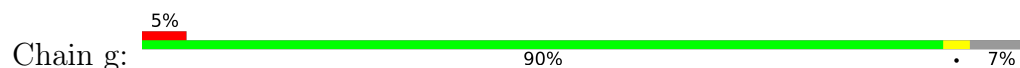
Chain e: 91% 8%



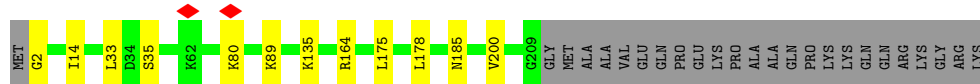
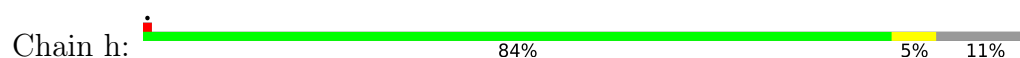
- Molecule 38: 50S ribosomal protein L36



- Molecule 39: 30S ribosomal protein S2



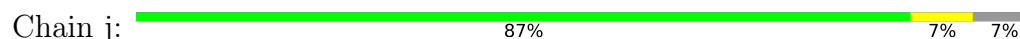
- Molecule 40: 30S ribosomal protein S3



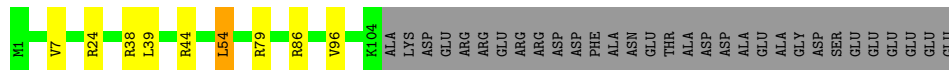
- Molecule 41: 30S ribosomal protein S4



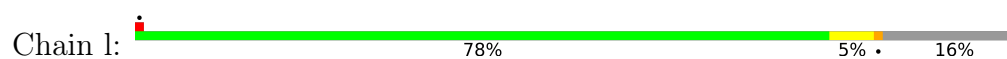
- Molecule 42: 30S ribosomal protein S5



- Molecule 43: 30S ribosomal protein S6

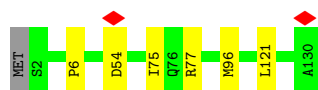


- Molecule 44: 30S ribosomal protein S7




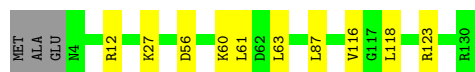
- Molecule 45: 30S ribosomal protein S8

Chain m:  95% 5%




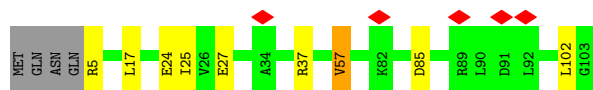
- Molecule 46: 30S ribosomal protein S9

Chain n:  90% 8%




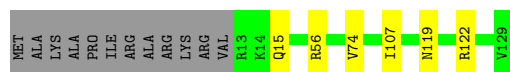
- Molecule 47: 30S ribosomal protein S10

Chain o:  5% 87% 8%



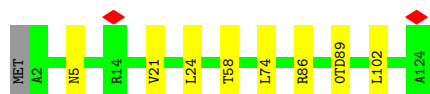
- Molecule 48: 30S ribosomal protein S11

Chain p:  86% 5% 9%




- Molecule 49: 30S ribosomal protein S12

Chain q:  93% 6%



- Molecule 50: 30S ribosomal protein S13

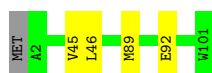
Chain r:  92% 6%



- Molecule 51: 30S ribosomal protein S14

Chain s:  95%





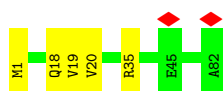
- Molecule 52: 30S ribosomal protein S15

Chain t: 83% 16% .



- Molecule 53: 30S ribosomal protein S16

Chain u: 94% 6%



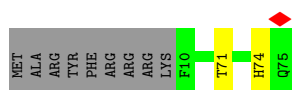
- Molecule 54: 30S ribosomal protein S17

Chain v: 92% 5%



- Molecule 55: 30S ribosomal protein S18

Chain w: 85% 12%



- Molecule 56: 30S ribosomal protein S19

Chain x: 83% 8% 10%

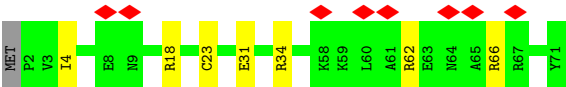
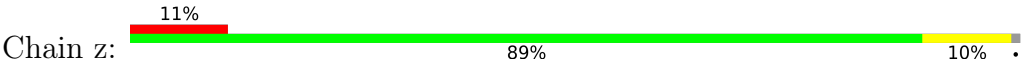


- Molecule 57: 30S ribosomal protein S20

Chain y: 95% 2%



- Molecule 58: 30S ribosomal protein S21



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141950	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	0.807	Depositor
Minimum map value	-0.456	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.05	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: PSU, FME, 7MG, 6MZ, H2U, ZN, 2MA, 5MC, MG, 5MU, 2MG, 3TD, MA6, 4SU, UR3, 1MG, 0TD, G7M, OMG, 8AN, 4OC, OMC, OMU

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	0.42	0/69285	0.74	28/108083 (0.0%)
2	2	0.36	0/36590	0.75	34/57074 (0.1%)
3	3	0.33	0/2872	0.70	0/4478
4	4	0.49	0/122	0.65	0/188
5	5	0.28	0/1672	0.71	0/2603
6	6	0.36	0/265	0.64	0/348
7	7	0.48	0/2741	0.78	0/3692
8	B	0.52	0/2121	0.82	0/2852
9	C	0.50	0/1586	0.73	0/2134
10	D	0.48	0/1571	0.78	2/2113 (0.1%)
11	E	0.48	0/1434	0.79	0/1926
12	F	0.39	0/1333	0.68	0/1805
13	G	0.43	0/1122	0.68	0/1515
14	H	0.49	0/993	0.73	0/1340
15	I	0.45	0/998	0.69	0/1348
16	J	0.55	0/1152	0.80	0/1551
17	K	0.48	0/955	0.80	0/1279
18	L	0.44	0/1062	0.81	0/1413
19	M	0.54	0/1093	0.82	0/1460
20	N	0.52	0/964	0.88	0/1289
21	O	0.49	0/902	0.82	0/1209
22	P	0.50	0/929	0.80	0/1242
23	Q	0.67	0/960	0.96	0/1278
24	R	0.42	0/829	0.73	0/1107
25	S	0.51	0/864	0.83	0/1156
26	T	0.50	0/752	0.76	0/1005
27	U	0.37	0/796	0.66	0/1062
28	V	0.46	0/766	0.72	0/1025
29	W	0.46	0/589	0.78	0/779
30	X	0.59	0/635	0.90	0/848
31	Y	0.53	0/502	0.86	0/667

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Z	0.47	0/452	0.80	0/605
33	a	0.41	0/531	0.70	0/709
34	b	0.46	0/450	0.81	0/599
35	c	0.40	0/433	0.69	0/576
36	d	0.59	0/380	1.06	0/498
37	e	0.47	0/513	0.84	0/676
38	f	0.44	0/303	0.82	1/397 (0.3%)
39	g	0.47	0/1791	0.70	0/2413
40	h	0.45	0/1663	0.79	1/2241 (0.0%)
41	i	0.48	0/1665	0.79	0/2227
42	j	0.49	0/1165	0.79	0/1568
43	k	0.48	0/867	0.78	1/1171 (0.1%)
44	l	0.50	0/1195	0.83	1/1602 (0.1%)
45	m	0.44	0/989	0.72	0/1326
46	n	0.43	0/1034	0.78	0/1375
47	o	0.40	0/800	0.76	0/1082
48	p	0.45	0/893	0.74	0/1205
49	q	0.46	0/960	0.80	0/1286
50	r	0.47	0/909	0.85	0/1215
51	s	0.53	0/817	0.84	0/1088
52	t	0.56	0/722	0.91	0/964
53	u	0.46	0/659	0.76	0/884
54	v	0.35	0/657	0.66	0/881
55	w	0.51	0/553	0.83	0/743
56	x	0.41	0/680	0.65	0/915
57	y	0.58	0/675	0.86	0/895
58	z	0.57	0/597	0.89	0/792
All	All	0.43	0/160808	0.75	68/239802 (0.0%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	h	2	GLY	N-CA-C	-14.12	77.80	113.10
2	2	928	G	N9-C1'-C2'	-12.87	97.26	114.00
2	2	1384	C	N1-C1'-C2'	-11.95	98.46	114.00
1	1	2252	G	N9-C1'-C2'	-11.10	99.57	114.00
1	1	1914	C	C4'-C3'-O3'	10.98	134.97	113.00
2	2	199	A	N9-C1'-C2'	-10.97	99.73	114.00
2	2	1277	C	N1-C1'-C2'	-10.72	100.06	114.00
2	2	1499	A	N9-C1'-C2'	-10.41	100.47	114.00
1	1	2315	G	N9-C1'-C2'	-9.92	101.09	112.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	927	G	N9-C1'-C2'	-9.52	101.53	112.00
2	2	148	G	N9-C1'-C2'	-9.21	101.86	112.00
1	1	1407	G	N9-C1'-C2'	-9.03	102.07	112.00
2	2	1206	G	N9-C1'-C2'	-8.91	102.20	112.00
2	2	1383	C	N1-C1'-C2'	-8.53	102.61	112.00
2	2	1391	U	N1-C1'-C2'	-8.44	102.72	112.00
1	1	1916	A	N9-C1'-C2'	-8.41	102.75	112.00
2	2	480	U	N1-C1'-C2'	-8.21	102.97	112.00
2	2	198	G	N9-C1'-C2'	-8.16	103.02	112.00
1	1	2314	A	N9-C1'-C2'	-8.03	103.17	112.00
1	1	2313	C	N1-C1'-C2'	-7.74	103.49	112.00
2	2	1276	G	N9-C1'-C2'	-7.48	103.77	112.00
1	1	2193	G	C2'-C3'-O3'	7.38	125.73	109.50
2	2	1276	G	C1'-C2'-O2'	-7.25	88.84	110.60
2	2	198	G	C4'-C3'-O3'	7.14	127.28	113.00
1	1	2245	U	N1-C1'-C2'	-7.06	104.23	112.00
2	2	147	G	N9-C1'-C2'	-7.06	104.23	112.00
1	1	754	U	N1-C1'-C2'	6.97	123.06	114.00
1	1	2313	C	C1'-C2'-O2'	-6.75	90.34	110.60
2	2	1390	U	N1-C1'-C2'	-6.51	104.84	112.00
10	D	69	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	1	2250	G	C4'-C3'-O3'	-6.44	95.88	109.40
2	2	480	U	C4'-C3'-O3'	6.36	125.72	113.00
2	2	1276	G	C4'-C3'-O3'	6.33	125.65	113.00
1	1	1379	U	C2'-C3'-O3'	6.30	123.78	113.70
10	D	69	ARG	NE-CZ-NH1	6.19	123.40	120.30
2	2	528	C	C1'-C2'-O2'	-6.06	92.42	110.60
1	1	2425	A	C2'-C3'-O3'	6.03	123.34	113.70
1	1	2313	C	C4'-C3'-O3'	5.84	124.68	113.00
1	1	748	G	C1'-O4'-C4'	-5.83	105.23	109.90
2	2	526	C	N1-C1'-C2'	-5.81	105.61	112.00
1	1	2243	U	N1-C1'-C2'	-5.76	105.66	112.00
44	1	109	ARG	NE-CZ-NH1	5.73	123.17	120.30
2	2	927	G	C4'-C3'-O3'	5.73	124.46	113.00
2	2	928	G	C4'-C3'-O3'	5.70	124.39	113.00
2	2	528	C	N1-C1'-C2'	-5.68	105.75	112.00
2	2	776	G	C2'-C3'-O3'	5.67	122.77	113.70
1	1	783	A	C4'-C3'-O3'	5.66	124.31	113.00
2	2	197	A	N9-C1'-C2'	5.66	121.35	114.00
2	2	196	A	N9-C1'-C2'	-5.59	105.85	112.00
1	1	2613	U	O4'-C1'-N1	5.55	112.64	108.20
2	2	528	C	C4'-C3'-O3'	5.49	123.98	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2252	G	C4'-C3'-O3'	5.46	123.92	113.00
1	1	1914	C	N1-C1'-C2'	-5.44	106.01	112.00
2	2	864	A	N9-C1'-C2'	5.42	121.04	114.00
2	2	529	G	N9-C1'-C2'	-5.39	106.07	112.00
1	1	953	G	C2'-C3'-O3'	5.32	122.21	113.70
1	1	1916	A	C4'-C3'-O3'	5.31	123.63	113.00
2	2	1206	G	C4'-C3'-O3'	5.22	123.45	113.00
2	2	526	C	C4'-C3'-O3'	5.20	123.40	113.00
1	1	1141	U	N1-C1'-C2'	5.19	120.75	114.00
1	1	2074	U	N1-C1'-C2'	5.13	120.67	114.00
1	1	2074	U	C2'-C3'-O3'	5.11	121.88	113.70
1	1	2296	U	C4'-C3'-O3'	5.08	123.15	113.00
2	2	198	G	C1'-C2'-O2'	-5.07	95.38	110.60
43	k	54	LEU	CA-CB-CG	5.07	126.96	115.30
2	2	1208	C	N1-C1'-C2'	-5.07	106.42	112.00
1	1	404	A	C2'-C3'-O3'	5.05	121.79	113.70
38	f	4	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	6	30/61 (49%)	24 (80%)	6 (20%)	0	100	100
7	7	335/365 (92%)	322 (96%)	11 (3%)	2 (1%)	25	55
8	B	269/273 (98%)	249 (93%)	18 (7%)	2 (1%)	22	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	C	207/209 (99%)	196 (95%)	10 (5%)	1 (0%)	29	60
10	D	199/201 (99%)	188 (94%)	10 (5%)	1 (0%)	29	60
11	E	175/179 (98%)	164 (94%)	10 (6%)	1 (1%)	25	55
12	F	173/177 (98%)	165 (95%)	8 (5%)	0	100	100
13	G	147/149 (99%)	132 (90%)	14 (10%)	1 (1%)	22	52
14	H	128/165 (78%)	106 (83%)	19 (15%)	3 (2%)	6	24
15	I	133/142 (94%)	116 (87%)	15 (11%)	2 (2%)	10	35
16	J	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
17	K	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
18	L	142/144 (99%)	135 (95%)	6 (4%)	1 (1%)	22	52
19	M	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
20	N	117/127 (92%)	106 (91%)	11 (9%)	0	100	100
21	O	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
22	P	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
23	Q	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17	47
24	R	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	7	27
25	S	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
26	T	92/100 (92%)	87 (95%)	5 (5%)	0	100	100
27	U	101/104 (97%)	96 (95%)	5 (5%)	0	100	100
28	V	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
29	W	74/85 (87%)	68 (92%)	5 (7%)	1 (1%)	11	36
30	X	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
31	Y	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
32	Z	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
33	a	64/70 (91%)	58 (91%)	6 (9%)	0	100	100
34	b	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
35	c	50/55 (91%)	47 (94%)	3 (6%)	0	100	100
36	d	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
37	e	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
38	f	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
39	g	223/241 (92%)	208 (93%)	14 (6%)	1 (0%)	34	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	h	206/233 (88%)	193 (94%)	12 (6%)	1 (0%)	29	60
41	i	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
42	j	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	25	55
43	k	102/135 (76%)	98 (96%)	3 (3%)	1 (1%)	15	45
44	l	149/179 (83%)	142 (95%)	6 (4%)	1 (1%)	22	52
45	m	127/130 (98%)	120 (94%)	5 (4%)	2 (2%)	9	33
46	n	125/130 (96%)	113 (90%)	11 (9%)	1 (1%)	19	50
47	o	97/103 (94%)	90 (93%)	6 (6%)	1 (1%)	15	45
48	p	115/129 (89%)	103 (90%)	10 (9%)	2 (2%)	9	32
49	q	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
50	r	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
51	s	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
52	t	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	13	40
53	u	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
54	v	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
55	w	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
56	x	81/92 (88%)	77 (95%)	4 (5%)	0	100	100
57	y	84/87 (97%)	84 (100%)	0	0	100	100
58	z	68/71 (96%)	68 (100%)	0	0	100	100
All	All	6234/6646 (94%)	5854 (94%)	350 (6%)	30 (0%)	32	60

