



## wwPDB EM Validation Summary 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 wwPDB EM Validation Summary 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:

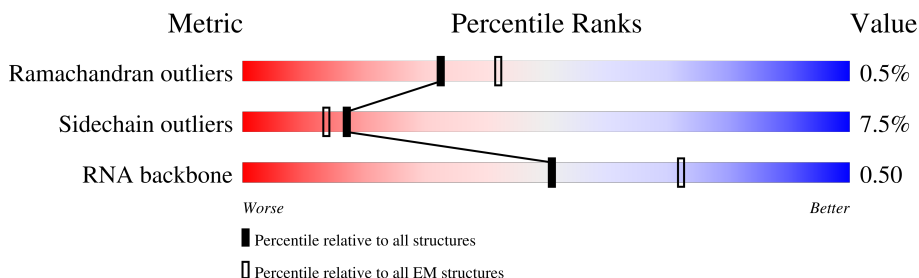
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et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



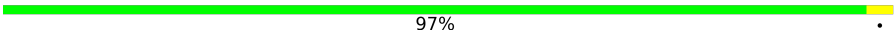
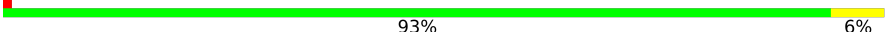

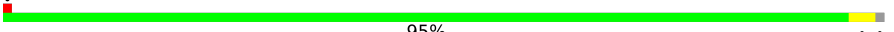








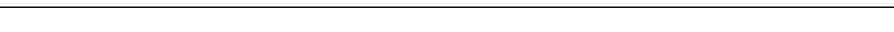

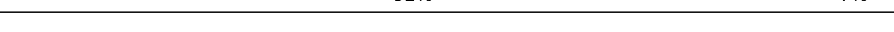
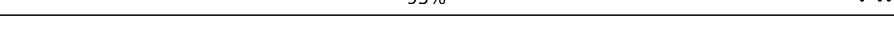
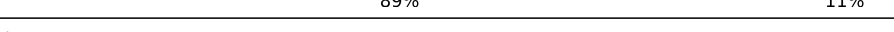
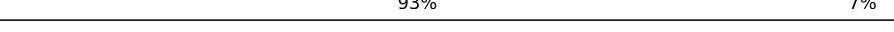

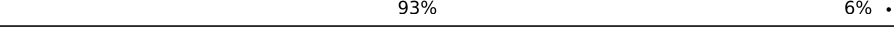
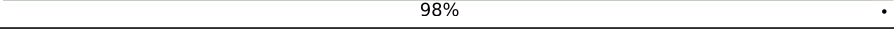




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	


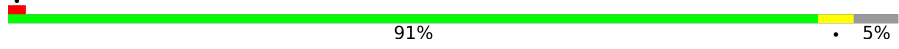

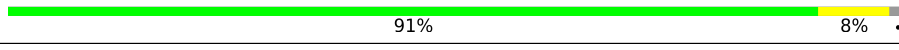

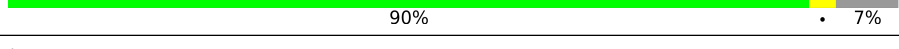
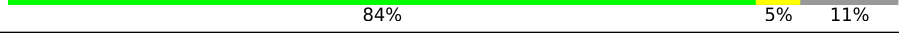
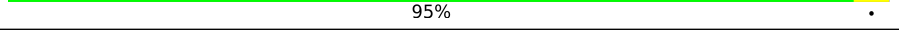
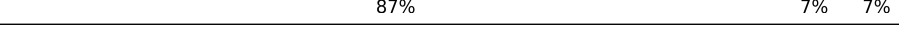
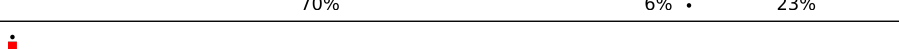
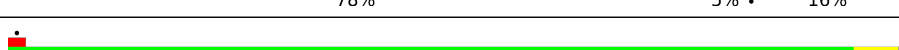
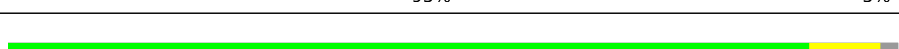
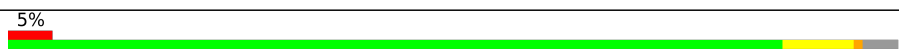

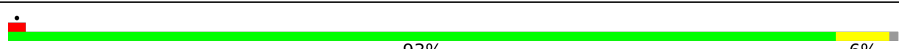

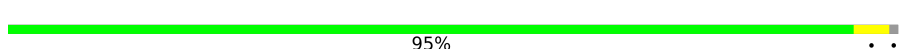

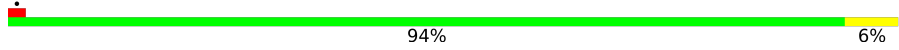
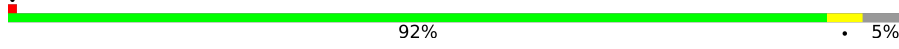
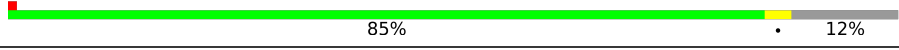
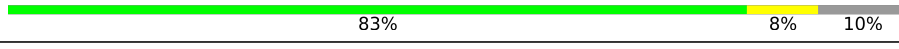
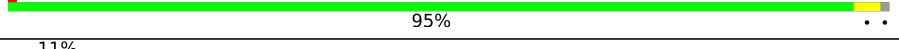


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Mol	Chain	Length	Quality of chain
9	C	209	
10	D	201	
11	E	179	
12	F	177	
13	G	149	
14	H	165	
15	I	142	
16	J	142	
17	K	123	
18	L	144	
19	M	136	
20	N	127	
21	O	117	
22	P	115	
23	Q	118	
24	R	103	
25	S	110	
26	T	100	
27	U	104	
28	V	94	
29	W	85	
30	X	78	
31	Y	63	
32	Z	59	
33	a	70	

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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		

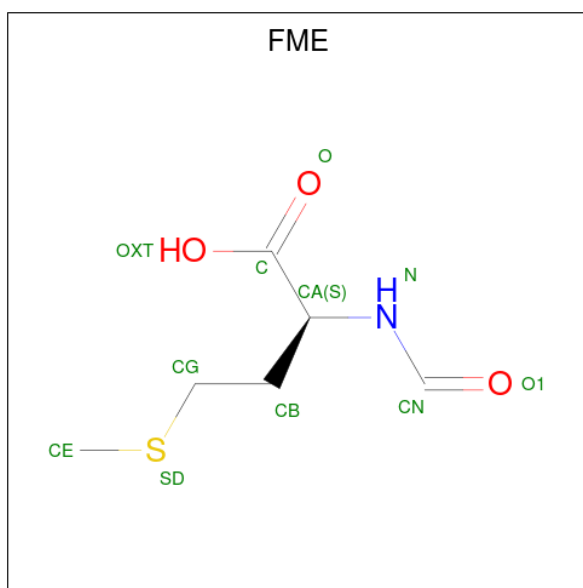
- Molecule 58 is a protein called 30S ribosomal protein S21.

