



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 01:29 pm GMT

PDB ID : 5MDV
EMDB ID : EMD-3489
Title : Structure of ArfA and RF2 bound to the 70S ribosome (accommodated state)
Authors : James, N.R.; Brown, A.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on : 2016-11-13
Resolution : 2.97 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, 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

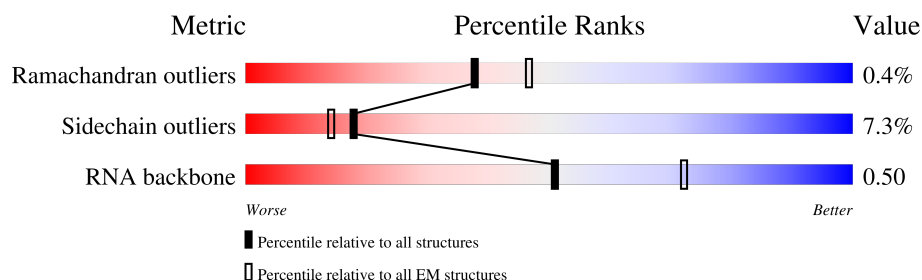
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.97 Å.

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



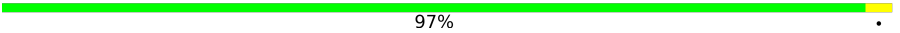


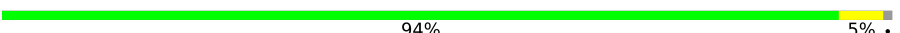












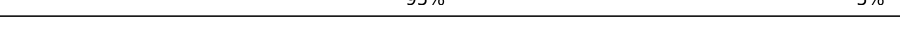
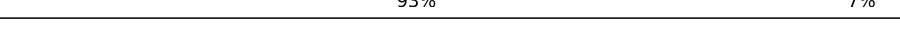

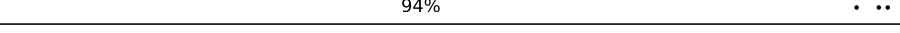
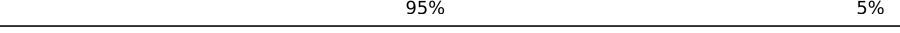

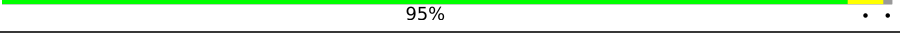
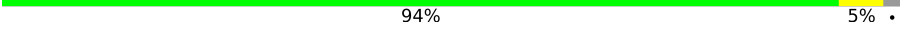

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	1	2904	79% 20% .
2	2	1534	79% 20% .
3	3	120	88% 12%
4	4	18	22% 6% 72%
5	5	78	62% 32% . .
6	6	61	72% . 25%
7	7	365	90% 9% .
8	B	273	95% 5% .



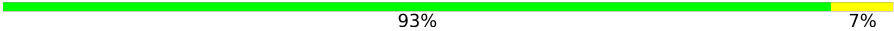
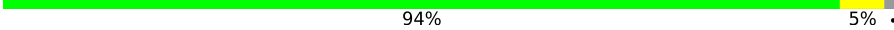



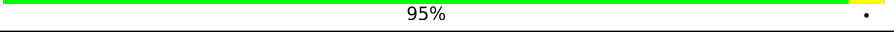



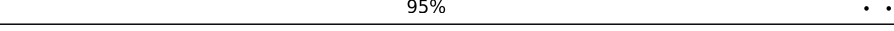





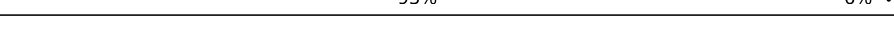

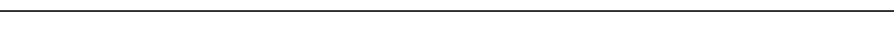

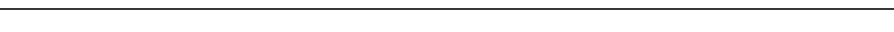
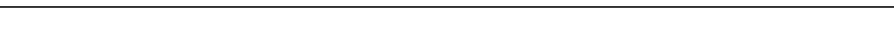


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Mol	Chain	Length	Quality of chain
9	C	209	 97% .
10	D	201	 93% 7%
11	E	179	 92% 7% .
12	F	177	 94% 5% .
13	G	149	 5% 93% 7%
14	H	165	 42% 69% 9% . 21%
15	I	142	 25% 85% 11% 5%
16	J	142	 . 94% 6%
17	K	123	 94% 6%
18	L	144	 . 93% 7%
19	M	136	 94% 6%
20	N	127	 89% 5% 6%
21	O	117	 94% 5% .
22	P	115	 93% 6% .
23	Q	118	 92% 8% .
24	R	103	 95% 5%
25	S	110	 93% 7%
26	T	100	 92% . 6%
27	U	104	 94% . .
28	V	94	 . 95% 5%
29	W	85	 87% . 11%
30	X	78	 95% . .
31	Y	63	 . 94% 5% .
32	Z	59	 93% 5% .
33	a	70	 . 87% 7% 6%

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Mol	Chain	Length	Quality of chain
34	b	57	 93% 5% .
35	c	55	 91% . 5%
36	d	46	 93% 7%
37	e	65	 94% 5% .
38	f	38	 92% 8%
39	g	241	 91% . 7%
40	h	233	 84% 5% 11%
41	i	206	 95% .
42	j	167	 84% 9% 7%
43	k	135	 71% 5% . 23%
44	l	179	 78% 6% . 15%
45	m	130	 95% . .
46	n	130	 91% 6% . .
47	o	103	 87% 8% . .
48	p	129	 85% 5% 9%
49	q	124	 91% 8% .
50	r	118	 90% 8% .
51	s	101	 93% 6% .
52	t	89	 87% 12% .
53	u	82	 93% 7%
54	v	84	 90% 5% 5%
55	w	75	 85% . 12%
56	x	92	 86% . 10%
57	y	87	 91% 8% .
58	z	71	 96% . .