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	B	158	ALA
46	n	56	ASP
7	7	137	GLY
11	E	62	GLY
14	H	117	LEU
23	Q	3	ARG
42	j	44	GLY
43	k	96	VAL
47	o	57	VAL
7	7	91	ASP
15	I	113	ALA

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Mol	Chain	Res	Type
40	h	80	LYS
44	l	130	ASN
52	t	21	ASP
8	B	240	PHE
10	D	142	ALA
14	H	51	TYR
24	R	37	GLU
48	p	119	ASN
13	G	89	LYS
14	H	55	VAL
9	C	94	GLN
29	W	29	GLU
39	g	74	ARG
45	m	6	PRO
15	I	136	GLY
48	p	74	VAL
18	L	28	GLY
24	R	44	GLY
45	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	6	27/52 (52%)	24 (89%)	3 (11%)	6	21
7	7	292/310 (94%)	260 (89%)	32 (11%)	6	22
8	B	216/218 (99%)	201 (93%)	15 (7%)	15	42
9	C	164/164 (100%)	159 (97%)	5 (3%)	41	69
10	D	165/165 (100%)	152 (92%)	13 (8%)	12	36
11	E	148/150 (99%)	137 (93%)	11 (7%)	13	39
12	F	136/138 (99%)	130 (96%)	6 (4%)	28	58
13	G	114/114 (100%)	102 (90%)	12 (10%)	7	23
14	H	99/123 (80%)	89 (90%)	10 (10%)	7	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	I	104/110 (94%)	95 (91%)	9 (9%)	10	33
16	J	116/116 (100%)	110 (95%)	6 (5%)	23	52
17	K	104/104 (100%)	98 (94%)	6 (6%)	20	48
18	L	103/103 (100%)	98 (95%)	5 (5%)	25	55
19	M	109/109 (100%)	100 (92%)	9 (8%)	11	35
20	N	99/103 (96%)	90 (91%)	9 (9%)	9	30
21	O	86/87 (99%)	79 (92%)	7 (8%)	11	35
22	P	99/100 (99%)	91 (92%)	8 (8%)	11	35
23	Q	89/90 (99%)	84 (94%)	5 (6%)	21	49
24	R	84/84 (100%)	75 (89%)	9 (11%)	6	23
25	S	93/93 (100%)	85 (91%)	8 (9%)	10	33
26	T	81/84 (96%)	78 (96%)	3 (4%)	34	64
27	U	84/85 (99%)	78 (93%)	6 (7%)	14	41
28	V	78/78 (100%)	76 (97%)	2 (3%)	46	72
29	W	58/63 (92%)	54 (93%)	4 (7%)	15	42
30	X	67/68 (98%)	61 (91%)	6 (9%)	9	30
31	Y	54/55 (98%)	49 (91%)	5 (9%)	9	29
32	Z	48/49 (98%)	42 (88%)	6 (12%)	4	16
33	a	59/62 (95%)	52 (88%)	7 (12%)	5	18
34	b	47/48 (98%)	42 (89%)	5 (11%)	6	23
35	c	47/49 (96%)	45 (96%)	2 (4%)	29	59
36	d	38/38 (100%)	31 (82%)	7 (18%)	1	6
37	e	51/52 (98%)	46 (90%)	5 (10%)	8	26
38	f	34/34 (100%)	31 (91%)	3 (9%)	10	32
39	g	187/199 (94%)	180 (96%)	7 (4%)	34	64
40	h	171/190 (90%)	161 (94%)	10 (6%)	20	48
41	i	172/173 (99%)	163 (95%)	9 (5%)	23	52
42	j	119/126 (94%)	109 (92%)	10 (8%)	11	34
43	k	91/116 (78%)	83 (91%)	8 (9%)	10	32
44	l	124/147 (84%)	113 (91%)	11 (9%)	9	31
45	m	104/105 (99%)	100 (96%)	4 (4%)	33	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	n	105/107 (98%)	96 (91%)	9 (9%)	10	33
47	o	86/90 (96%)	77 (90%)	9 (10%)	7	23
48	p	90/99 (91%)	86 (96%)	4 (4%)	28	58
49	q	102/103 (99%)	95 (93%)	7 (7%)	15	42
50	r	94/96 (98%)	87 (93%)	7 (7%)	13	39
51	s	83/84 (99%)	79 (95%)	4 (5%)	25	55
52	t	76/77 (99%)	63 (83%)	13 (17%)	2	7
53	u	65/65 (100%)	60 (92%)	5 (8%)	13	38
54	v	74/78 (95%)	71 (96%)	3 (4%)	30	61
55	w	57/65 (88%)	55 (96%)	2 (4%)	36	66
56	x	72/79 (91%)	65 (90%)	7 (10%)	8	27
57	y	65/66 (98%)	62 (95%)	3 (5%)	27	57
58	z	60/61 (98%)	53 (88%)	7 (12%)	5	19
All	All	5190/5424 (96%)	4802 (92%)	388 (8%)	17	39

All (388) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	17	GLU
6	6	18	THR
6	6	20	LEU
7	7	14	LEU
7	7	17	ARG
7	7	27	TYR
7	7	31	LYS
7	7	42	GLU
7	7	54	GLN
7	7	79	ASP
7	7	86	LEU
7	7	102	GLU
7	7	107	GLU
7	7	112	GLN
7	7	114	GLU
7	7	117	ARG
7	7	122	GLU
7	7	123	TYR
7	7	124	ASP

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Mol	Chain	Res	Type
7	7	186	ASP
7	7	195	GLU
7	7	242	ASP
7	7	258	GLU
7	7	270	ILE
7	7	272	THR
7	7	276	ASN
7	7	279	SER
7	7	285	ASP
7	7	288	MET
7	7	292	LYS
7	7	324	ARG
7	7	337	ARG
7	7	343	ARG
7	7	354	ASP
7	7	362	LYS
8	B	51	THR
8	B	52	ARG
8	B	115	GLN
8	B	125	LYS
8	B	156	ARG
8	B	174	LEU
8	B	189	ARG
8	B	202	LEU
8	B	203	ARG
8	B	204	VAL
8	B	242	LYS
8	B	252	THR
8	B	257	THR
8	B	258	ARG
8	B	261	LYS
9	C	2	ILE
9	C	4	LEU
9	C	13	ARG
9	C	46	ARG
9	C	59	ARG
10	D	9	GLN
10	D	21	ARG
10	D	40	ARG
10	D	48	THR
10	D	57	LYS
10	D	67	ARG

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Mol	Chain	Res	Type
10	D	69	ARG
10	D	77	ILE
10	D	105	LEU
10	D	108	ILE
10	D	109	LEU
10	D	122	GLU
10	D	149	ILE
11	E	10	ASP
11	E	57	LEU
11	E	80	ARG
11	E	95	ARG
11	E	115	ARG
11	E	117	LEU
11	E	122	PHE
11	E	123	ASP
11	E	133	ARG
11	E	140	GLU
11	E	152	LEU
12	F	32	GLU
12	F	95	ARG
12	F	104	ASN
12	F	114	ASP
12	F	152	ARG
12	F	176	LYS
13	G	1	MET
13	G	11	ASN
13	G	12	LEU
13	G	15	LEU
13	G	41	LYS
13	G	51	ARG
13	G	66	ASN
13	G	72	ILE
13	G	87	GLU
13	G	96	THR
13	G	97	ARG
13	G	114	GLU
14	H	3	LEU
14	H	7	ASP
14	H	9	GLN
14	H	29	ASP
14	H	37	LYS
14	H	40	GLU

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Mol	Chain	Res	Type
14	H	57	ASN
14	H	109	LYS
14	H	114	GLU
14	H	123	ILE
15	I	10	LEU
15	I	11	GLN
15	I	38	CYS
15	I	44	LYS
15	I	71	LYS
15	I	78	LEU
15	I	79	LEU
15	I	95	ASP
15	I	137	LEU
16	J	5	THR
16	J	30	THR
16	J	40	HIS
16	J	65	THR
16	J	70	THR
16	J	108	MET
17	K	17	ARG
17	K	49	ARG
17	K	53	LYS
17	K	70	ARG
17	K	91	SER
17	K	99	ILE
18	L	2	ARG
18	L	42	SER
18	L	48	ARG
18	L	59	ARG
18	L	78	ARG
19	M	6	ARG
19	M	14	LYS
19	M	18	ARG
19	M	40	ARG
19	M	95	LEU
19	M	110	GLU
19	M	115	GLU
19	M	126	ILE
19	M	134	THR
20	N	1	MET
20	N	2	ARG
20	N	20	MET

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Mol	Chain	Res	Type
20	N	46	ARG
20	N	51	LEU
20	N	59	SER
20	N	63	ARG
20	N	69	ARG
20	N	95	THR
21	O	8	ILE
21	O	19	GLN
21	O	20	GLU
21	O	31	THR
21	O	48	LEU
21	O	94	ARG
21	O	102	ARG
22	P	8	LEU
22	P	11	GLU
22	P	26	VAL
22	P	27	GLU
22	P	81	VAL
22	P	109	ARG
22	P	110	ILE
22	P	114	LEU
23	Q	3	ARG
23	Q	51	ARG
23	Q	75	SER
23	Q	91	ASP
23	Q	117	LEU
24	R	10	LYS
24	R	39	LEU
24	R	40	MET
24	R	48	LYS
24	R	55	ASP
24	R	68	ARG
24	R	71	LYS
24	R	72	VAL
24	R	86	GLN
25	S	7	HIS
25	S	12	SER
25	S	19	LEU
25	S	67	ASP
25	S	69	LEU
25	S	107	VAL
25	S	108	SER

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Mol	Chain	Res	Type
25	S	110	ARG
26	T	1	MET
26	T	25	GLU
26	T	78	SER
27	U	6	ARG
27	U	8	ASP
27	U	22	ARG
27	U	52	LEU
27	U	68	SER
27	U	99	ASN
28	V	1	MET
28	V	40	ILE
29	W	10	THR
29	W	11	ARG
29	W	64	ASP
29	W	70	GLU
30	X	11	ARG
30	X	25	THR
30	X	33	LEU
30	X	48	THR
30	X	54	LYS
30	X	56	MET
31	Y	7	ARG
31	Y	18	LEU
31	Y	48	ARG
31	Y	49	ASP
31	Y	57	LEU
32	Z	6	LYS
32	Z	10	THR
32	Z	11	ARG
32	Z	31	ARG
32	Z	36	VAL
32	Z	45	ARG
33	a	16	CYS
33	a	24	ILE
33	a	43	PHE
33	a	45	THR
33	a	47	LYS
33	a	56	ARG
33	a	63	ARG
34	b	9	THR
34	b	11	SER