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	

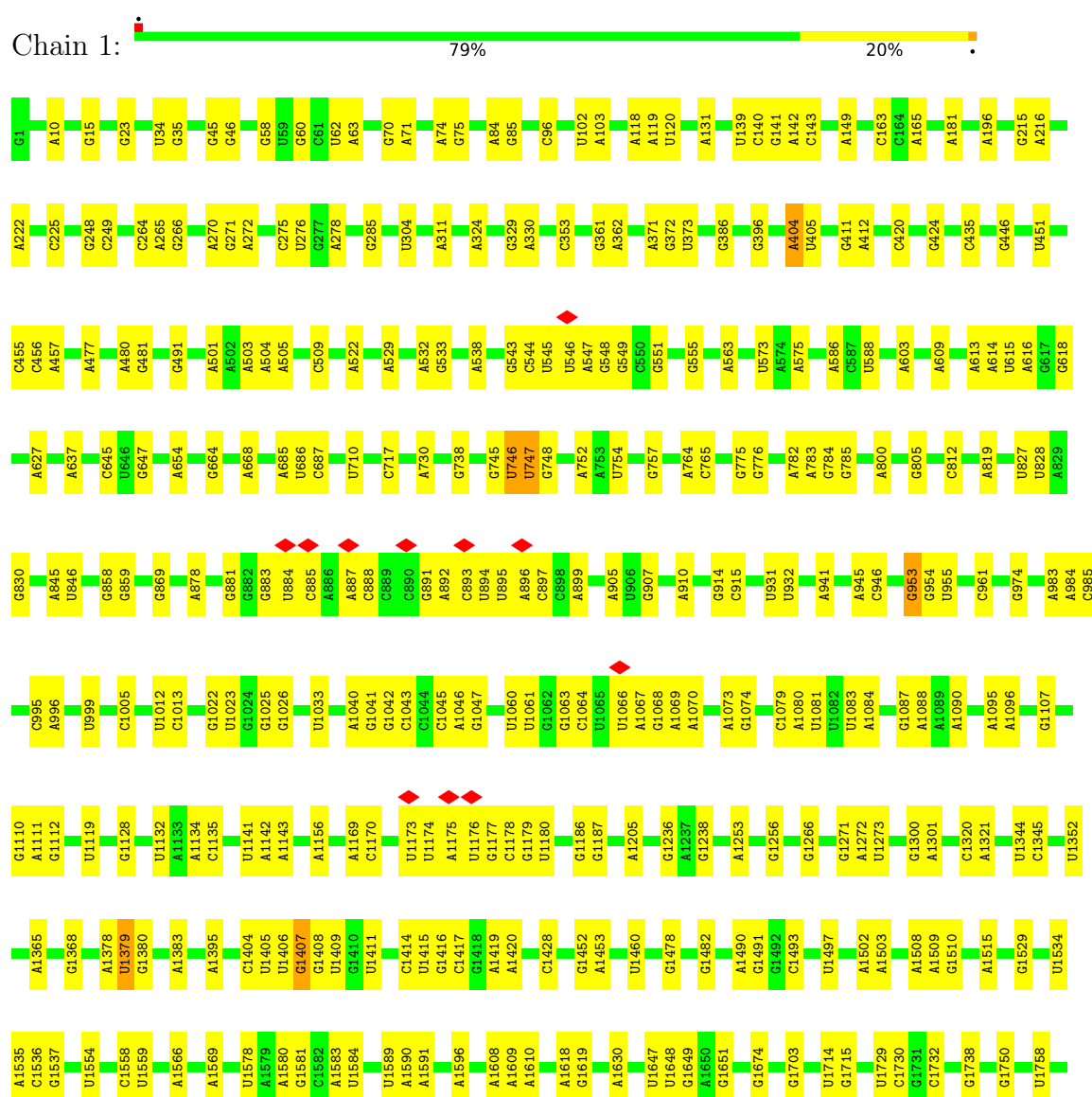
- Molecule 62 is water.

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

### 3 Residue-property plots

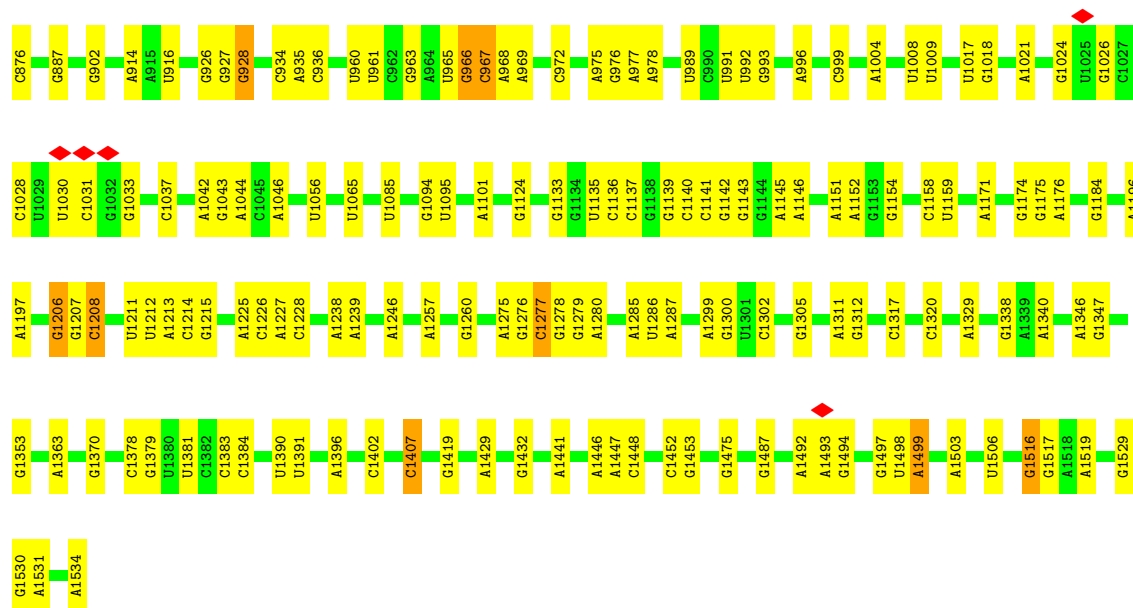
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



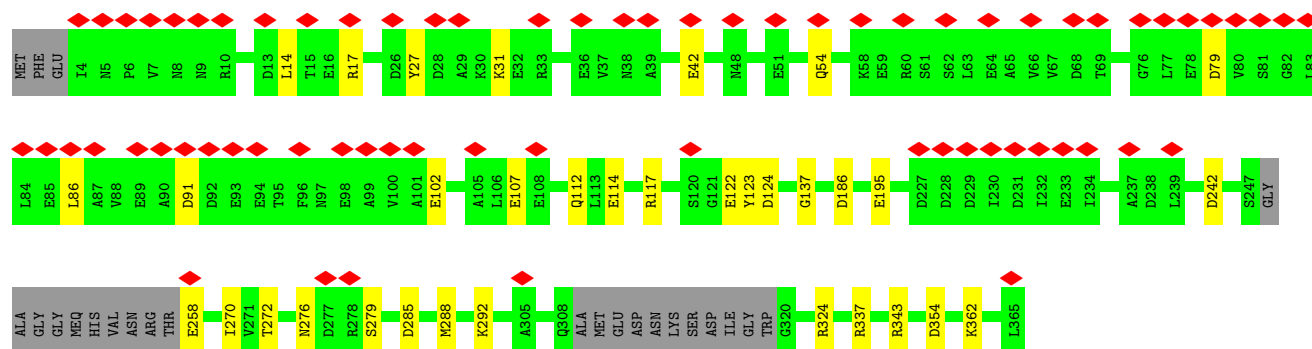
- Molecule 6: Alternative ribosome-rescue factor A

Chain 6: 48% 5% 48%



- Molecule 7: Peptide chain release factor 2

Chain 7: 19% 84% 9% 7%



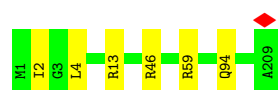
- Molecule 8: 50S ribosomal protein L2

Chain B: 93% 6%



- Molecule 9: 50S ribosomal protein L3

Chain C: 97%



- Molecule 10: 50S ribosomal protein L4

Chain D: 93% 6%



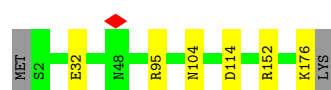
- Molecule 11: 50S ribosomal protein L5

Chain E: 92% 7%

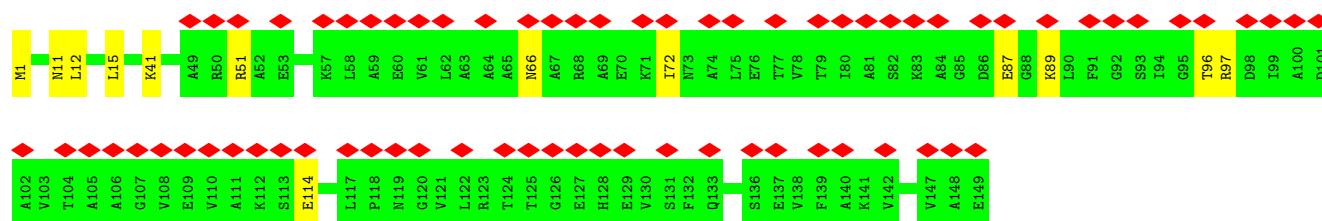
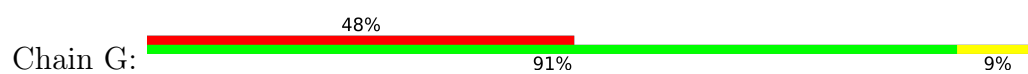