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 149892 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	46	Total	C	N	O	S	0	0
			377	234	77	64	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	0	HIS	-	expression tag	UNP P36675

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	362	Total	C	N	O	S	0	0
			2863	1762	501	590	10		

- 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	152	Total	C	N	O	S	0	0
			1191	741	230	216	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		

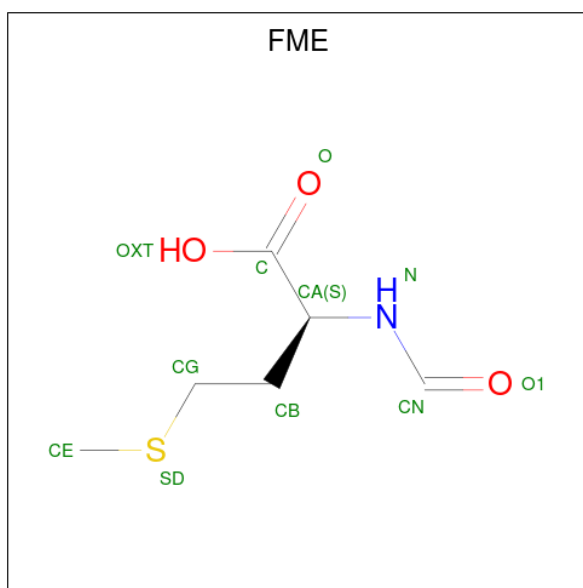
- Molecule 58 is a protein called 30S ribosomal protein S21.

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	296	Total	Mg	0
			296	296	
59	2	129	Total	Mg	0
			129	129	
59	3	9	Total	Mg	0
			9	9	
59	5	4	Total	Mg	0
			4	4	
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.

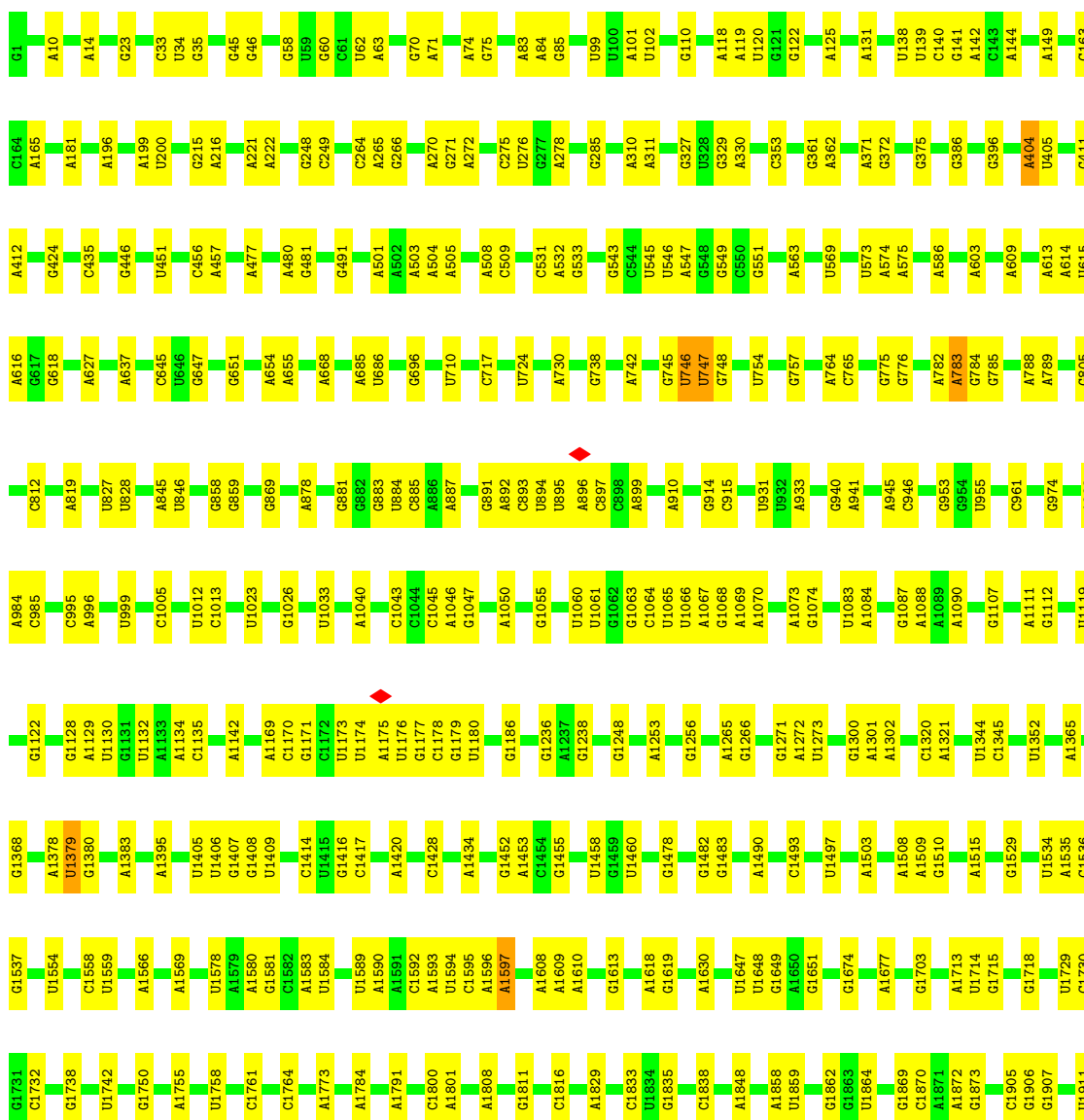
Mol	Chain	Residues	Atoms		AltConf
62	B	2	Total	O	0
			2	2	