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Mol	Chain	Res	Type
34	b	12	LYS
34	b	27	SER
34	b	40	ARG
35	c	5	ILE
35	c	13	SER
36	d	3	ARG
36	d	12	ARG
36	d	24	THR
36	d	41	ARG
36	d	42	LEU
36	d	43	THR
36	d	45	SER
37	e	16	LYS
37	e	30	ARG
37	e	31	HIS
37	e	54	ASP
37	e	55	LEU
38	f	3	VAL
38	f	6	SER
38	f	26	ILE
39	g	23	TRP
39	g	105	LYS
39	g	117	LEU
39	g	128	LYS
39	g	129	LEU
39	g	132	LYS
39	g	220	THR
40	h	14	ILE
40	h	33	LEU
40	h	35	SER
40	h	89	LYS
40	h	135	LYS
40	h	164	ARG
40	h	175	LEU
40	h	178	LEU
40	h	185	ASN
40	h	200	VAL
41	i	5	LEU
41	i	47	ARG
41	i	95	GLU
41	i	104	ARG
41	i	116	GLN

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Mol	Chain	Res	Type
41	i	138	SER
41	i	143	VAL
41	i	197	GLU
41	i	206	LYS
42	j	10	GLU
42	j	15	LEU
42	j	18	VAL
42	j	60	ILE
42	j	65	GLU
42	j	114	VAL
42	j	115	LEU
42	j	138	ARG
42	j	141	ILE
42	j	142	ASP
43	k	7	VAL
43	k	24	ARG
43	k	38	ARG
43	k	39	LEU
43	k	44	ARG
43	k	54	LEU
43	k	79	ARG
43	k	86	ARG
44	l	7	ILE
44	l	17	LYS
44	l	21	GLU
44	l	23	LEU
44	l	27	VAL
44	l	79	ARG
44	l	97	ASN
44	l	109	ARG
44	l	123	GLU
44	l	130	ASN
44	l	146	GLU
45	m	54	ASP
45	m	77	ARG
45	m	96	MET
45	m	121	LEU
46	n	12	ARG
46	n	27	LYS
46	n	60	LYS
46	n	61	LEU
46	n	63	LEU

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Mol	Chain	Res	Type
46	n	87	LEU
46	n	116	VAL
46	n	118	LEU
46	n	123	ARG
47	o	5	ARG
47	o	17	LEU
47	o	24	GLU
47	o	25	ILE
47	o	27	GLU
47	o	37	ARG
47	o	57	VAL
47	o	85	ASP
47	o	102	LEU
48	p	15	GLN
48	p	56	ARG
48	p	107	ILE
48	p	122	ARG
49	q	5	ASN
49	q	21	VAL
49	q	24	LEU
49	q	58	THR
49	q	74	LEU
49	q	86	ARG
49	q	102	LEU
50	r	16	VAL
50	r	25	VAL
50	r	29	ARG
50	r	59	GLU
50	r	76	SER
50	r	93	ARG
50	r	104	THR
51	s	45	VAL
51	s	46	LEU
51	s	89	MET
51	s	92	GLU
52	t	10	LYS
52	t	17	ARG
52	t	18	ASP
52	t	22	THR
52	t	39	LEU
52	t	40	GLN
52	t	61	SER

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Mol	Chain	Res	Type
52	t	64	ARG
52	t	66	LEU
52	t	67	LEU
52	t	70	LEU
52	t	84	ARG
52	t	85	LEU
53	u	1	MET
53	u	18	GLN
53	u	19	VAL
53	u	20	VAL
53	u	35	ARG
54	v	67	LEU
54	v	75	LEU
54	v	79	VAL
55	w	71	THR
55	w	74	HIS
56	x	12	ASP
56	x	21	LYS
56	x	33	THR
56	x	58	VAL
56	x	69	HIS
56	x	79	THR
56	x	81	ARG
57	y	6	SER
57	y	10	ARG
57	y	54	MET
58	z	4	ILE
58	z	18	ARG
58	z	23	CYS
58	z	31	GLU
58	z	34	ARG
58	z	62	ARG
58	z	66	ARG

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

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2897/2904 (99%)	559 (19%)	70 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	1528/1534 (99%)	309 (20%)	34 (2%)
3	3	119/120 (99%)	18 (15%)	0
4	4	4/18 (22%)	1 (25%)	0
5	5	73/78 (93%)	20 (27%)	8 (10%)
All	All	4621/4654 (99%)	907 (19%)	112 (2%)

All (907) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	23	G
1	1	34	U
1	1	35	G
1	1	45	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	84	A
1	1	85	G
1	1	96	C
1	1	102	U
1	1	103	A
1	1	118	A
1	1	119	A
1	1	120	U
1	1	131	A
1	1	139	U
1	1	140	C
1	1	141	G
1	1	142	A
1	1	143	C
1	1	149	A
1	1	163	C
1	1	165	A
1	1	181	A
1	1	196	A
1	1	215	G

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Mol	Chain	Res	Type
1	1	216	A
1	1	222	A
1	1	225	C
1	1	248	G
1	1	249	C
1	1	264	C
1	1	265	A
1	1	266	G
1	1	270	A
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	304	U
1	1	311	A
1	1	324	A
1	1	329	G
1	1	330	A
1	1	353	C
1	1	361	G
1	1	362	A
1	1	371	A
1	1	372	G
1	1	373	U
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	455	C
1	1	456	C
1	1	457	A
1	1	477	A
1	1	480	A
1	1	481	G
1	1	491	G

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Mol	Chain	Res	Type
1	1	501	A
1	1	503	A
1	1	504	A
1	1	505	A
1	1	509	C
1	1	522	A
1	1	529	A
1	1	532	A
1	1	533	G
1	1	538	A
1	1	543	G
1	1	544	C
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	573	U
1	1	575	A
1	1	586	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	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	687	C
1	1	710	U
1	1	717	C
1	1	730	A

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Mol	Chain	Res	Type
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
1	1	782	A
1	1	784	G
1	1	785	G
1	1	800	A
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	830	G
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	887	A
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	905	A
1	1	907	G
1	1	910	A
1	1	914	G
1	1	915	C
1	1	931	U

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Mol	Chain	Res	Type
1	1	932	U
1	1	941	A
1	1	945	A
1	1	946	C
1	1	953	G
1	1	954	G
1	1	961	C
1	1	974	G
1	1	983	A
1	1	984	A
1	1	985	C
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1012	U
1	1	1013	C
1	1	1022	G
1	1	1023	U
1	1	1025	G
1	1	1026	G
1	1	1033	U
1	1	1040	A
1	1	1041	G
1	1	1042	G
1	1	1043	C
1	1	1045	C
1	1	1046	A
1	1	1047	G
1	1	1060	U
1	1	1061	U
1	1	1063	G
1	1	1064	C
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1069	A
1	1	1070	A
1	1	1073	A
1	1	1074	G
1	1	1079	C
1	1	1080	A

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Mol	Chain	Res	Type
1	1	1081	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
1	1	1132	U
1	1	1134	A
1	1	1135	C
1	1	1142	A
1	1	1143	A
1	1	1156	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	1187	G
1	1	1236	G
1	1	1238	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	1300	G
1	1	1301	A
1	1	1321	A

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Mol	Chain	Res	Type
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	1395	A
1	1	1404	C
1	1	1405	U
1	1	1406	U
1	1	1407	G
1	1	1408	G
1	1	1409	U
1	1	1411	U
1	1	1414	C
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	1491	G
1	1	1493	C
1	1	1497	U
1	1	1502	A
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

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Mol	Chain	Res	Type
1	1	1537	G
1	1	1554	U
1	1	1558	C
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	1583	A
1	1	1584	U
1	1	1589	U
1	1	1590	A
1	1	1591	A
1	1	1596	A
1	1	1608	A
1	1	1609	A
1	1	1610	A
1	1	1619	G
1	1	1630	A
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G
1	1	1674	G
1	1	1703	G
1	1	1714	U
1	1	1715	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1750	G
1	1	1758	U
1	1	1764	C
1	1	1773	A
1	1	1791	A
1	1	1800	C
1	1	1808	A
1	1	1811	G
1	1	1816	C
1	1	1829	A

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Mol	Chain	Res	Type
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	1917	PSU
1	1	1918	A
1	1	1919	A
1	1	1923	U
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	1960	A
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	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

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Mol	Chain	Res	Type
1	1	2027	G
1	1	2033	A
1	1	2036	C
1	1	2041	U
1	1	2043	C
1	1	2049	G
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	2080	A
1	1	2093	G
1	1	2097	A
1	1	2099	U
1	1	2101	A
1	1	2108	A
1	1	2110	G
1	1	2111	U
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2120	G
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

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Mol	Chain	Res	Type
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	2186	G
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
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	2243	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

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Mol	Chain	Res	Type
1	1	2288	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	2336	A
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2352	A
1	1	2357	G
1	1	2361	G
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
1	1	2435	A
1	1	2436	G
1	1	2441	U
1	1	2445	2MG
1	1	2447	G
1	1	2448	A
1	1	2459	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

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Mol	Chain	Res	Type
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	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	2584	U
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	2630	G
1	1	2663	G
1	1	2671	G
1	1	2682	A
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2720	U
1	1	2726	A
1	1	2733	A
1	1	2744	G
1	1	2746	U
1	1	2748	A
1	1	2758	A

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Mol	Chain	Res	Type
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	2825	G
1	1	2836	U
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	9	G
2	2	22	G
2	2	32	A
2	2	39	G
2	2	41	G
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	58	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

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Mol	Chain	Res	Type
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	116	A
2	2	120	A
2	2	121	U
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	161	A
2	2	164	G
2	2	173	U
2	2	181	A
2	2	182	A
2	2	196	A
2	2	197	A
2	2	198	G
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	214	C
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	258	G
2	2	262	A
2	2	266	G
2	2	267	C
2	2	271	C

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Mol	Chain	Res	Type
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	330	C
2	2	332	G
2	2	347	G
2	2	352	C
2	2	354	G
2	2	355	C
2	2	367	U
2	2	372	C
2	2	373	A
2	2	374	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	428	G
2	2	429	U
2	2	446	G
2	2	451	A
2	2	457	G
2	2	458	U
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	469	C

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Mol	Chain	Res	Type
2	2	478	A
2	2	479	U
2	2	480	U
2	2	481	G
2	2	482	A
2	2	484	G
2	2	485	U
2	2	486	U
2	2	505	G
2	2	511	C
2	2	516	PSU
2	2	517	G
2	2	518	C
2	2	519	C
2	2	528	C
2	2	529	G
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	564	C
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	607	A
2	2	628	G
2	2	633	G
2	2	642	A
2	2	650	G
2	2	653	U
2	2	665	A
2	2	666	G
2	2	700	G
2	2	723	U
2	2	724	G
2	2	731	G

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Mol	Chain	Res	Type
2	2	733	G
2	2	747	A
2	2	748	G
2	2	755	G
2	2	763	G
2	2	777	A
2	2	793	U
2	2	794	A
2	2	799	G
2	2	810	C
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	846	G
2	2	849	G
2	2	851	G
2	2	874	G
2	2	876	C
2	2	887	G
2	2	902	G
2	2	914	A
2	2	916	U
2	2	926	G
2	2	928	G
2	2	934	C
2	2	935	A
2	2	936	C
2	2	960	U
2	2	961	U
2	2	963	G
2	2	965	U
2	2	966	2MG
2	2	967	5MC
2	2	968	A
2	2	969	A
2	2	972	C
2	2	975	A

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Mol	Chain	Res	Type
2	2	976	G
2	2	977	A
2	2	978	A
2	2	989	U
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	1033	G
2	2	1037	C
2	2	1042	A
2	2	1043	G
2	2	1044	A
2	2	1046	A
2	2	1056	U
2	2	1065	U
2	2	1085	U
2	2	1094	G
2	2	1095	U
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

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Mol	Chain	Res	Type
2	2	1145	A
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1154	G
2	2	1158	C
2	2	1159	U
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	1212	U
2	2	1213	A
2	2	1214	C
2	2	1215	G
2	2	1225	A
2	2	1226	C
2	2	1227	A
2	2	1228	C
2	2	1238	A
2	2	1239	A
2	2	1246	A
2	2	1257	A
2	2	1260	G
2	2	1275	A
2	2	1277	C
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	1311	A

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Mol	Chain	Res	Type
2	2	1312	G
2	2	1317	C
2	2	1320	C
2	2	1329	A
2	2	1338	G
2	2	1340	A
2	2	1346	A
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	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	1493	A
2	2	1494	G
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	1531	A
2	2	1534	A
3	3	2	G
3	3	9	G
3	3	13	G
3	3	16	G
3	3	17	C

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Mol	Chain	Res	Type
3	3	21	G
3	3	35	C
3	3	45	A
3	3	51	G
3	3	56	G
3	3	57	A
3	3	66	A
3	3	67	G
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	3	G
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	31	G
5	5	47	U
5	5	48	C
5	5	55	PSU
5	5	57	A
5	5	60	U
5	5	69	C
5	5	74	C

All (112) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	62	U
1	1	70	G
1	1	140	C
1	1	142	A