- Molecule 12: 50S ribosomal protein L6

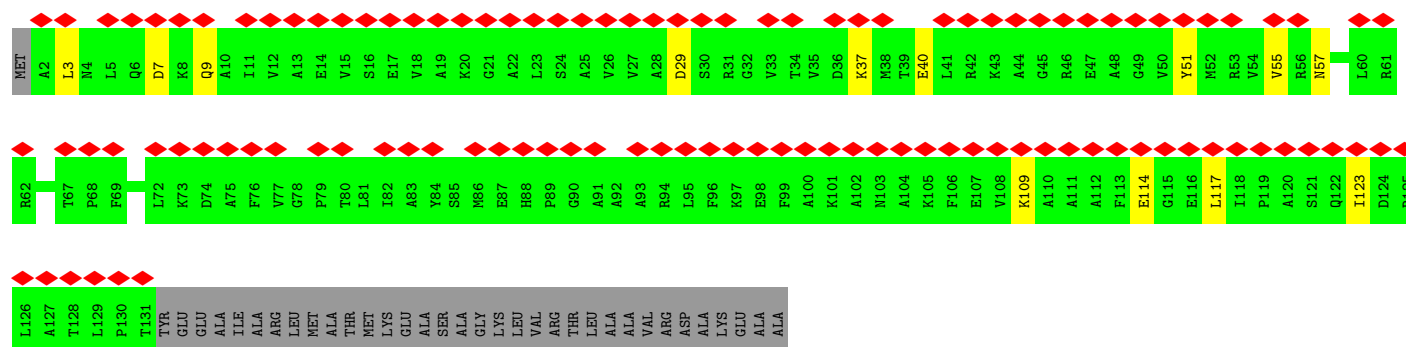
Chain F: 95%



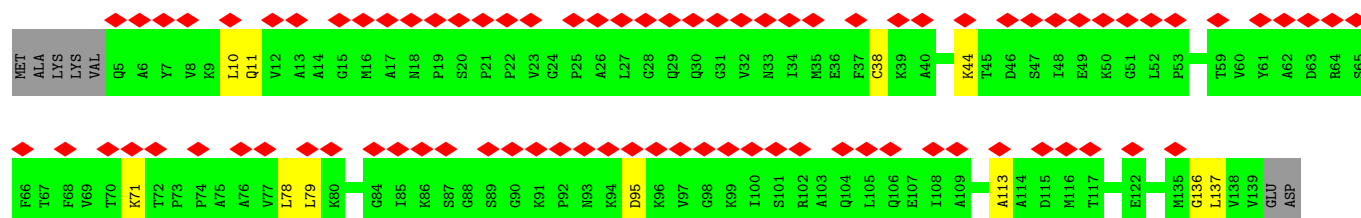
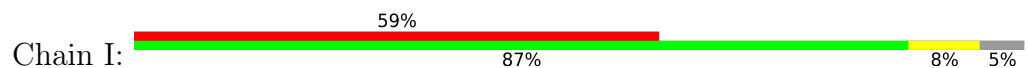
- Molecule 13: 50S ribosomal protein L9



• Molecule 14: 50S ribosomal protein L10



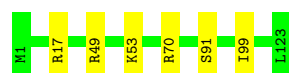
• Molecule 15: 50S ribosomal protein L11



• Molecule 16: 50S ribosomal protein L13

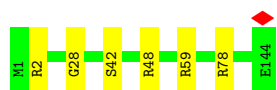


• Molecule 17: 50S ribosomal protein L14



- 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%




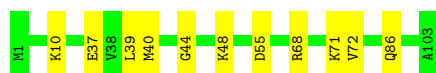
- Molecule 23: 50S ribosomal protein L20

Chain Q:  95%




- Molecule 24: 50S ribosomal protein L21

Chain R:  89% 11%



- Molecule 25: 50S ribosomal protein L22

Chain S:  93% 7%



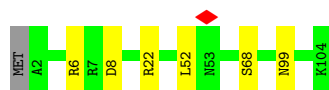
- Molecule 26: 50S ribosomal protein L23

Chain T:  91% 6%



- Molecule 27: 50S ribosomal protein L24

Chain U:  93% 6%




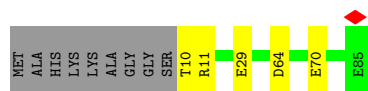
- Molecule 28: 50S ribosomal protein L25

Chain V:  98%



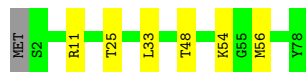
- Molecule 29: 50S ribosomal protein L27

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%



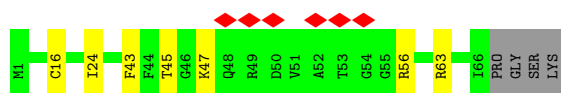
- Molecule 32: 50S ribosomal protein L30

Chain Z: 88% 10%



- Molecule 33: 50S ribosomal protein L31

Chain a: 9% 84% 10% 6%



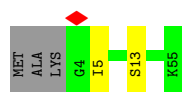
- Molecule 34: 50S ribosomal protein L32

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%

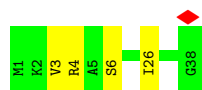
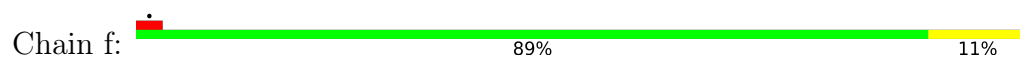


- Molecule 37: 50S ribosomal protein L35

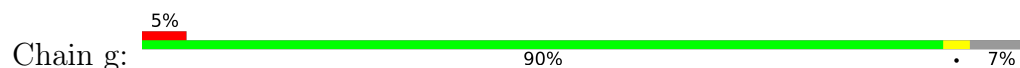
Chain e: 91% 8%



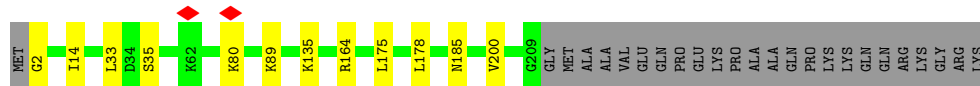
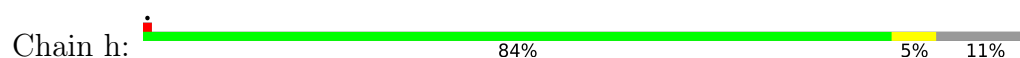
- Molecule 38: 50S ribosomal protein L36



- Molecule 39: 30S ribosomal protein S2



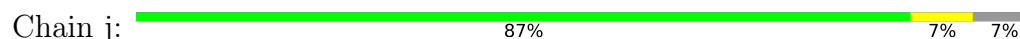
- Molecule 40: 30S ribosomal protein S3



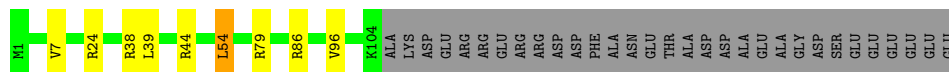
- Molecule 41: 30S ribosomal protein S4



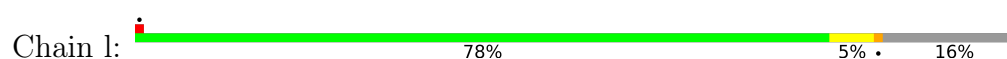
- Molecule 42: 30S ribosomal protein S5



- Molecule 43: 30S ribosomal protein S6

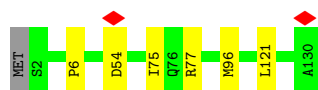


- Molecule 44: 30S ribosomal protein S7




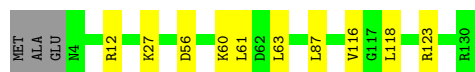
- Molecule 45: 30S ribosomal protein S8

Chain m:  95% 5%




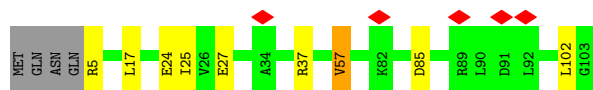
- Molecule 46: 30S ribosomal protein S9

Chain n:  90% 8%




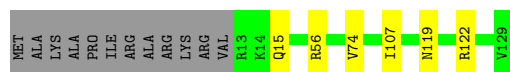
- Molecule 47: 30S ribosomal protein S10

Chain o:  5% 87% 8%



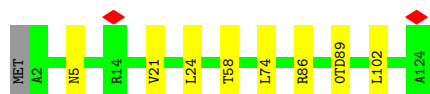
- Molecule 48: 30S ribosomal protein S11

Chain p:  86% 5% 9%




- Molecule 49: 30S ribosomal protein S12

Chain q:  93% 6%



- Molecule 50: 30S ribosomal protein S13

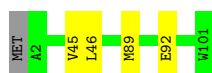
Chain r:  92% 6%



- Molecule 51: 30S ribosomal protein S14

Chain s:  95%





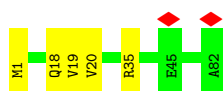
- Molecule 52: 30S ribosomal protein S15

Chain t: 83% 16% .