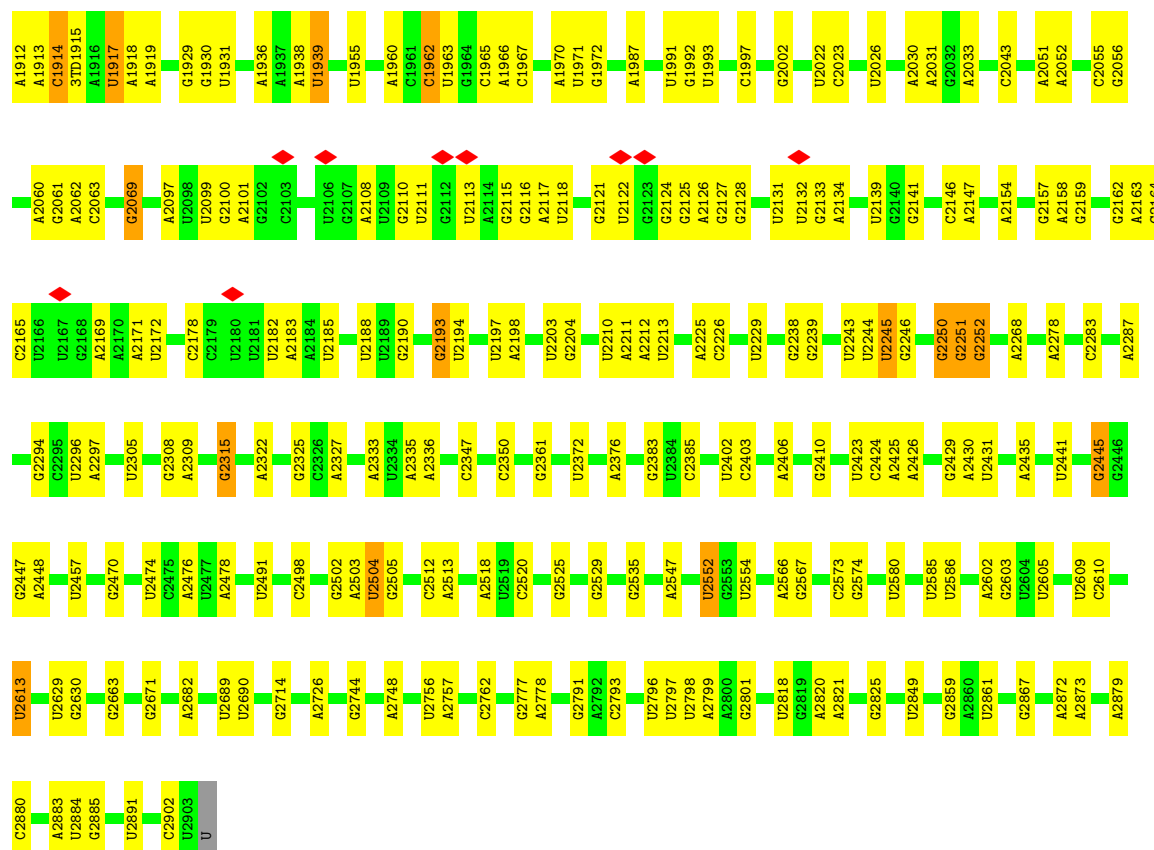
3 Residue-property plots

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

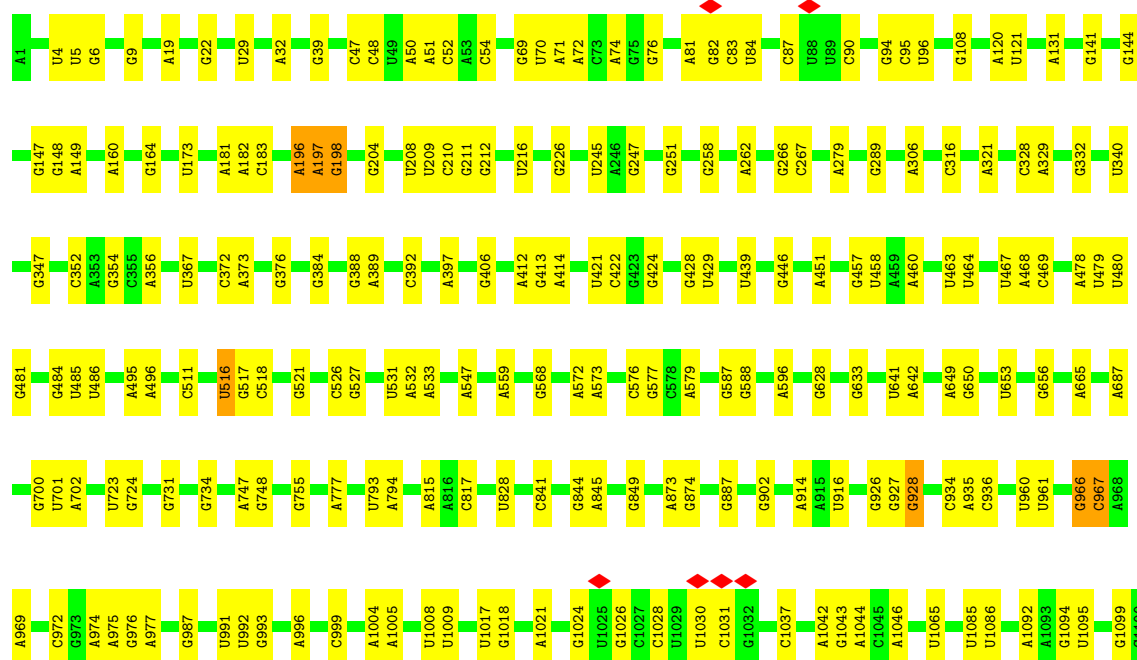
Chain 1:  79% 20% .

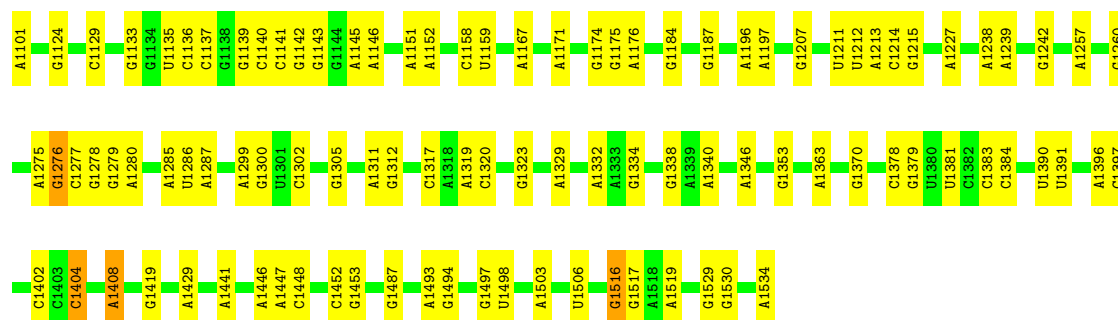




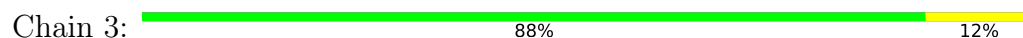
• Molecule 2: 16S ribosomal RNA

Chain 2: 79% 20% .