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Mol	Chain	Res	Type
1	1	271	G
1	1	404	A
1	1	446	G
1	1	503	A
1	1	532	A
1	1	545	U
1	1	548	G
1	1	555	G
1	1	685	A
1	1	752	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	1045	C
1	1	1063	G
1	1	1064	C
1	1	1069	A
1	1	1110	G
1	1	1128	G
1	1	1142	A
1	1	1173	U
1	1	1177	G
1	1	1205	A
1	1	1253	A
1	1	1320	C
1	1	1344	U
1	1	1379	U
1	1	1415	U
1	1	1490	A
1	1	1509	A
1	1	1583	A
1	1	1584	U
1	1	1608	A
1	1	1847	A
1	1	1900	A
1	1	1912	A
1	1	1913	A
1	1	1918	A

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Mol	Chain	Res	Type
1	1	1962	5MC
1	1	2062	A
1	1	2074	U
1	1	2146	C
1	1	2162	G
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	2308	G
1	1	2324	U
1	1	2326	C
1	1	2425	A
1	1	2447	G
1	1	2506	U
1	1	2572	A
1	1	2585	U
1	1	2610	C
1	1	2798	U
1	1	2849	U
1	1	2873	A
2	2	70	U
2	2	106	C
2	2	181	A
2	2	183	C
2	2	197	A
2	2	209	U
2	2	428	G
2	2	438	U
2	2	481	G
2	2	517	G
2	2	527	7MG
2	2	531	U
2	2	560	A
2	2	641	U
2	2	722	G
2	2	793	U
2	2	966	2MG
2	2	967	5MC

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Mol	Chain	Res	Type
2	2	991	U
2	2	992	U
2	2	1145	A
2	2	1196	A
2	2	1211	U
2	2	1213	A
2	2	1214	C
2	2	1225	A
2	2	1299	A
2	2	1363	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	8	4SU
5	5	16	C
5	5	17	U
5	5	18	G
5	5	20	H2U
5	5	21	A
5	5	47	U
5	5	60	U

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

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	$\# Z  > 2$
1	PSU	1	1917	1	18,21,22	0.91	1 (5%)	22,30,33	1.01	1 (4%)
5	4OC	5	32	5	20,23,24	0.59	0	26,32,35	1.21	2 (7%)
1	PSU	1	746	59,1	18,21,22	2.14	1 (5%)	22,30,33	2.11	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	5MC	2	967	2	18,22,23	0.85	1 (5%)	26,32,35	1.45	3 (11%)
1	5MU	1	1939	59,1	19,22,23	0.84	1 (5%)	28,32,35	0.99	3 (10%)
2	PSU	2	516	2,59	18,21,22	1.57	1 (5%)	22,30,33	1.61	2 (9%)
2	UR3	2	1498	2	19,22,23	1.35	2 (10%)	26,32,35	1.24	5 (19%)
1	1MG	1	745	1	18,26,27	1.62	2 (11%)	19,39,42	2.04	4 (21%)
2	2MG	2	1516	2	18,26,27	1.26	3 (16%)	16,38,41	1.59	3 (18%)
2	MA6	2	1519	2	19,26,27	0.57	0	18,38,41	0.85	1 (5%)
1	G7M	1	2069	1	20,26,27	1.64	1 (5%)	17,39,42	2.53	5 (29%)
1	OMG	1	2251	5,1	18,26,27	1.67	4 (22%)	19,38,41	2.15	5 (26%)
5	PSU	5	55	5	18,21,22	1.86	1 (5%)	22,30,33	1.57	3 (13%)
1	PSU	1	2504	1	18,21,22	1.64	1 (5%)	22,30,33	1.65	3 (13%)
1	2MG	1	2445	1	18,26,27	1.24	2 (11%)	16,38,41	1.64	3 (18%)
1	PSU	1	2605	1	18,21,22	1.98	1 (5%)	22,30,33	1.70	3 (13%)
1	PSU	1	2457	1	18,21,22	2.15	1 (5%)	22,30,33	1.54	4 (18%)
1	6MZ	1	1618	1	18,25,26	0.95	1 (5%)	16,36,39	1.65	2 (12%)
2	4OC	2	1402	2	20,23,24	1.18	2 (10%)	26,32,35	1.12	2 (7%)
5	8AN	5	76	5,59,60,1	19,24,25	0.68	0	13,35,38	0.83	1 (7%)
2	7MG	2	527	2,59	22,26,27	1.47	4 (18%)	29,39,42	2.86	12 (41%)
2	2MG	2	1207	2	18,26,27	1.63	4 (22%)	16,38,41	1.07	1 (6%)
2	MA6	2	1518	2	19,26,27	0.57	0	18,38,41	0.78	0
1	2MA	1	2503	59,1	17,25,26	1.17	3 (17%)	17,37,40	3.14	6 (35%)
5	5MU	5	54	5	19,22,23	0.64	0	28,32,35	1.00	3 (10%)
49	0TD	q	89	49	7,9,10	6.74	5 (71%)	6,11,13	4.11	2 (33%)
1	5MC	1	1962	1	18,22,23	0.85	1 (5%)	26,32,35	1.52	4 (15%)
1	6MZ	1	2030	1	18,25,26	1.23	1 (5%)	16,36,39	2.10	5 (31%)
5	4SU	5	8	5	18,21,22	1.64	3 (16%)	26,30,33	2.75	9 (34%)
2	5MC	2	1407	2	18,22,23	0.90	1 (5%)	26,32,35	1.30	3 (11%)
1	3TD	1	1915	1	18,22,23	2.35	2 (11%)	22,32,35	2.63	6 (27%)
1	PSU	1	955	1	18,21,22	2.17	2 (11%)	22,30,33	1.57	3 (13%)
1	PSU	1	1911	1	18,21,22	1.44	4 (22%)	22,30,33	2.08	4 (18%)
1	2MG	1	1835	1	18,26,27	1.21	3 (16%)	16,38,41	1.61	3 (18%)
1	5MU	1	747	1	19,22,23	0.75	1 (5%)	28,32,35	1.01	3 (10%)
5	H2U	5	20	5	18,21,22	0.63	0	21,30,33	1.93	4 (19%)
1	OMU	1	2552	1	19,22,23	0.48	0	26,31,34	0.82	1 (3%)
1	PSU	1	2580	1	18,21,22	1.83	1 (5%)	22,30,33	1.61	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMC	1	2498	59,1	19,22,23	1.14	2 (10%)	26,31,34	1.63	4 (15%)
2	2MG	2	966	2	18,26,27	1.21	3 (16%)	16,38,41	2.15	3 (18%)

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
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
5	4OC	5	32	5	-	0/9/29/30	0/2/2/2
1	PSU	1	746	59,1	-	2/7/25/26	0/2/2/2
2	5MC	2	967	2	-	5/7/25/26	0/2/2/2
1	5MU	1	1939	59,1	-	0/7/25/26	0/2/2/2
2	PSU	2	516	2,59	-	2/7/25/26	0/2/2/2
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
2	MA6	2	1519	2	-	6/7/29/30	0/3/3/3
1	G7M	1	2069	1	-	2/3/25/26	0/3/3/3
1	OMG	1	2251	5,1	-	0/5/27/28	0/3/3/3
5	PSU	5	55	5	-	3/7/25/26	0/2/2/2
1	PSU	1	2504	1	-	1/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	6MZ	1	1618	1	-	4/5/27/28	0/3/3/3
2	4OC	2	1402	2	-	0/9/29/30	0/2/2/2
5	8AN	5	76	5,59,60,1	-	3/3/25/26	0/3/3/3
2	7MG	2	527	2,59	-	0/7/37/38	0/3/3/3
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
2	MA6	2	1518	2	-	0/7/29/30	0/3/3/3
1	2MA	1	2503	59,1	-	1/3/25/26	0/3/3/3
5	5MU	5	54	5	-	0/7/25/26	0/2/2/2
49	0TD	q	89	49	-	2/7/12/14	-
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
1	6MZ	1	2030	1	-	2/5/27/28	0/3/3/3
5	4SU	5	8	5	-	2/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	3TD	1	1915	1	-	5/7/25/26	0/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1911	1	-	1/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	0/5/27/28	0/3/3/3
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
5	H2U	5	20	5	-	4/7/38/39	0/2/2/2
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2498	59,1	-	2/9/27/28	0/2/2/2
2	2MG	2	966	2	-	3/5/27/28	0/3/3/3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	q	89	0TD	CB-SB	-16.93	1.65	1.82
1	1	1915	3TD	C1'-C5	-9.08	1.29	1.50
1	1	746	PSU	C2'-C1'	-8.86	1.42	1.53
1	1	955	PSU	C2'-C1'	-8.65	1.42	1.53
1	1	2457	PSU	C2'-C1'	-8.61	1.42	1.53
1	1	2605	PSU	C2'-C1'	-7.97	1.43	1.53
5	5	55	PSU	C2'-C1'	-7.67	1.43	1.53
1	1	2580	PSU	C2'-C1'	-7.43	1.44	1.53
1	1	2504	PSU	C2'-C1'	-6.55	1.45	1.53
2	2	516	PSU	C2'-C1'	-6.32	1.45	1.53
1	1	2069	G7M	C2'-C1'	-6.30	1.44	1.53
5	5	8	4SU	C4-S4	-4.73	1.59	1.68
1	1	745	1MG	C2'-C1'	-4.69	1.46	1.53
1	1	2251	OMG	C3'-C2'	-4.42	1.43	1.52
1	1	2030	6MZ	C2'-C1'	-4.05	1.47	1.53
2	2	1207	2MG	C2'-C1'	-3.61	1.48	1.53
2	2	527	7MG	C4-N9	-3.52	1.33	1.37
1	1	2498	OMC	C3'-C2'	-3.48	1.45	1.52
49	q	89	0TD	CA-N	-3.17	1.37	1.47
2	2	1207	2MG	C6-N1	3.17	1.42	1.37
1	1	2445	2MG	C5-C6	-3.15	1.41	1.47
5	5	8	4SU	C5-C4	-2.97	1.38	1.42
1	1	1911	PSU	C4-N3	-2.95	1.33	1.38
2	2	1516	2MG	C5-C6	-2.95	1.41	1.47
1	1	745	1MG	C5-C6	-2.90	1.38	1.47
1	1	1835	2MG	C5-C6	-2.89	1.41	1.47
2	2	527	7MG	C5-N7	-2.88	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	527	7MG	C6-N1	-2.87	1.33	1.38
1	1	1962	5MC	C2'-C1'	-2.76	1.44	1.53
1	1	1939	5MU	C2'-C1'	-2.76	1.44	1.53
1	1	2251	OMG	C6-N1	2.75	1.42	1.37
2	2	966	2MG	C5-C6	-2.73	1.41	1.47
49	q	89	0TD	OD2-CG	-2.70	1.21	1.30
49	q	89	0TD	CB-CG	-2.68	1.47	1.52
1	1	2498	OMC	C2'-C1'	-2.66	1.46	1.53
2	2	966	2MG	C6-N1	2.65	1.41	1.37
1	1	1618	6MZ	C2'-C1'	-2.64	1.49	1.53
2	2	527	7MG	C5-C4	2.61	1.46	1.38
2	2	1498	UR3	O4-C4	-2.57	1.18	1.23
49	q	89	0TD	CSB-SB	-2.53	1.74	1.79
2	2	1516	2MG	C6-N1	2.51	1.41	1.37
1	1	1911	PSU	C6-C5	2.50	1.38	1.35
2	2	967	5MC	C2'-C1'	-2.48	1.45	1.53
2	2	1207	2MG	C5-C4	-2.48	1.36	1.43
1	1	2445	2MG	C5-C4	-2.45	1.36	1.43
1	1	1915	3TD	C4-N3	-2.43	1.35	1.40
2	2	1407	5MC	C2'-C1'	-2.39	1.45	1.53
1	1	2503	2MA	C2'-C3'	-2.38	1.46	1.53
1	1	1835	2MG	C5-C4	-2.36	1.37	1.43
1	1	2251	OMG	C5-C6	-2.32	1.42	1.47
2	2	1402	4OC	C6-N1	-2.30	1.32	1.38
2	2	966	2MG	C5-C4	-2.27	1.37	1.43
1	1	1917	PSU	C2'-C1'	-2.22	1.50	1.53
1	1	955	PSU	C3'-C2'	-2.22	1.47	1.53
2	2	1516	2MG	C5-C4	-2.21	1.37	1.43
1	1	2251	OMG	C5-C4	-2.20	1.37	1.43
1	1	1835	2MG	C6-N1	2.18	1.41	1.37
1	1	1911	PSU	C2-N3	-2.16	1.33	1.37
1	1	747	5MU	C2'-C1'	-2.14	1.46	1.53
1	1	1911	PSU	C2-N1	-2.13	1.33	1.36
2	2	1498	UR3	C6-N1	-2.13	1.32	1.38
2	2	1207	2MG	C5-C6	-2.10	1.43	1.47
1	1	2503	2MA	C5-C4	-2.09	1.37	1.43
1	1	2503	2MA	C8-N7	-2.07	1.31	1.35
5	5	8	4SU	C4-N3	-2.05	1.35	1.37
2	2	1402	4OC	C2-N3	-2.01	1.32	1.36