- Molecule 53: 30S ribosomal protein S16

Chain u: 94% 6%



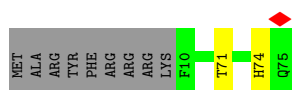
- Molecule 54: 30S ribosomal protein S17

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%

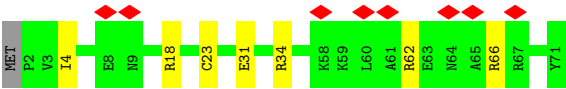
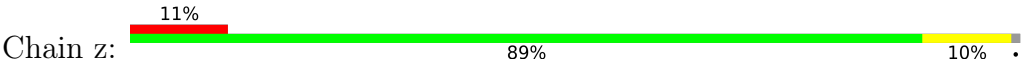


- Molecule 57: 30S ribosomal protein S20

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.

The worst 5 of 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

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	z	68/71 (96%)	68 (100%)	0	0	100	100
All	All	6234/6646 (94%)	5854 (94%)	350 (6%)	30 (0%)	32	60

5 of 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

### 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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 388 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	b	40	ARG
43	k	24	ARG
36	d	42	LEU
40	h	135	LYS
44	l	109	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%)
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%)

5 of 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

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Mol	Chain	Res	Type
1	1	35	G

5 of 112 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	2296	U
5	5	47	U
2	2	106	C
5	5	21	A
2	2	1407	5MC

## 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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2MG	1	2445	1	18,26,27	1.24	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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 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

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(°)	Ideal(°)
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



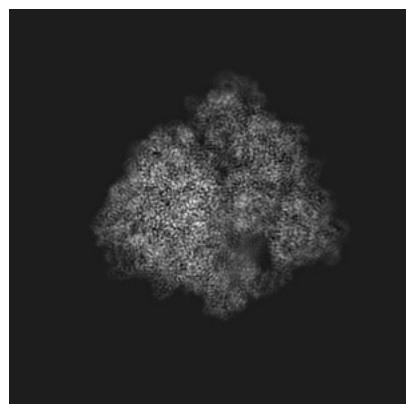
## 6 Map visualisation [i](#)

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.

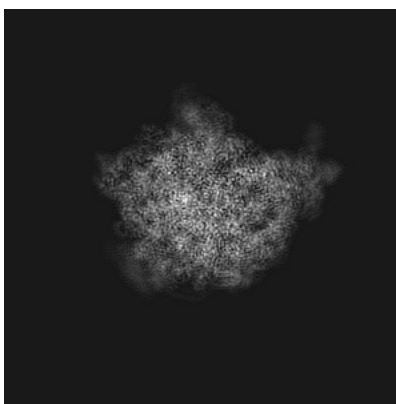
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

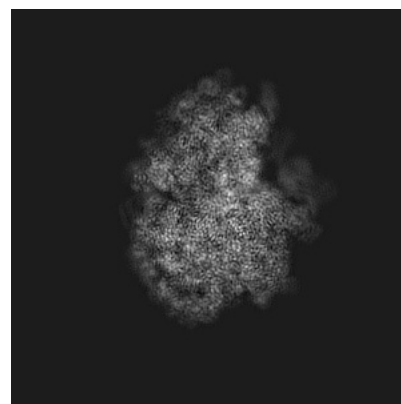
#### 6.1.1 Primary map



X

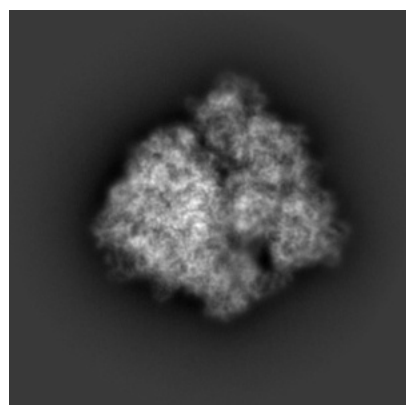


Y

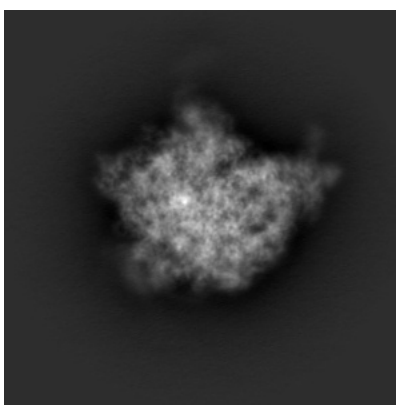


Z

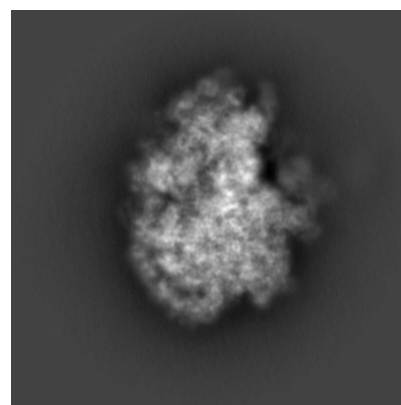
#### 6.1.2 Raw map



X



Y

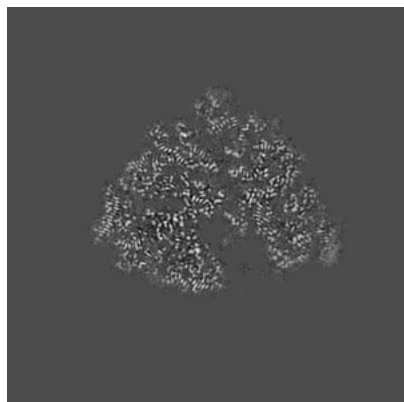


Z

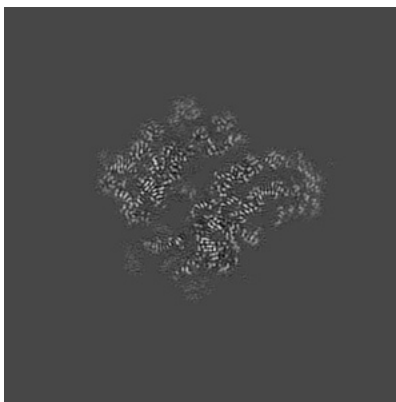
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