• Molecule 3: 5S ribosomal RNA



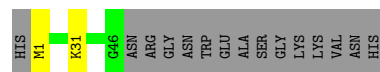
• Molecule 4: mRNA



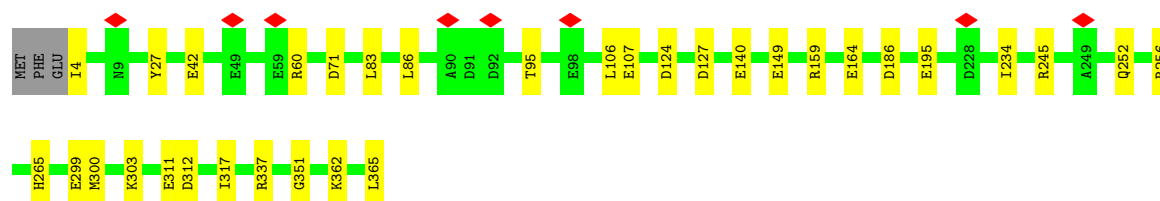
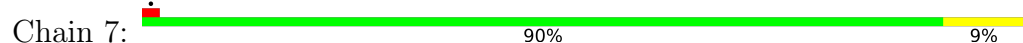
• Molecule 5: fMet-NH-tRNA(fMet)



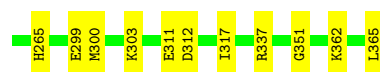
• Molecule 6: Alternative ribosome-rescue factor A