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	527	7MG	N9-C4-N3	8.97	138.88	125.47
1	1	2503	2MA	C3'-C2'-C1'	-8.82	87.69	100.98
1	1	746	PSU	C3'-C2'-C1'	7.73	110.64	101.64
1	1	1915	3TD	O5'-C5'-C4'	7.70	135.17	108.99
49	q	89	0TD	CB-CA-N	-7.52	93.08	109.10
5	5	8	4SU	C5-C4-N3	7.17	121.34	114.69
2	2	966	2MG	O3'-C3'-C4'	6.98	131.23	111.05
5	5	8	4SU	C4-N3-C2	-6.94	120.60	127.34
1	1	2069	G7M	O2'-C2'-C3'	6.63	133.26	111.82
1	1	1911	PSU	N1-C2-N3	6.31	122.28	115.13
49	q	89	0TD	CSB-SB-CB	6.19	113.63	102.44
1	1	1915	3TD	N1-C2-N3	6.01	120.88	116.14
5	5	8	4SU	C5-C4-S4	-5.98	116.77	124.47
2	2	967	5MC	O3'-C3'-C4'	5.70	127.52	111.05
1	1	745	1MG	C3'-C2'-C1'	5.57	109.37	100.98
2	2	527	7MG	C5-C4-N3	-5.51	117.62	128.13
2	2	516	PSU	O2'-C2'-C3'	5.47	129.52	111.82
2	2	527	7MG	N9-C8-N7	-5.24	95.89	103.38
1	1	1962	5MC	O3'-C3'-C4'	5.21	126.12	111.05
1	1	2498	OMC	O2'-C2'-C1'	5.21	119.24	109.08
1	1	2251	OMG	C3'-C2'-C1'	5.20	112.66	102.89
1	1	1618	6MZ	O3'-C3'-C4'	5.14	125.90	111.05
1	1	2498	OMC	O3'-C3'-C2'	5.11	125.69	111.17
5	5	55	PSU	O2'-C2'-C3'	5.11	128.34	111.82
1	1	2069	G7M	C3'-C2'-C1'	-5.04	93.39	100.98
1	1	2580	PSU	O2'-C2'-C3'	4.98	127.93	111.82
1	1	2504	PSU	O2'-C2'-C3'	4.92	127.73	111.82
5	5	20	H2U	O2'-C2'-C3'	4.89	127.66	111.82
2	2	1407	5MC	O3'-C3'-C2'	4.80	127.34	111.82
1	1	2504	PSU	O2'-C2'-C1'	4.73	122.52	111.23
1	1	2030	6MZ	O3'-C3'-C4'	4.69	124.60	111.05
1	1	955	PSU	O2'-C2'-C3'	4.67	126.93	111.82
1	1	2030	6MZ	C3'-C2'-C1'	-4.67	93.95	100.98
2	2	1516	2MG	O3'-C3'-C2'	4.64	126.85	111.82
1	1	2605	PSU	O2'-C2'-C3'	4.61	126.74	111.82
1	1	2605	PSU	O2'-C2'-C1'	4.59	122.19	111.23
5	5	20	H2U	O3'-C3'-C2'	4.54	126.50	111.82
1	1	2457	PSU	O2'-C2'-C3'	4.53	126.49	111.82
1	1	2503	2MA	O4'-C1'-C2'	4.51	113.52	106.93
1	1	2503	2MA	O2'-C2'-C1'	4.48	127.40	110.85
1	1	1911	PSU	C4-N3-C2	-4.38	120.03	126.34
1	1	746	PSU	O2'-C2'-C3'	4.36	125.94	111.82
1	1	2503	2MA	O3'-C3'-C4'	4.36	123.66	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2445	2MG	O3'-C3'-C2'	4.33	125.82	111.82
5	5	32	4OC	O3'-C3'-C2'	4.31	123.40	111.17
1	1	2251	OMG	O3'-C3'-C4'	4.27	123.39	111.05
1	1	1915	3TD	C5'-C4'-C3'	-4.25	99.26	115.18
1	1	2503	2MA	O3'-C3'-C2'	4.20	125.40	111.82
2	2	527	7MG	C2-N3-C4	4.10	119.61	112.30
1	1	745	1MG	O3'-C3'-C4'	4.09	122.89	111.05
1	1	1835	2MG	O3'-C3'-C4'	4.05	122.76	111.05
5	5	20	H2U	O3'-C3'-C4'	4.05	122.76	111.05
1	1	745	1MG	O3'-C3'-C2'	4.03	124.85	111.82
5	5	55	PSU	O2'-C2'-C1'	4.01	120.80	111.23
1	1	1915	3TD	C4-N3-C2	-3.99	120.28	124.61
1	1	1911	PSU	O2-C2-N1	-3.96	118.43	122.79
1	1	955	PSU	O2'-C2'-C1'	3.85	120.40	111.23
1	1	2251	OMG	O3'-C3'-C2'	3.79	121.93	111.17
1	1	2069	G7M	O2'-C2'-C1'	3.77	124.78	110.85
1	1	2580	PSU	O2'-C2'-C1'	3.60	119.82	111.23
2	2	516	PSU	O2'-C2'-C1'	3.53	119.66	111.23
1	1	2457	PSU	O2'-C2'-C1'	3.45	119.46	111.23
2	2	527	7MG	O4'-C4'-C3'	-3.44	98.30	105.11
1	1	1835	2MG	O3'-C3'-C2'	3.41	122.86	111.82
1	1	2580	PSU	C3'-C2'-C1'	3.41	105.61	101.64
5	5	20	H2U	O2'-C2'-C1'	3.38	121.34	110.02
2	2	527	7MG	O3'-C3'-C2'	3.29	122.45	111.82
5	5	8	4SU	C1'-N1-C2	3.24	123.43	117.57
1	1	1917	PSU	C3'-C2'-C1'	3.19	105.35	101.64
1	1	2030	6MZ	O3'-C3'-C2'	3.16	122.06	111.82
5	5	8	4SU	N3-C2-N1	3.16	119.08	114.89
2	2	966	2MG	C2'-C3'-C4'	-3.14	96.54	102.64
1	1	2030	6MZ	C2-N1-C6	3.11	119.26	116.59
1	1	1618	6MZ	C2-N1-C6	3.05	119.20	116.59
5	5	32	4OC	O3'-C3'-C4'	2.98	119.68	111.05
1	1	955	PSU	C2'-C3'-C4'	-2.98	96.85	102.64
2	2	1498	UR3	O4'-C1'-C2'	-2.97	100.17	106.64
1	1	746	PSU	O2'-C2'-C1'	2.94	118.25	111.23
2	2	1516	2MG	O3'-C3'-C4'	2.93	119.53	111.05
1	1	1962	5MC	O3'-C3'-C2'	2.92	121.27	111.82
1	1	2069	G7M	O3'-C3'-C2'	2.87	121.12	111.82
1	1	2251	OMG	O2'-C2'-C1'	2.84	114.72	109.09
1	1	2445	2MG	C3'-C2'-C1'	2.82	105.23	100.98
1	1	2605	PSU	C2'-C3'-C4'	-2.80	97.21	102.64
1	1	2445	2MG	O3'-C3'-C4'	2.78	119.09	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	527	7MG	O3'-C3'-C4'	2.78	119.09	111.05
1	1	2457	PSU	C2'-C3'-C4'	-2.77	97.27	102.64
1	1	745	1MG	O2'-C2'-C3'	2.72	120.63	111.82
1	1	2503	2MA	O2'-C2'-C3'	2.72	120.62	111.82
2	2	527	7MG	C5-C6-N1	2.68	115.72	110.99
1	1	1962	5MC	C2'-C1'-N1	2.66	120.76	113.22
1	1	2069	G7M	C2'-C3'-C4'	-2.65	97.50	102.64
5	5	54	5MU	C2'-C1'-N1	2.58	120.54	113.22
2	2	1402	4OC	O4'-C4'-C3'	-2.58	100.00	105.11
1	1	747	5MU	C2'-C1'-N1	2.58	120.52	113.22
1	1	1835	2MG	C3'-C2'-C1'	2.55	104.82	100.98
5	5	8	4SU	C4'-O4'-C1'	-2.54	103.86	109.47
1	1	2251	OMG	C5'-C4'-C3'	2.54	124.71	115.18
1	1	1939	5MU	C2'-C1'-N1	2.51	120.32	113.22
2	2	1498	UR3	O2-C2-N3	-2.44	117.90	121.34
2	2	527	7MG	C3'-C2'-C1'	-2.44	96.80	101.43
1	1	2498	OMC	O3'-C3'-C4'	2.43	118.07	111.05
2	2	1402	4OC	O2-C2-N3	-2.41	118.42	122.33
5	5	55	PSU	C3'-C2'-C1'	2.40	104.43	101.64
1	1	2504	PSU	C2'-C3'-C4'	-2.40	97.98	102.64
2	2	527	7MG	O6-C6-C5	-2.37	121.73	127.54
1	1	1962	5MC	C3'-C2'-C1'	2.36	105.92	101.43
2	2	1519	MA6	C2'-C3'-C4'	-2.36	98.05	102.64
5	5	8	4SU	O4'-C1'-N1	2.35	113.74	108.36
5	5	8	4SU	O4'-C1'-C2'	-2.27	101.70	106.64
1	1	1939	5MU	C4-N3-C2	-2.26	124.43	127.35
2	2	1207	2MG	O2'-C2'-C1'	-2.26	102.52	110.85
1	1	1939	5MU	N3-C2-N1	2.26	117.88	114.89
1	1	2457	PSU	C3'-C2'-C1'	2.24	104.24	101.64
2	2	527	7MG	C5-C4-N9	-2.23	103.45	106.35
1	1	1915	3TD	O4'-C4'-C5'	-2.18	102.19	109.37
1	1	747	5MU	N3-C2-N1	2.17	117.77	114.89
2	2	1407	5MC	O3'-C3'-C4'	2.15	117.28	111.05
2	2	1498	UR3	C1'-N1-C2	2.15	120.62	116.99
1	1	1915	3TD	C3'-C2'-C1'	2.12	104.11	101.64
5	5	54	5MU	N3-C2-N1	2.11	117.70	114.89
1	1	2552	OMU	N3-C2-N1	2.11	117.69	114.89
2	2	1516	2MG	C3'-C2'-C1'	2.10	104.14	100.98
1	1	2498	OMC	C3'-C2'-C1'	2.10	106.84	102.89
2	2	967	5MC	O3'-C3'-C2'	2.10	118.61	111.82
2	2	1498	UR3	C4-N3-C2	-2.08	122.61	124.56
2	2	527	7MG	O4'-C1'-N9	2.08	112.13	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	8	4SU	C6-C5-C4	-2.07	118.16	119.95
2	2	966	2MG	C3'-C2'-C1'	2.05	104.06	100.98
2	2	967	5MC	C2'-C1'-N1	2.04	119.00	113.22
1	1	2030	6MZ	O4'-C1'-C2'	2.04	109.91	106.93
2	2	1498	UR3	O3'-C3'-C4'	-2.03	105.18	111.05
5	5	54	5MU	C4-N3-C2	-2.03	124.73	127.35
5	5	76	8AN	C5-C6-N6	2.02	123.42	120.35
2	2	1407	5MC	O4'-C1'-C2'	2.01	111.03	106.64
1	1	1911	PSU	C5-C6-N1	-2.01	119.10	122.11
1	1	747	5MU	C4-N3-C2	-2.00	124.76	127.35

There are no chirality outliers.

All (52) 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'
2	2	966	2MG	O4'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
2	2	966	2MG	N3-C2-N2-CM2
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C9
2	2	1519	MA6	C5-C6-N6-C10
49	q	89	0TD	SB-CB-CG-OD2
5	5	20	H2U	O4'-C4'-C5'-O5'
5	5	20	H2U	O4'-C1'-N1-C6
5	5	55	PSU	C3'-C4'-C5'-O5'
1	1	1915	3TD	C3'-C4'-C5'-O5'
1	1	2069	G7M	O4'-C4'-C5'-O5'
2	2	967	5MC	C3'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'
5	5	20	H2U	O4'-C1'-N1-C2
5	5	76	8AN	C3'-C4'-C5'-O5'
1	1	1915	3TD	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
2	2	516	PSU	C3'-C4'-C5'-O5'
2	2	516	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
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	76	8AN	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C5-C6-N6-C9
5	5	8	4SU	O4'-C1'-N1-C2
49	q	89	0TD	CG-CB-SB-CSB
5	5	8	4SU	O4'-C1'-N1-C6
1	1	2069	G7M	C4'-C5'-O5'-P
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2498	OMC	O4'-C4'-C5'-O5'
1	1	1911	PSU	O4'-C4'-C5'-O5'
2	2	967	5MC	C4'-C5'-O5'-P
1	1	2498	OMC	C3'-C4'-C5'-O5'
2	2	967	5MC	C2'-C1'-N1-C6
1	1	746	PSU	O4'-C1'-C5-C6
1	1	1915	3TD	C4'-C5'-O5'-P
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C4'-C5'-O5'
2	2	967	5MC	C2'-C1'-N1-C2
5	5	55	PSU	C4'-C5'-O5'-P
2	2	1519	MA6	C4'-C5'-O5'-P
1	1	2504	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 441 ligands modelled in this entry, 440 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	$\# Z  > 2$
60	FME	5	101	5	8,9,10	0.54	0	7,9,11	1.22	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
60	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( $^{\circ}$ )	Ideal( $^{\circ}$ )
60	5	101	FME	O-C-CA	-3.16	116.50	124.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	5	101	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1



All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	2196:C	O3'	2197:U	P	2.55

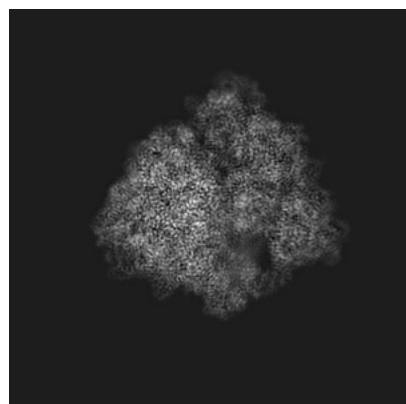
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3490. These allow visual inspection of the internal detail of the map and identification of artifacts.