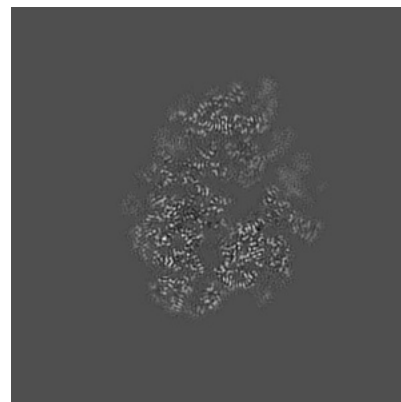
### 6.2.1 Primary map



X Index: 200

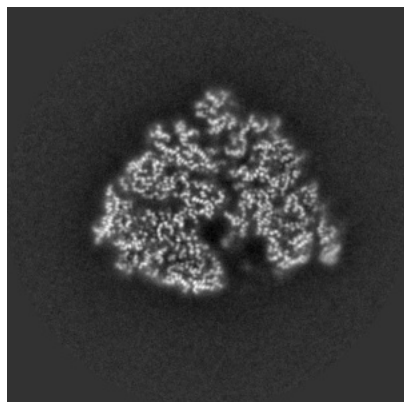


Y Index: 200

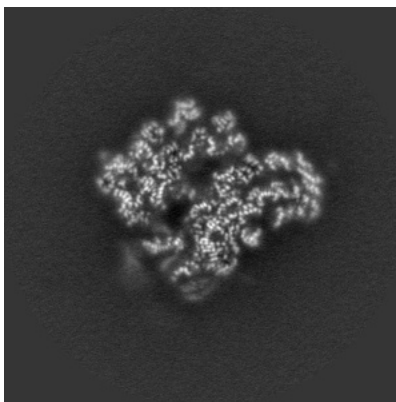


Z Index: 200

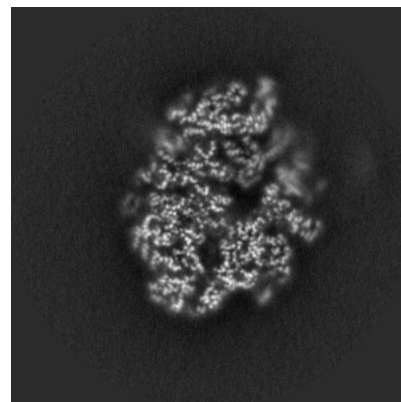
### 6.2.2 Raw map



X Index: 200



Y Index: 200

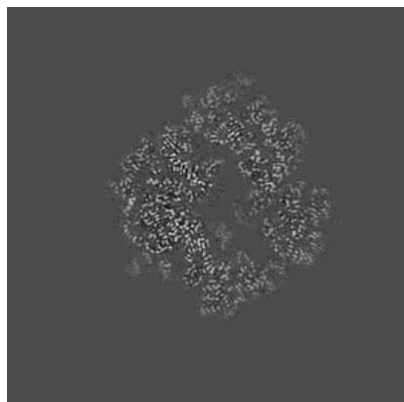


Z Index: 200

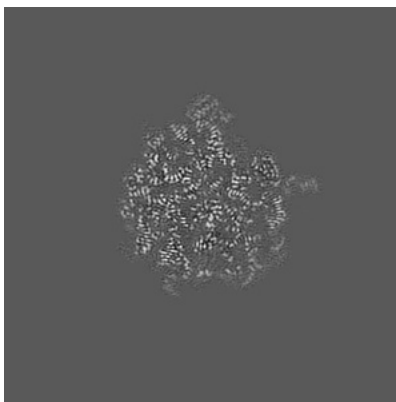
The images above show central slices of the map in three orthogonal directions.

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

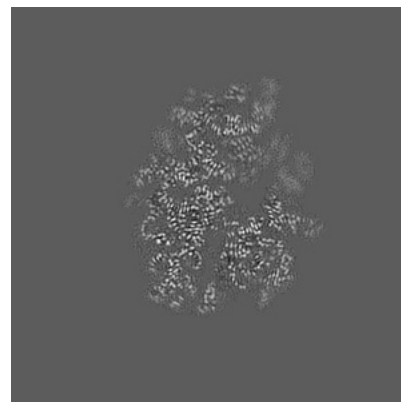
### 6.3.1 Primary map



X Index: 225

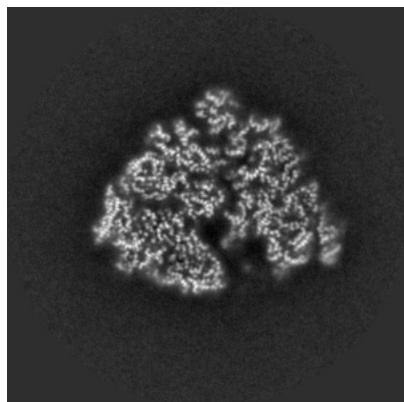


Y Index: 181

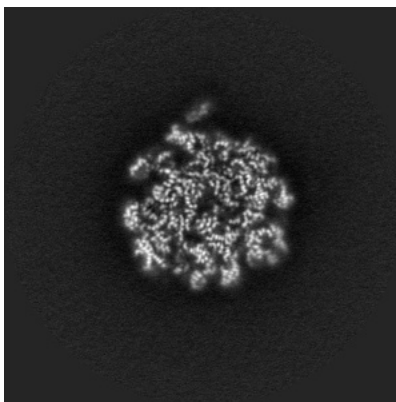


Z Index: 205

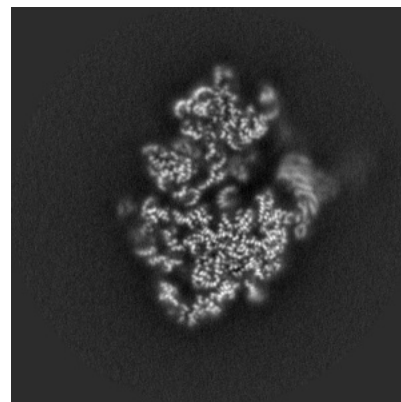
### 6.3.2 Raw map



X Index: 201



Y Index: 169

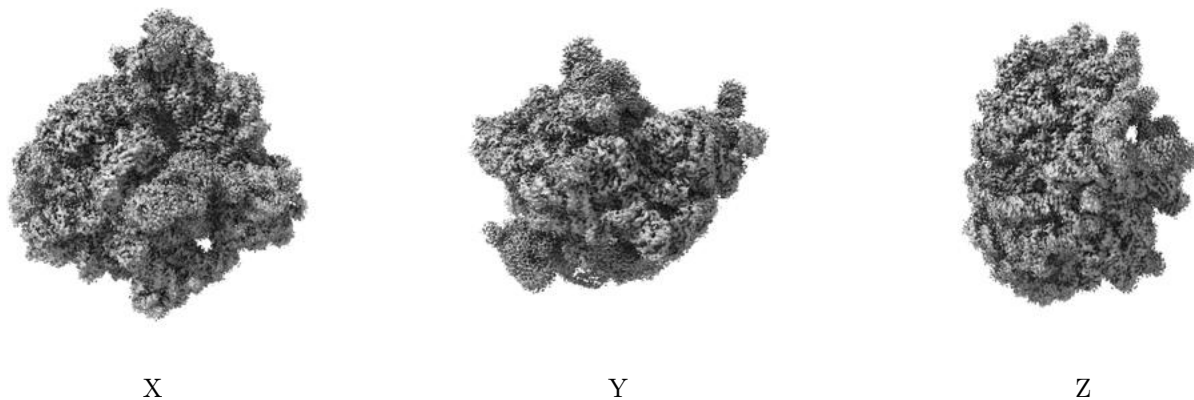


Z Index: 185

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

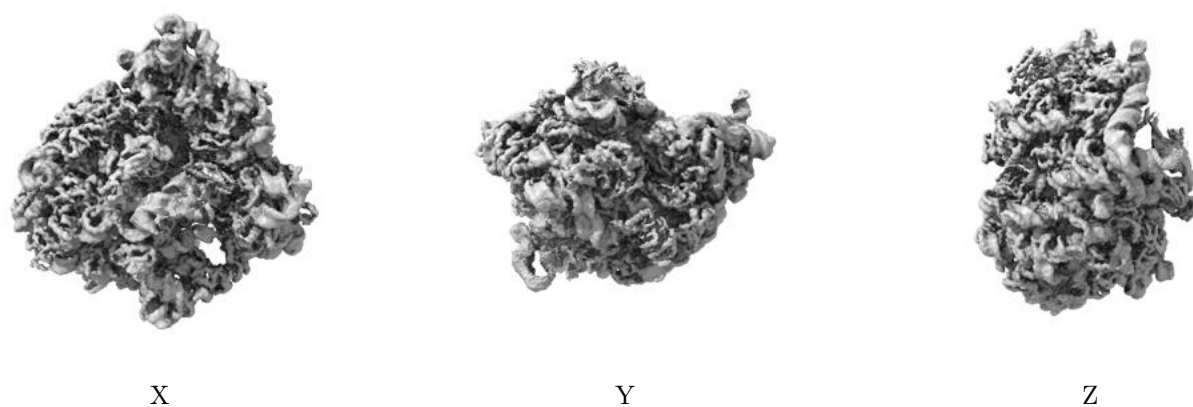
## 6.4 Orthogonal surface views [i](#)