• Molecule 7: Peptide chain release factor 2



• Molecule 8: 50S ribosomal protein L2



Chain B:  95% 5%



- Molecule 9: 50S ribosomal protein L3

Chain C:  97%



- Molecule 10: 50S ribosomal protein L4

Chain D:  93% 7%



- Molecule 11: 50S ribosomal protein L5

Chain E:  92% 7%



- Molecule 12: 50S ribosomal protein L6

Chain F:  94% 5%




- Molecule 13: 50S ribosomal protein L9

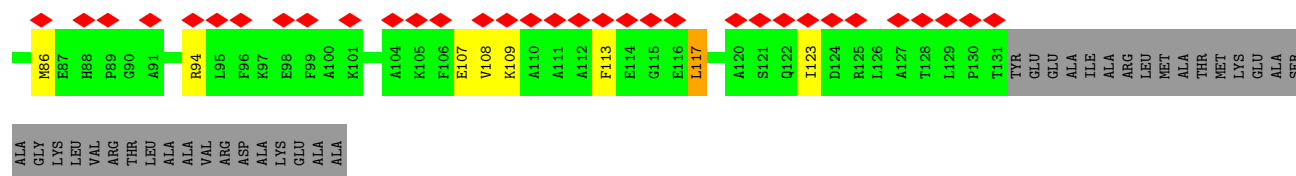
Chain G:  5% 93% 7%



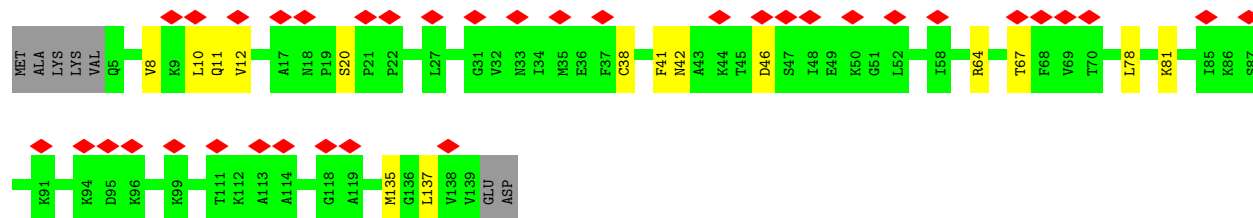
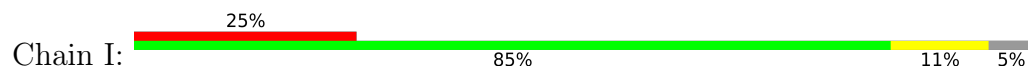
- Molecule 14: 50S ribosomal protein L10

Chain H:  42% 69% 9% 21%

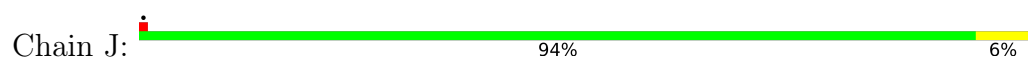




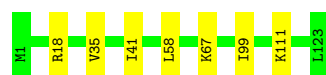
- Molecule 15: 50S ribosomal protein L11



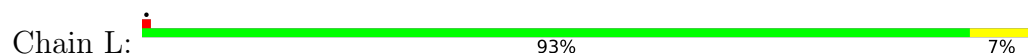
- Molecule 16: 50S ribosomal protein L13



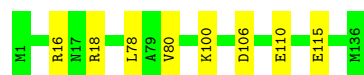
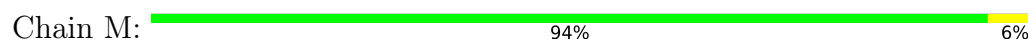
- Molecule 17: 50S ribosomal protein L14



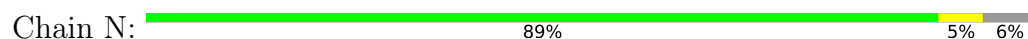
- Molecule 18: 50S ribosomal protein L15



- Molecule 19: 50S ribosomal protein L16



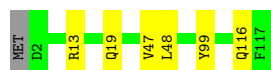
- Molecule 20: 50S ribosomal protein L17





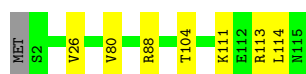
- Molecule 21: 50S ribosomal protein L18

Chain O: 94% 5%



- Molecule 22: 50S ribosomal protein L19

Chain P: 93% 6%



- Molecule 23: 50S ribosomal protein L20

Chain Q: 92% 8%



- Molecule 24: 50S ribosomal protein L21

Chain R: 95% 5%



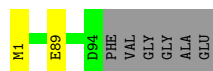
- Molecule 25: 50S ribosomal protein L22

Chain S: 93% 7%



- Molecule 26: 50S ribosomal protein L23

Chain T: 92% 6%



- Molecule 27: 50S ribosomal protein L24

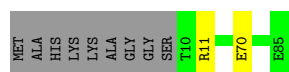
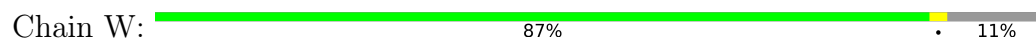
Chain U: 94% 5%



- Molecule 28: 50S ribosomal protein L25



- Molecule 29: 50S ribosomal protein L27



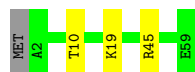
- Molecule 30: 50S ribosomal protein L28



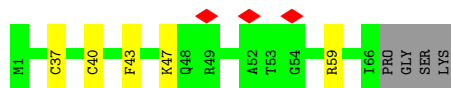
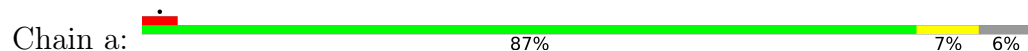
- Molecule 31: 50S ribosomal protein L29