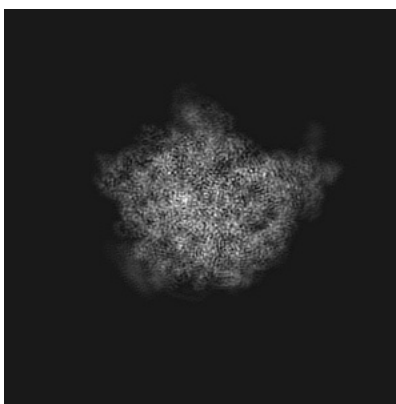
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

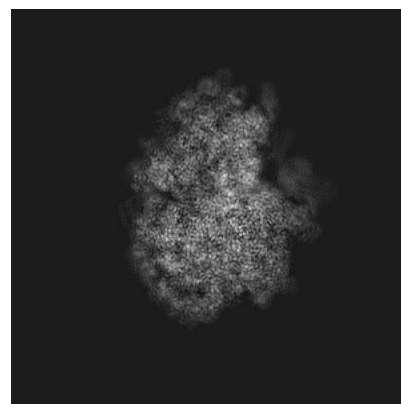
#### 6.1.1 Primary map



X

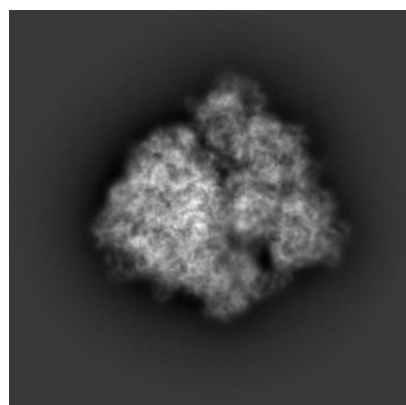


Y

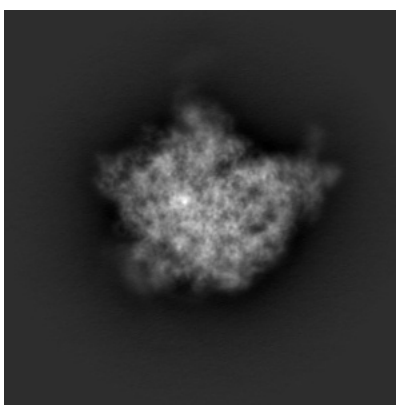


Z

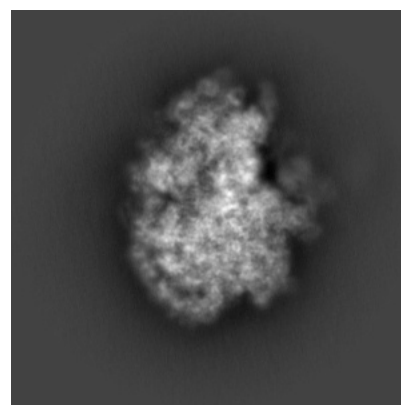
#### 6.1.2 Raw map



X



Y

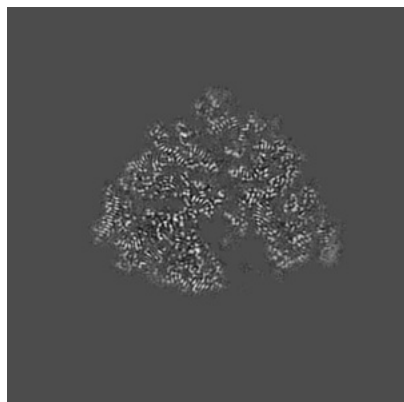


Z

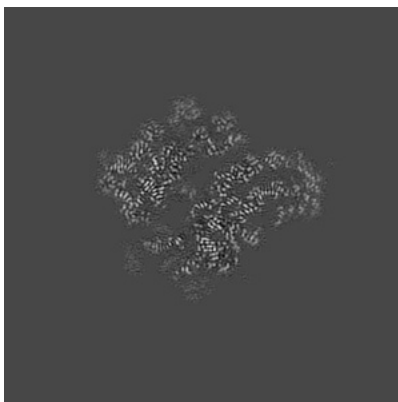
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

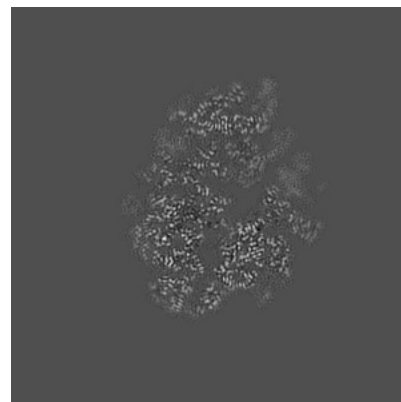
### 6.2.1 Primary map



X Index: 200

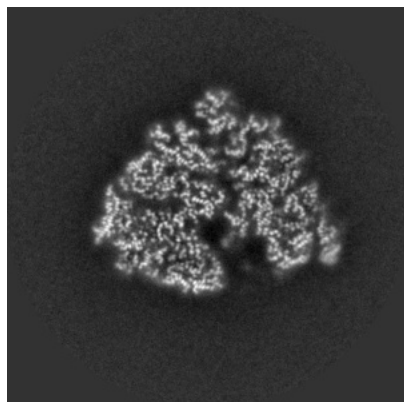


Y Index: 200

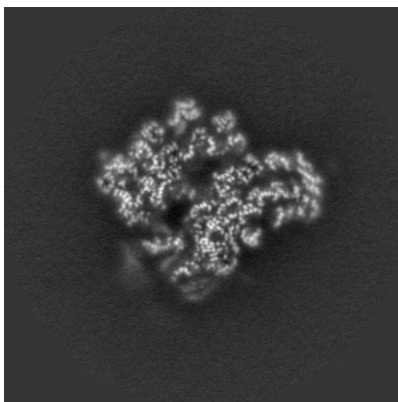


Z Index: 200

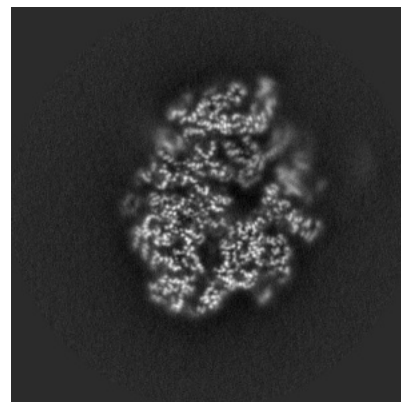
### 6.2.2 Raw map



X Index: 200



Y Index: 200

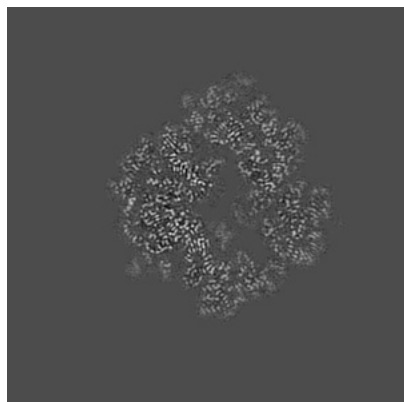


Z Index: 200

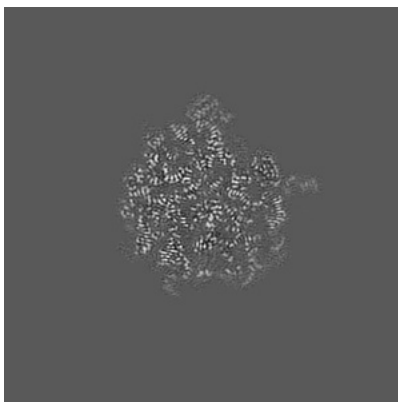
The images above show central slices of the map in three orthogonal directions.

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

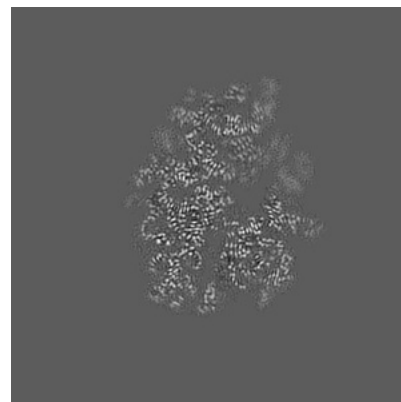
### 6.3.1 Primary map



X Index: 225

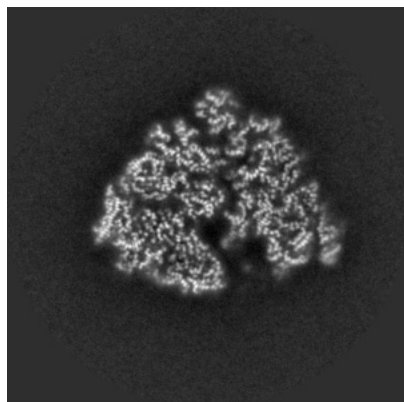


Y Index: 181

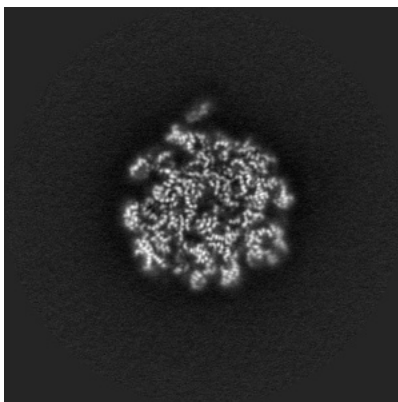


Z Index: 205

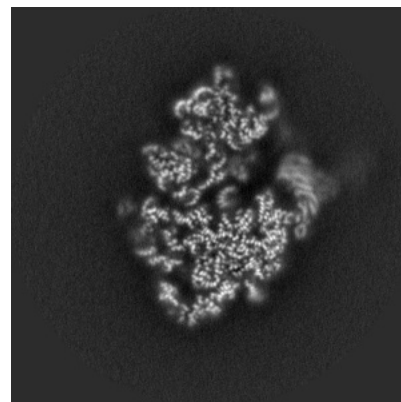
### 6.3.2 Raw map



X Index: 201



Y Index: 169

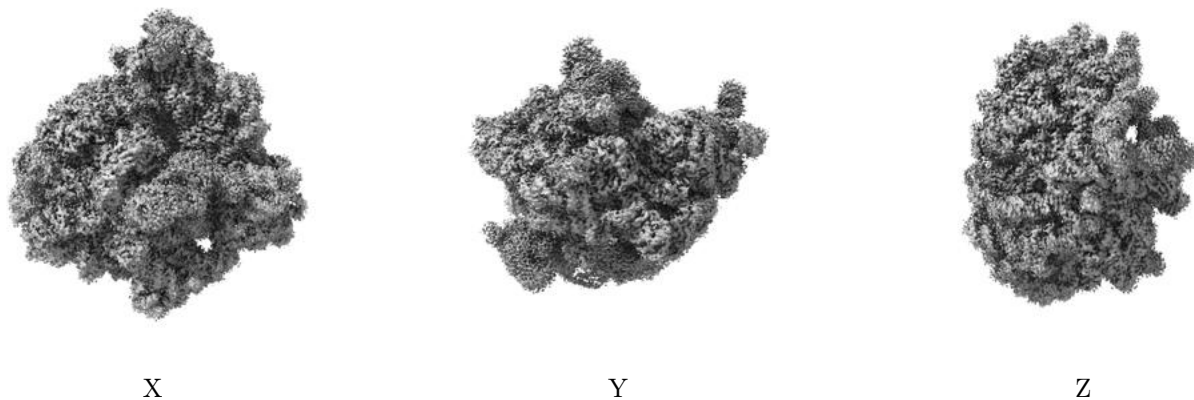


Z Index: 185

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

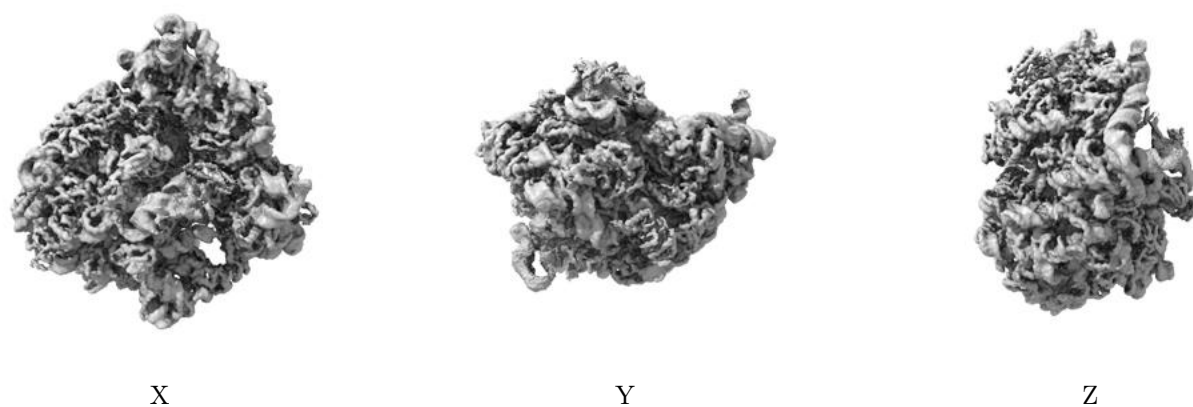
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