### 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.

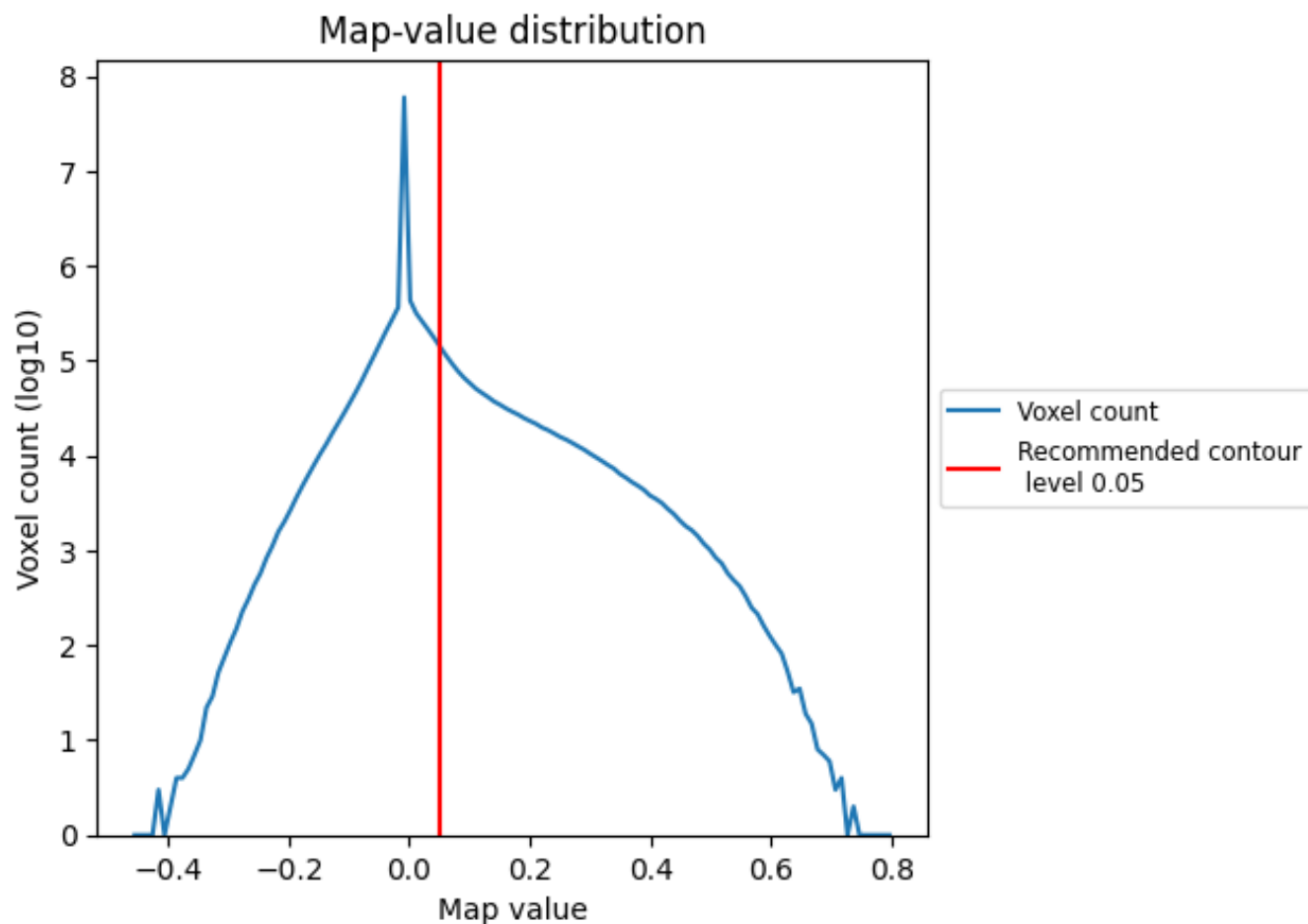
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

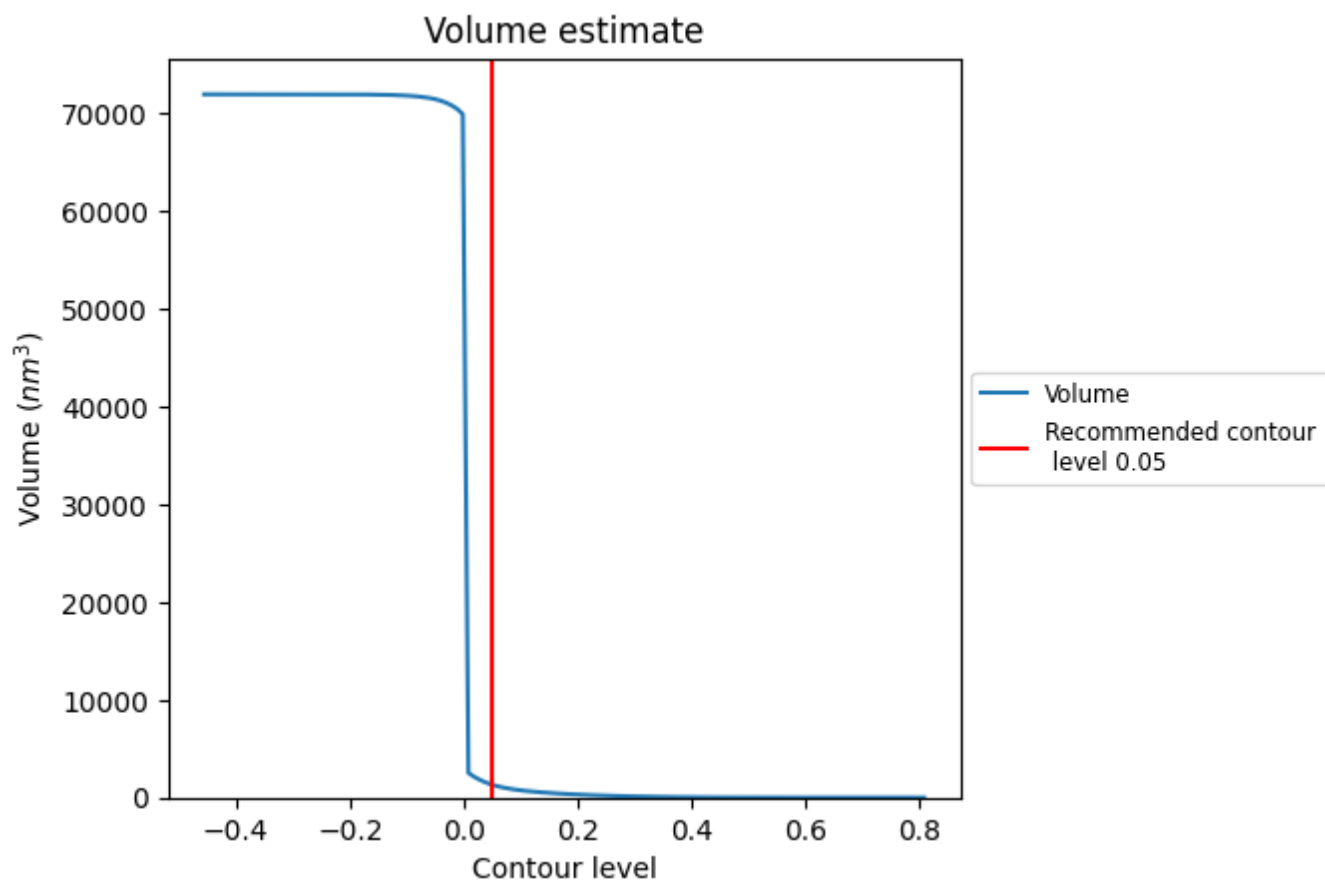
This section contains the results of statistical analysis of the map.