- Molecule 32: 50S ribosomal protein L30



- Molecule 33: 50S ribosomal protein L31



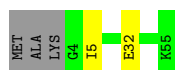
- Molecule 34: 50S ribosomal protein L32





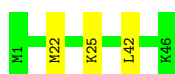
- Molecule 35: 50S ribosomal protein L33

Chain c: 91% 5%



- Molecule 36: 50S ribosomal protein L34

Chain d: 93% 7%



- Molecule 37: 50S ribosomal protein L35

Chain e: 94% 5%



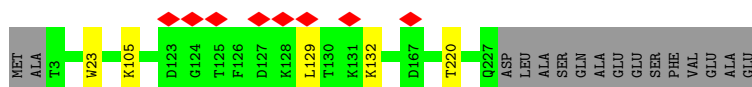
- Molecule 38: 50S ribosomal protein L36

Chain f: 92% 8%



- Molecule 39: 30S ribosomal protein S2

Chain g: 91% 7%



- Molecule 40: 30S ribosomal protein S3

Chain h: 84% 5% 11%



- Molecule 41: 30S ribosomal protein S4

Chain i: 95% 5%



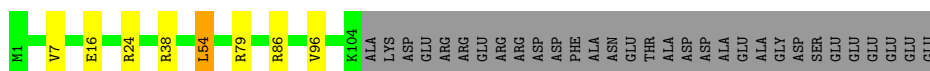
- Molecule 42: 30S ribosomal protein S5

Chain j: 84% 9% 7%



- Molecule 43: 30S ribosomal protein S6

Chain k: 71% 5% 23%



- Molecule 44: 30S ribosomal protein S7

Chain l: 78% 6% 15%



- Molecule 45: 30S ribosomal protein S8

Chain m: 95% 4% 1%



- Molecule 46: 30S ribosomal protein S9

Chain n: 91% 6% 3%



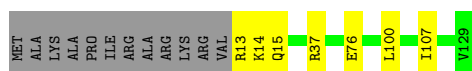
- Molecule 47: 30S ribosomal protein S10

Chain o: 87% 8% 5%

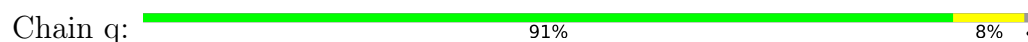


- Molecule 48: 30S ribosomal protein S11

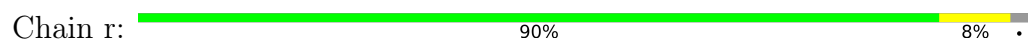
Chain p: 85% 5% 9%



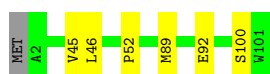
- Molecule 49: 30S ribosomal protein S12



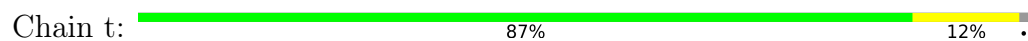
- Molecule 50: 30S ribosomal protein S13



- Molecule 51: 30S ribosomal protein S14



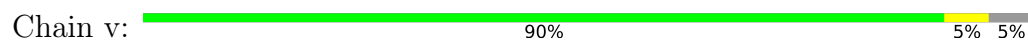
- Molecule 52: 30S ribosomal protein S15



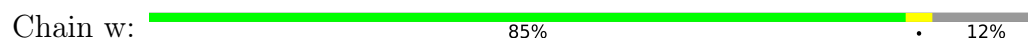
- Molecule 53: 30S ribosomal protein S16

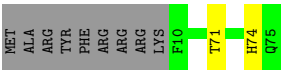


- Molecule 54: 30S ribosomal protein S17

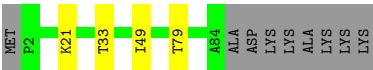
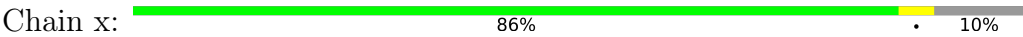