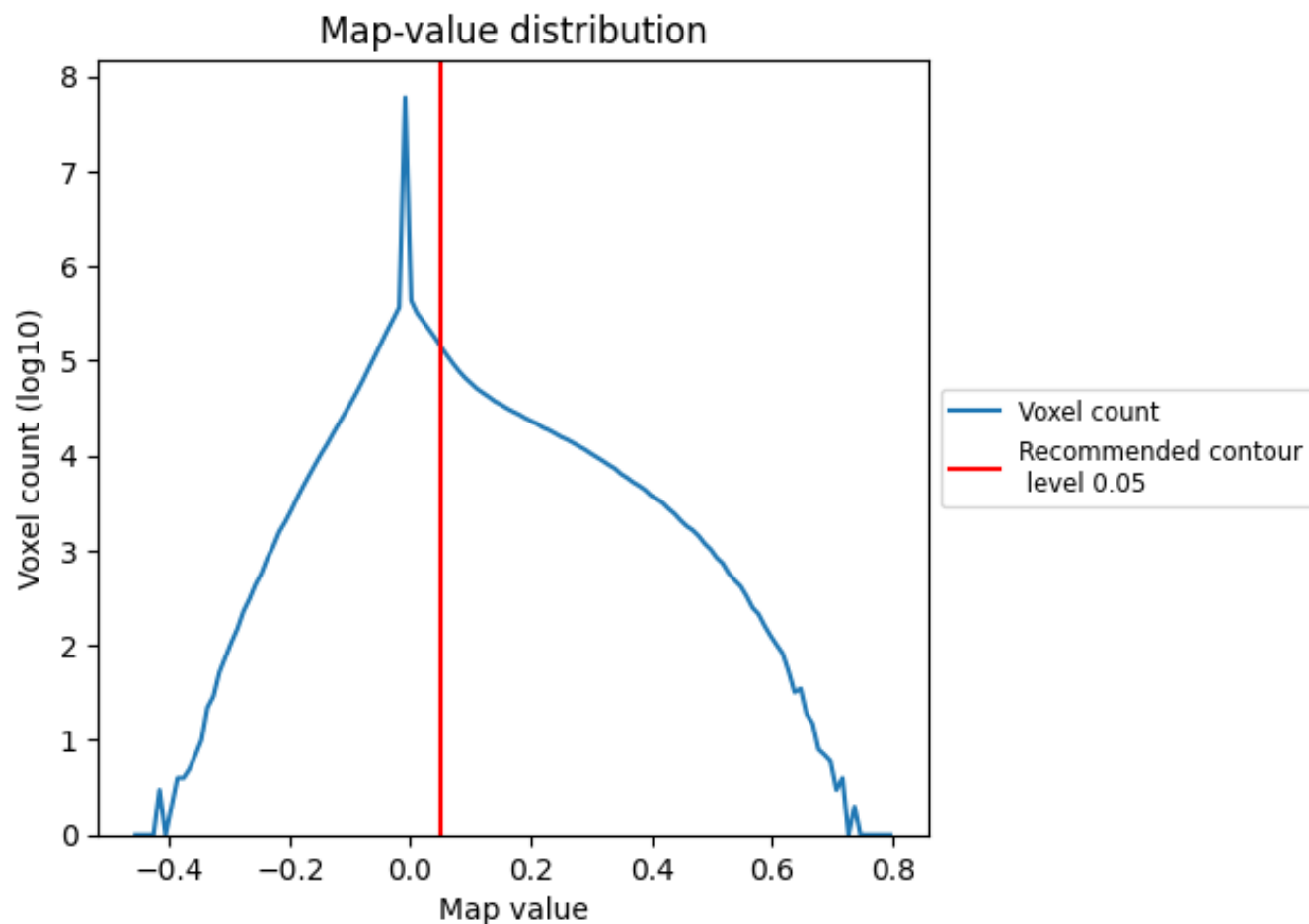
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

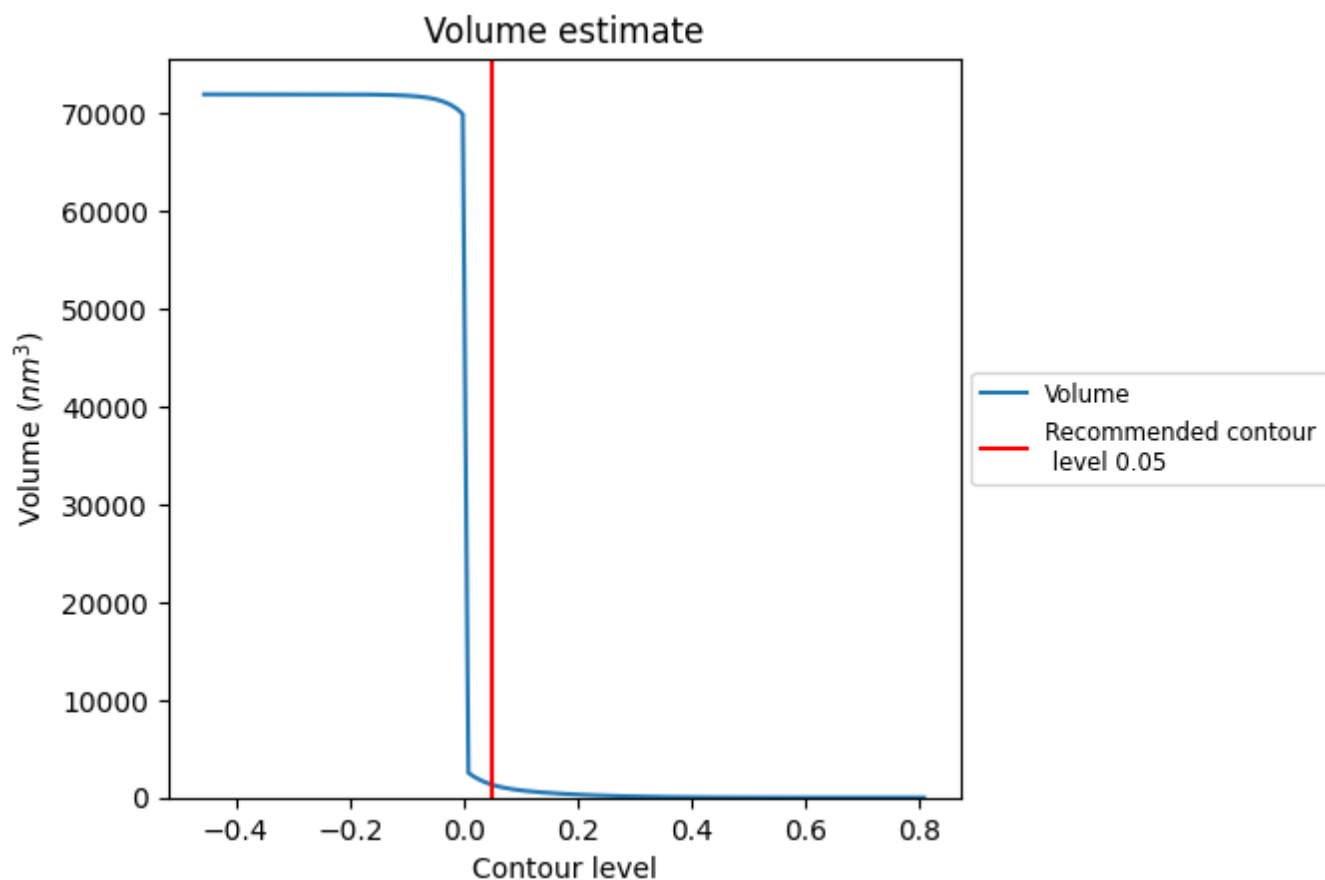
This section contains the results of statistical analysis of the map.

### 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.

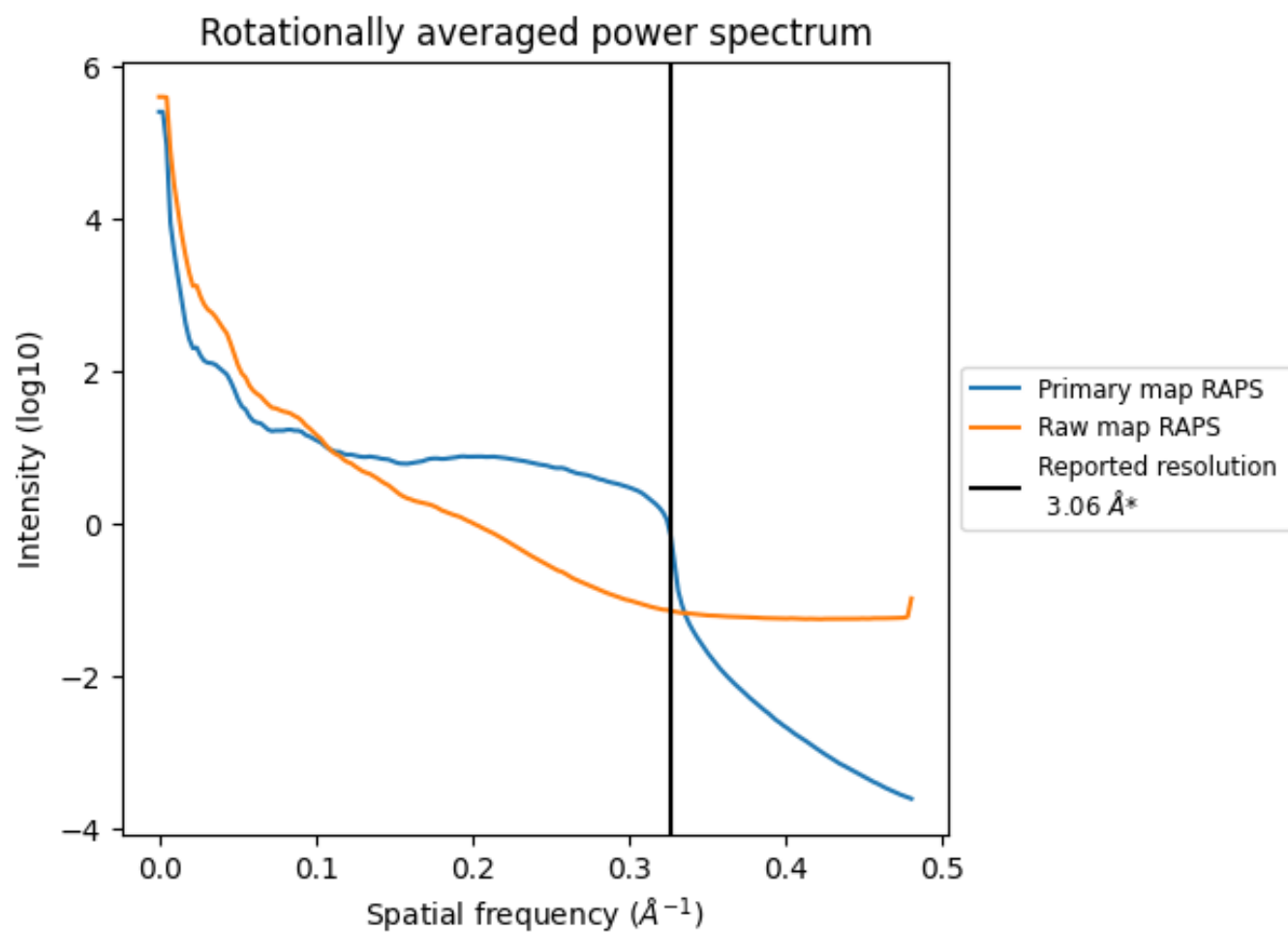
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1309 nm<sup>3</sup>; this corresponds to an approximate mass of 1182 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 ⓘ