### 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.

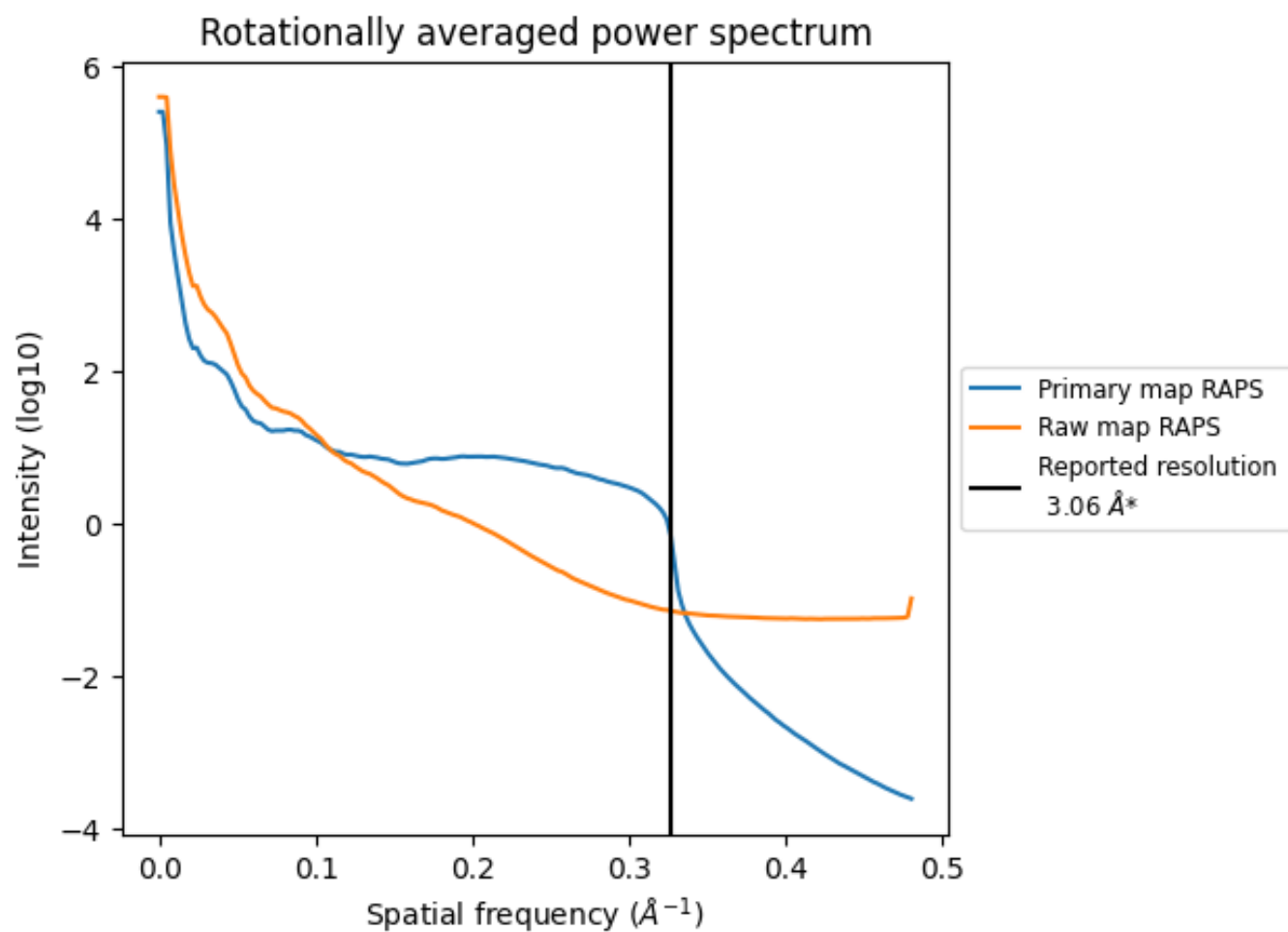
## 7.2 Volume estimate [i](#)



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 ⓘ

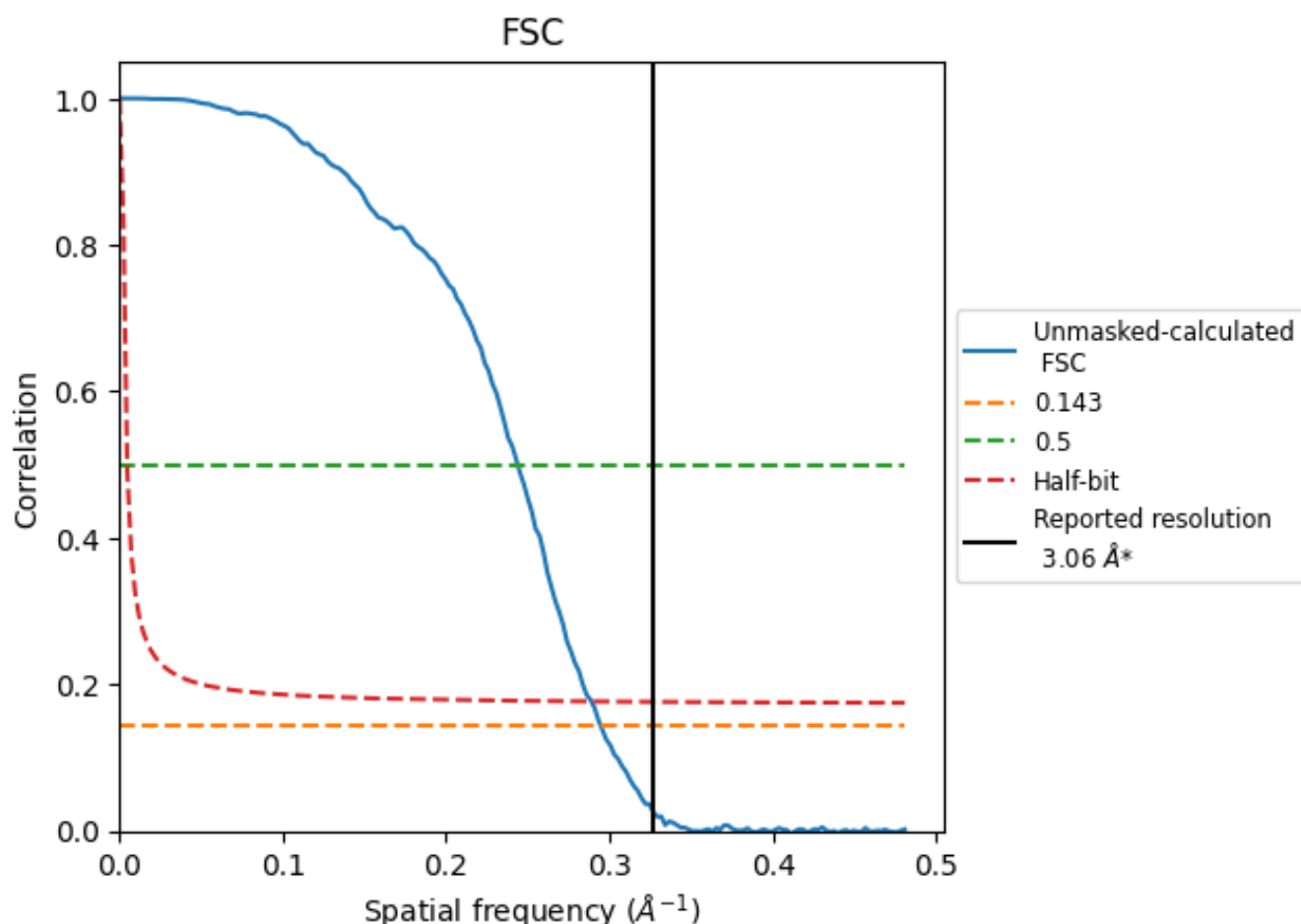


\*Reported resolution corresponds to spatial frequency of 0.327 Å<sup>-1</sup>

## 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](#)

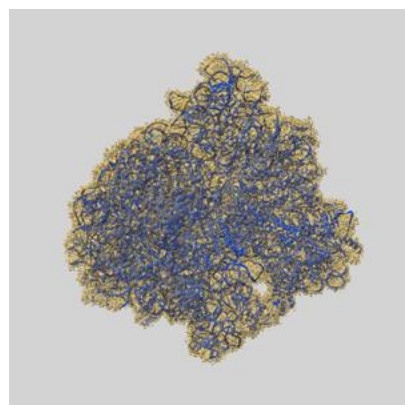
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.39	4.10	3.46

\*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 %

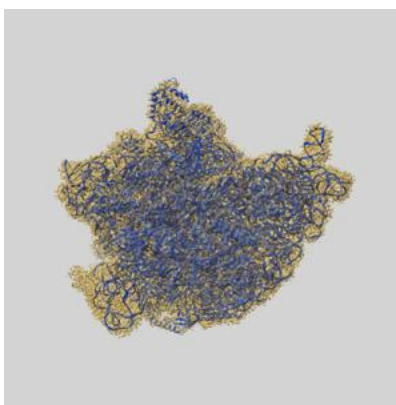
## 9 Map-model fit [i](#)

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.