- Molecule 55: 30S ribosomal protein S18

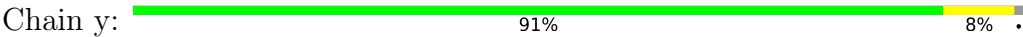




• Molecule 56: 30S ribosomal protein S19



• Molecule 57: 30S ribosomal protein S20



• 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	139792	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	1.105	Depositor
Minimum map value	-0.583	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.04	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: 6MZ, 4OC, MG, G7M, OMG, 8AN, 2MA, 0TD, UR3, MA6, 2MG, 5MU, 4SU, OMU, 7MG, FME, 1MG, 5MC, MEQ, PSU, OMC, H2U, 3TD, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.35	0/69286	0.72	22/108087 (0.0%)
2	2	0.35	0/36590	0.73	19/57074 (0.0%)
3	3	0.26	0/2872	0.69	0/4478
4	4	0.34	0/122	0.60	0/188
5	5	0.29	0/1672	0.73	0/2603
6	6	0.41	0/383	0.68	0/504
7	7	0.49	0/2892	0.76	0/3897
8	B	0.39	0/2121	0.78	0/2852
9	C	0.40	0/1586	0.68	0/2134
10	D	0.45	0/1571	0.77	1/2113 (0.0%)
11	E	0.46	0/1434	0.78	0/1926
12	F	0.39	0/1333	0.67	0/1805
13	G	0.43	0/1122	0.67	0/1515
14	H	0.50	0/993	0.74	0/1340
15	I	0.46	0/998	0.68	0/1348
16	J	0.44	0/1152	0.72	0/1551
17	K	0.39	0/955	0.75	0/1279
18	L	0.43	0/1062	0.78	0/1413
19	M	0.44	0/1093	0.78	0/1460
20	N	0.49	0/964	0.87	0/1289
21	O	0.47	0/902	0.80	0/1209
22	P	0.41	0/929	0.77	0/1242
23	Q	0.57	0/960	0.89	0/1278
24	R	0.34	0/829	0.64	0/1107
25	S	0.47	0/864	0.82	0/1156
26	T	0.41	0/752	0.72	0/1005
27	U	0.34	0/796	0.61	0/1062
28	V	0.40	0/766	0.67	0/1025
29	W	0.42	0/589	0.75	0/779
30	X	0.46	0/635	0.80	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	0.43	0/452	0.76	0/605
33	a	0.39	0/531	0.73	0/709
34	b	0.43	0/450	0.78	0/599
35	c	0.37	0/433	0.69	0/576
36	d	0.51	0/380	0.96	0/498
37	e	0.45	0/513	0.82	0/676
38	f	0.38	0/303	0.79	0/397
39	g	0.46	0/1791	0.70	0/2413
40	h	0.47	0/1663	0.74	0/2241
41	i	0.47	0/1665	0.78	0/2227
42	j	0.50	0/1165	0.79	0/1568
43	k	0.43	0/867	0.75	1/1171 (0.1%)
44	l	0.51	0/1206	0.85	1/1617 (0.1%)
45	m	0.42	0/989	0.69	0/1326
46	n	0.44	0/1034	0.81	1/1375 (0.1%)
47	o	0.41	0/800	0.76	0/1082
48	p	0.41	0/893	0.74	0/1205
49	q	0.46	0/960	0.81	0/1286
50	r	0.48	0/909	0.85	0/1215
51	s	0.50	0/817	0.80	0/1088
52	t	0.56	0/722	0.86	0/964
53	u	0.46	0/659	0.78	0/884
54	v	0.34	0/657	0.66	0/881
55	w	0.46	0/553	0.79	0/743
56	x	0.39	0/680	0.68	0/915
57	y	0.59	0/675	0.86	0/895
58	z	0.55	0/597	0.88	0/792
All	All	0.38	0/161089	0.73	45/240182 (0.0%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	198	G	N9-C1'-C2'	-10.10	100.87	114.00
2	2	1408	A	N9-C1'-C2'	-9.66	101.38	112.00
2	2	1404	C	N1-C1'-C2'	-9.40	101.66	112.00
2	2	928	G	N9-C1'-C2'	-9.08	102.01	112.00
2	2	927	G	N9-C1'-C2'	-8.22	102.96	112.00
44	l	109	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	1	2245	U	N1-C1'-C2'	-8.00	103.19	112.00
1	1	1914	C	N1-C1'-C2'	-7.97	103.23	112.00
1	1	2243	U	N1-C1'-C2'	-7.91	103.30	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2193	G	C2'-C3'-O3'	7.17	125.26	109.50
1	1	1597	A	N9-C1'-C2'	-7.14	104.14	112.00
1	1	2252	G	N9-C1'-C2'	-7.03	104.27	112.00
1	1	754	U	N1-C1'-C2'	6.46	122.39	114.00
2	2	1391	U	N1-C1'-C2'	-6.41	104.94	112.00
2	2	1276	G	C1'-C2'-O2'	-6.39	91.42	110.60
2	2	197	A	N9-C1'-C2'	6.39	122.30	114.00
2	2	927	G	C1'-C2'-O2'	-6.26	91.82	110.60
1	1	1379	U	C2'-C3'-O3'	6.24	123.69	113.70
1	1	2244	U	C1'-C2'-O2'	-6.20	92.01	110.60
1	1	375	G	C2'-C3'-O3'	6.10	123.46	113.70
46	n	41	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	1	2315	G	N9-C1'-C2'	-5.95	105.46	112.00
2	2	927	G	C4'-C3'-O3'	5.93	124.86	113.00
1	1	2244	U	C4'-C3'-O3'	5.89	124.77	113.00
2	2	1390	U	N1-C1'-C2'	-5.83	105.58	112.00
2	2	1390	U	C1'-C2'-O2'	-5.70	93.51	110.60
1	1	742	A	C8-N9-C1'	-5.64	117.56	127.70
1	1	2250	G	C4'-C3'-O3'	-5.60	97.64	109.40
2	2	1390	U	C4'-C3'-O3'	5.56	124.11	113.00
1	1	2252	G	C4'-C3'-O3'	5.52	124.03	113.00
1	1	742	A	C4-N9-C1'	5.47	136.15	126.30
1	1	783	A	C4'-C3'-O3'	5.47	123.94	113.00
43	k	54	LEU	CA-CB-CG	5.47	127.87	115.30
2	2	439	U	N1-C1'-C2'	5.46	121.11	114.00
1	1	2613	U	O4'-C1'-N1	5.40	112.52	108.20
1	1	1914	C	C4'-C3'-O3'	5.34	123.69	113.00
2	2	356	A	C2'-C3'-O3'	5.32	122.21	113.70
1	1	742	A	N9-C1'-C2'	5.31	120.90	114.00
2	2	928	G	C4'-C3'-O3'	5.30	123.59	113.00
10	D	69	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	1	404	A	C2'-C3'-O3'	5.25	122.09	113.70
2	2	1408	A	C4'-C3'-O3'	5.24	123.47	113.00
2	2	1384	C	N1-C1'-C2'	-5.17	106.32	112.00
2	2	196	A	N9-C1'-C2'	-5.10	106.39	112.00
1	1	1838	C	N1-C1'-C2'	5.03	120.54	114.00