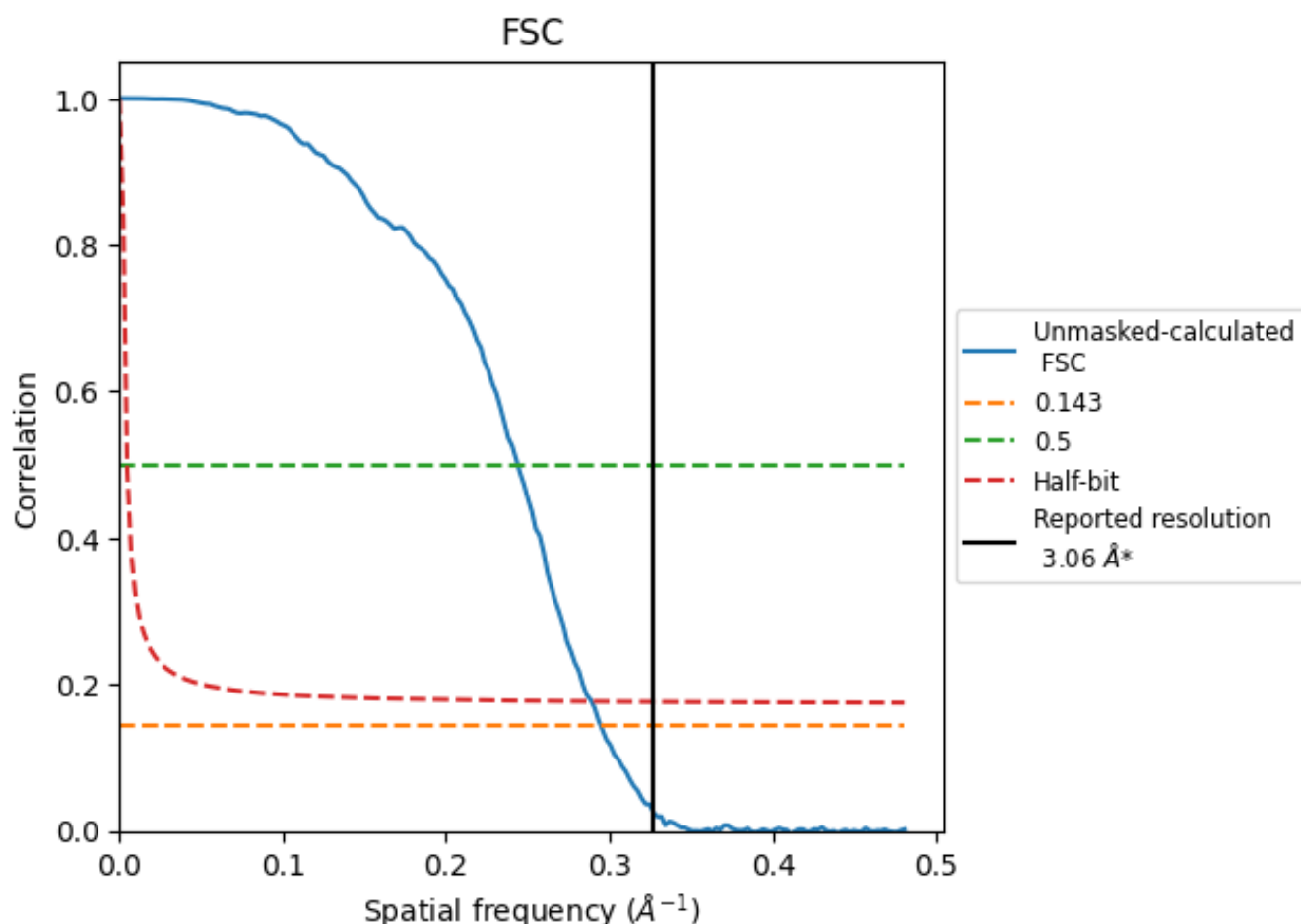
\*Reported resolution corresponds to spatial frequency of 0.327 Å<sup>-1</sup>



## 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 0.327 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

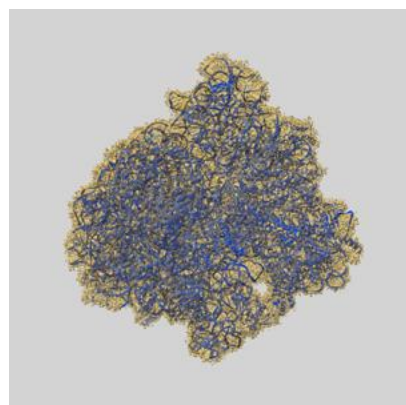
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.39	4.10	3.46

\*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 3.39 differs from the reported value 3.06 by more than 10 %

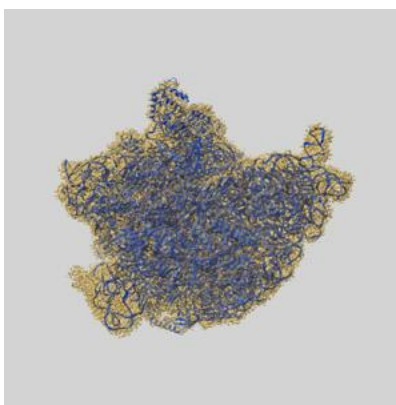
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3490 and PDB model 5MDW. Per-residue inclusion information can be found in section 3 on page 15.

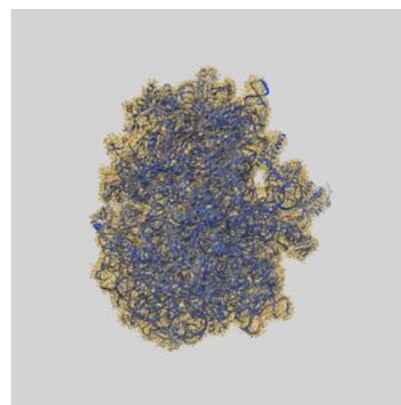
### 9.1 Map-model overlay [i](#)



X



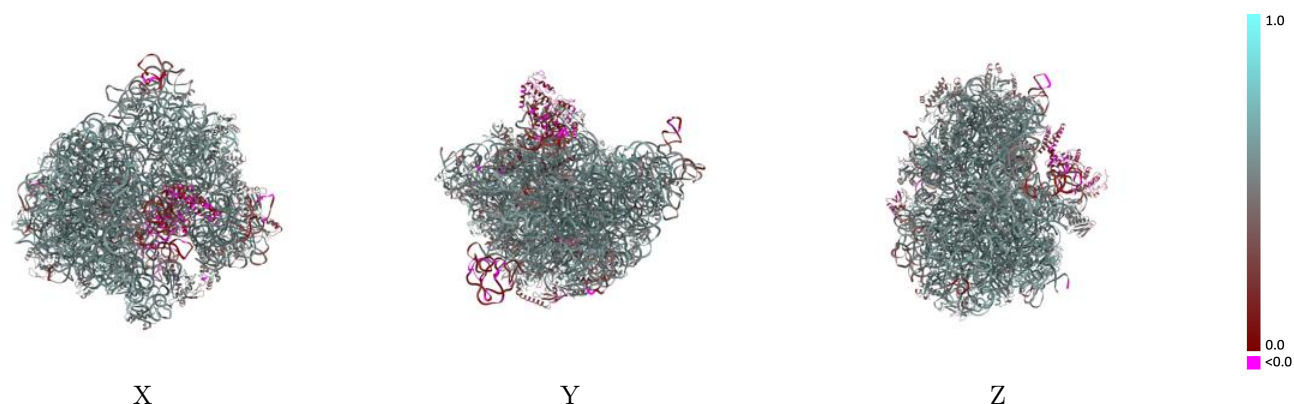
Y



Z

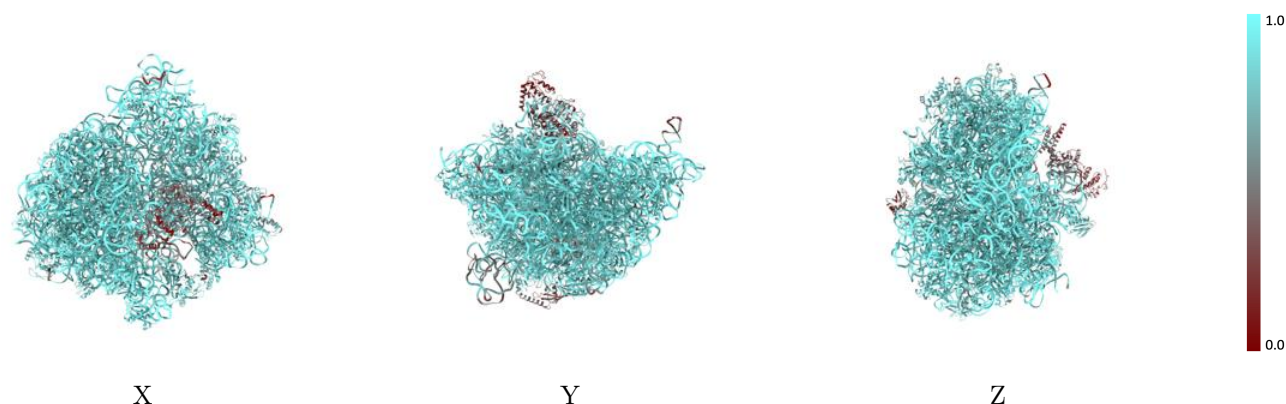
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



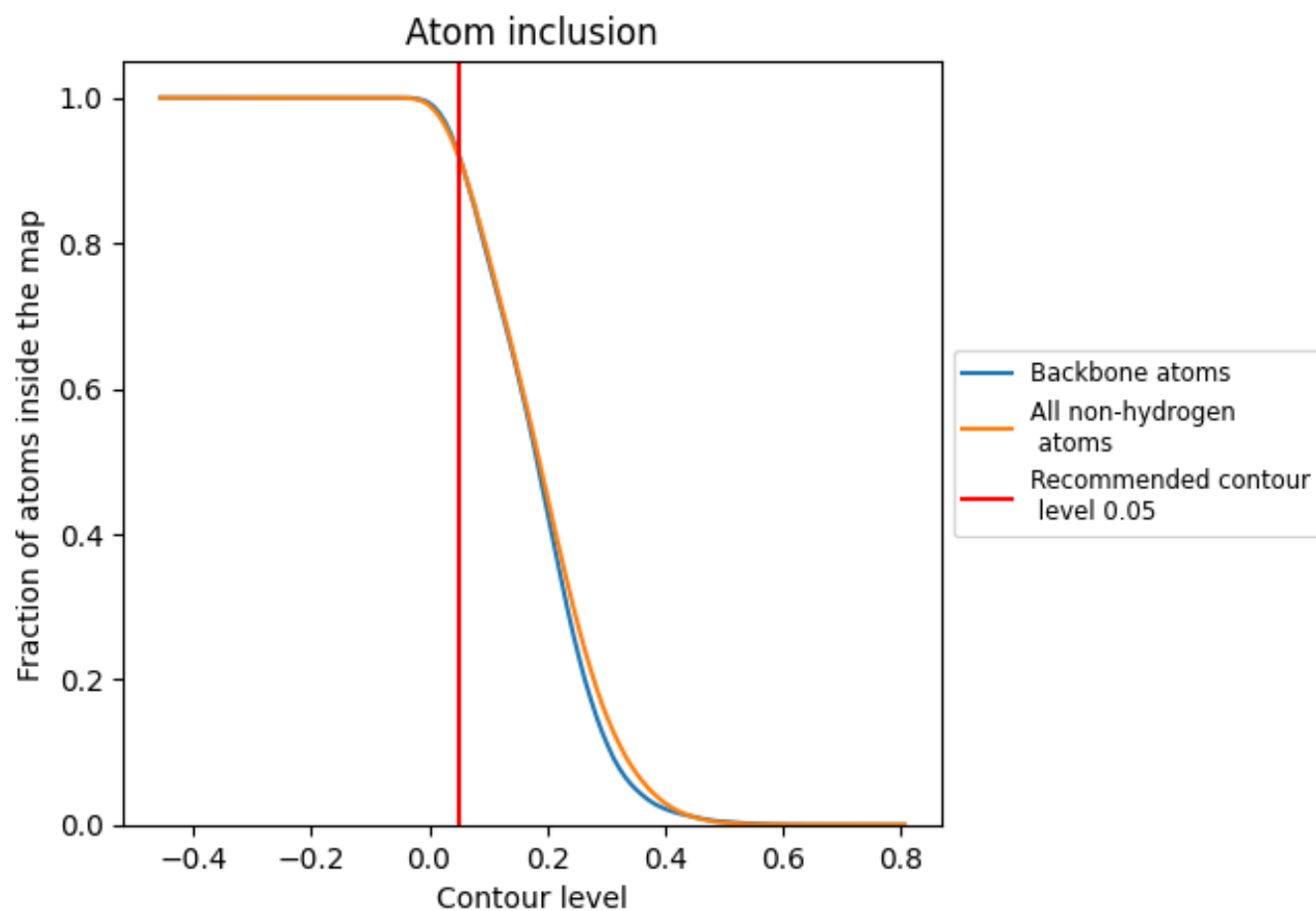
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9201	 0.5310
1	 0.9609	 0.5470
2	 0.9690	 0.5530
3	 0.9779	 0.5620
4	 0.9541	 0.5460
5	 0.9315	 0.5180
6	 0.8465	 0.5290
7	 0.6359	 0.3400
B	 0.9410	 0.5830
C	 0.9226	 0.5690
D	 0.8822	 0.5170
E	 0.8696	 0.4920
F	 0.8524	 0.4700
G	 0.4699	 0.2810
H	 0.1729	 0.0610
I	 0.3419	 0.0690
J	 0.9236	 0.5610
K	 0.9099	 0.5580
L	 0.9102	 0.5470
M	 0.9203	 0.5590
N	 0.9266	 0.5670
O	 0.9061	 0.5360
P	 0.9144	 0.5610
Q	 0.9262	 0.5720
R	 0.9310	 0.5570
S	 0.8995	 0.5530
T	 0.8781	 0.5240
U	 0.8892	 0.5150
V	 0.8862	 0.5270
W	 0.9276	 0.5780
X	 0.9268	 0.5720
Y	 0.8548	 0.4940
Z	 0.9151	 0.5520
a	 0.7891	 0.3910
b	 0.9044	 0.5640



*Continued on next page...*

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Chain	Atom inclusion	Q-score
c	 0.8589	 0.5320
d	 0.9099	 0.5820
e	 0.9348	 0.5860
f	 0.9249	 0.5600
g	 0.7426	 0.4440
h	 0.8830	 0.5130
i	 0.8768	 0.5150
j	 0.9115	 0.5540
k	 0.8561	 0.4870
l	 0.8374	 0.4730
m	 0.8854	 0.5400
n	 0.8662	 0.5010
o	 0.8183	 0.4560
p	 0.9039	 0.5410
q	 0.9090	 0.5620
r	 0.8721	 0.5070
s	 0.9005	 0.5350
t	 0.8986	 0.5320
u	 0.8947	 0.5340
v	 0.8671	 0.5130
w	 0.8948	 0.5280
x	 0.9042	 0.5140
y	 0.8853	 0.5150
z	 0.7567	 0.4250