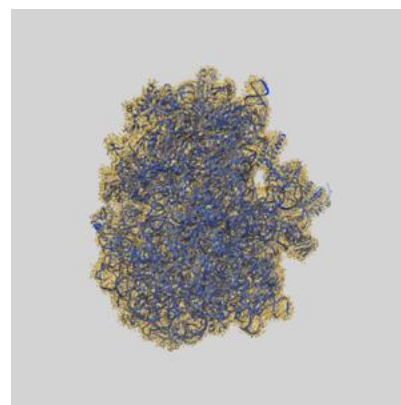
### 9.1 Map-model overlay [i](#)



X



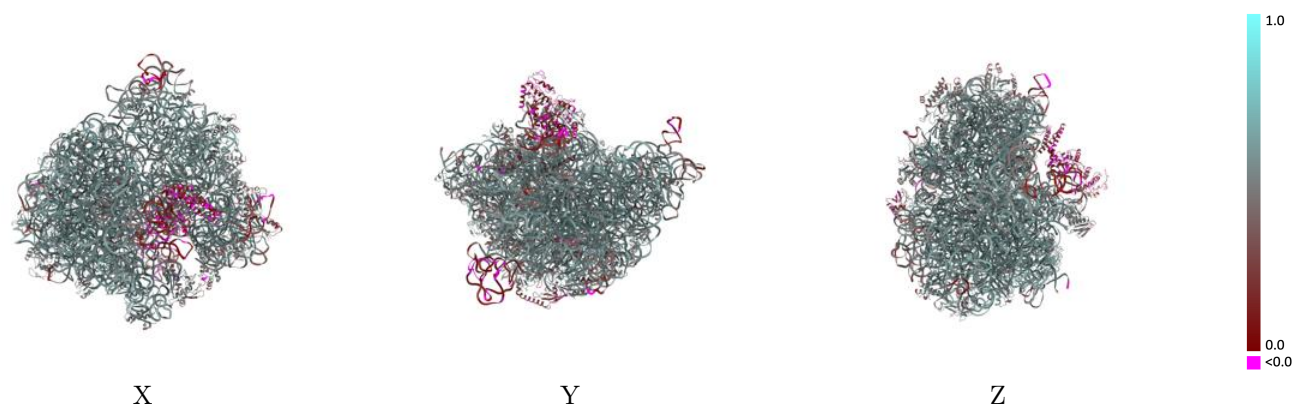
Y



Z

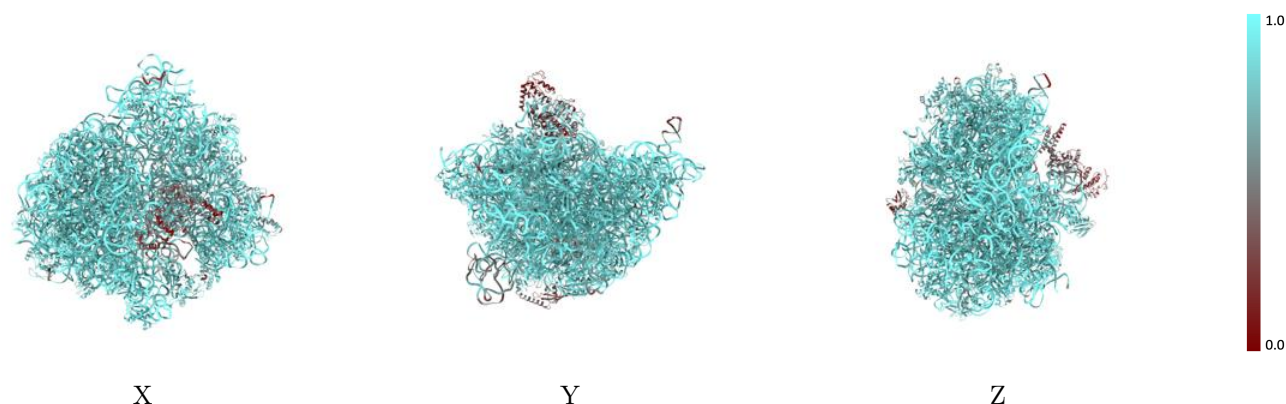
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



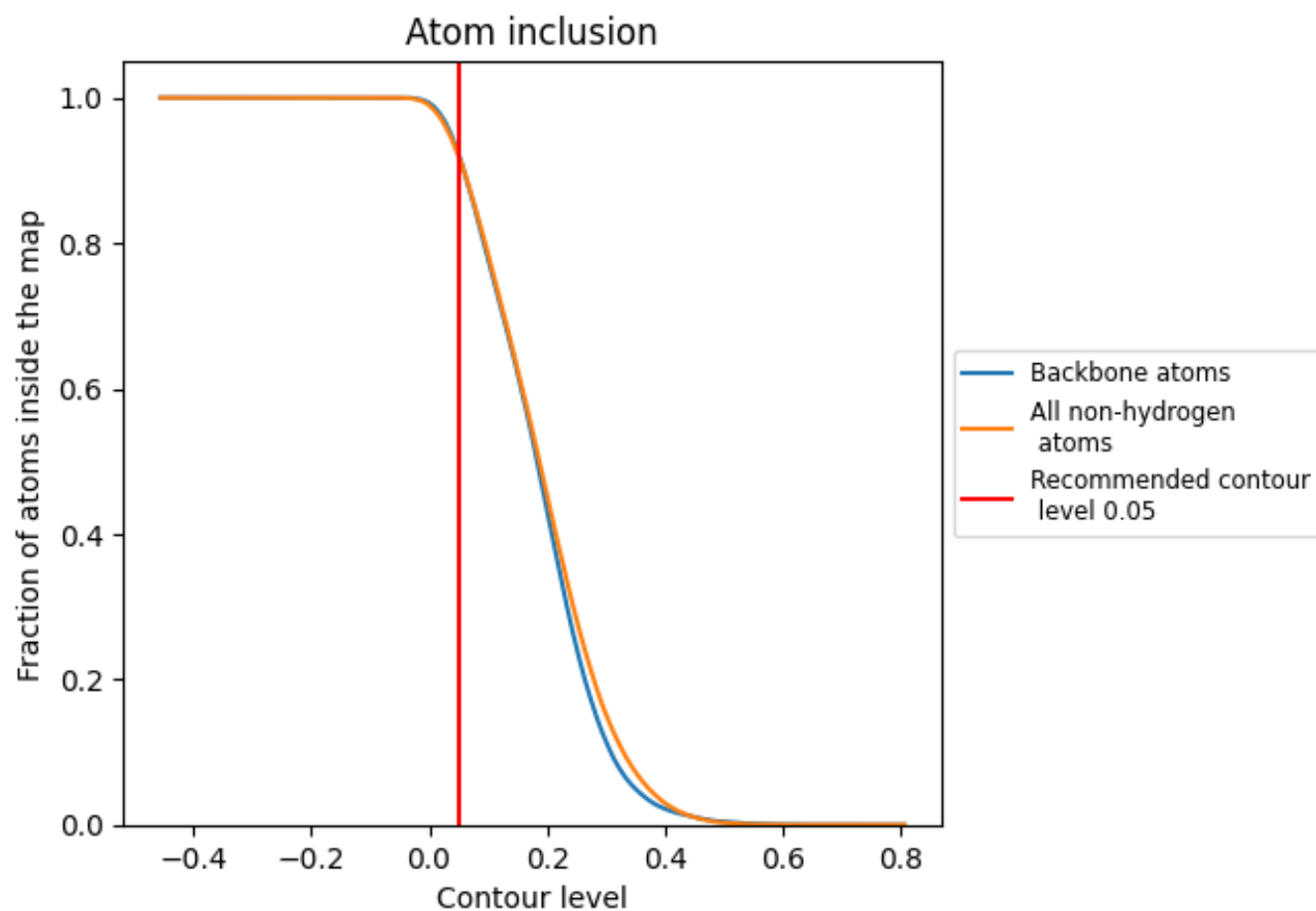
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).







































































## 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