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	44/61 (72%)	39 (89%)	5 (11%)	0	100	100
7	7	359/365 (98%)	344 (96%)	14 (4%)	1 (0%)	41	74
8	B	269/273 (98%)	255 (95%)	13 (5%)	1 (0%)	34	70
9	C	207/209 (99%)	198 (96%)	8 (4%)	1 (0%)	29	66
10	D	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
11	E	175/179 (98%)	166 (95%)	8 (5%)	1 (1%)	25	61
12	F	173/177 (98%)	161 (93%)	12 (7%)	0	100	100
13	G	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
14	H	128/165 (78%)	104 (81%)	20 (16%)	4 (3%)	4	20
15	I	133/142 (94%)	114 (86%)	17 (13%)	2 (2%)	10	39
16	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
17	K	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
18	L	142/144 (99%)	133 (94%)	7 (5%)	2 (1%)	11	41
19	M	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
20	N	117/127 (92%)	106 (91%)	11 (9%)	0	100	100
21	O	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	17	53
22	P	112/115 (97%)	104 (93%)	8 (7%)	0	100	100
23	Q	115/118 (98%)	112 (97%)	2 (2%)	1 (1%)	17	53
24	R	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
25	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
26	T	92/100 (92%)	90 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	U	101/104 (97%)	97 (96%)	3 (3%)	1 (1%)	15	50
28	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
29	W	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
30	X	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
31	Y	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
32	Z	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
33	a	64/70 (91%)	62 (97%)	2 (3%)	0	100	100
34	b	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
35	c	50/55 (91%)	50 (100%)	0	0	100	100
36	d	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
37	e	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
38	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
39	g	223/241 (92%)	213 (96%)	10 (4%)	0	100	100
40	h	206/233 (88%)	197 (96%)	6 (3%)	3 (2%)	10	39
41	i	203/206 (98%)	194 (96%)	9 (4%)	0	100	100
42	j	154/167 (92%)	145 (94%)	8 (5%)	1 (1%)	25	61
43	k	102/135 (76%)	98 (96%)	3 (3%)	1 (1%)	15	50
44	l	150/179 (84%)	143 (95%)	6 (4%)	1 (1%)	22	58
45	m	127/130 (98%)	120 (94%)	6 (5%)	1 (1%)	19	55
46	n	125/130 (96%)	116 (93%)	7 (6%)	2 (2%)	9	38
47	o	97/103 (94%)	90 (93%)	6 (6%)	1 (1%)	15	50
48	p	115/129 (89%)	104 (90%)	11 (10%)	0	100	100
49	q	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
50	r	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
51	s	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
52	t	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
53	u	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
54	v	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
55	w	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
56	x	81/92 (88%)	78 (96%)	3 (4%)	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%)	67 (98%)	1 (2%)	0	100	100
All	All	6273/6646 (94%)	5943 (95%)	305 (5%)	25 (0%)	38	70

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	L	36	LYS
27	U	7	ARG
46	n	56	ASP
47	o	57	VAL
8	B	240	PHE
9	C	149	ASN
14	H	117	LEU
23	Q	3	ARG
44	l	130	ASN
15	I	64	ARG
18	L	99	ASN
40	h	14	ILE
11	E	62	GLY
40	h	60	PRO
40	h	80	LYS
14	H	51	TYR
14	H	113	PHE
21	O	99	TYR
43	k	96	VAL
45	m	75	ILE
14	H	108	VAL
7	7	351	GLY
15	I	12	VAL
42	j	27	GLY
46	n	50	GLN

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	39/51 (76%)	37 (95%)	2 (5%)	24	57
7	7	306/310 (99%)	275 (90%)	31 (10%)	7	27
8	B	216/218 (99%)	204 (94%)	12 (6%)	21	54
9	C	164/164 (100%)	159 (97%)	5 (3%)	41	73
10	D	165/165 (100%)	150 (91%)	15 (9%)	9	32
11	E	148/150 (99%)	136 (92%)	12 (8%)	11	37
12	F	136/138 (99%)	128 (94%)	8 (6%)	19	52
13	G	114/114 (100%)	103 (90%)	11 (10%)	8	30
14	H	99/123 (80%)	86 (87%)	13 (13%)	4	17
15	I	104/110 (94%)	91 (88%)	13 (12%)	4	18
16	J	116/116 (100%)	108 (93%)	8 (7%)	15	46
17	K	104/104 (100%)	97 (93%)	7 (7%)	16	47
18	L	103/103 (100%)	95 (92%)	8 (8%)	12	40
19	M	109/109 (100%)	101 (93%)	8 (7%)	14	42
20	N	99/103 (96%)	93 (94%)	6 (6%)	18	51
21	O	86/87 (99%)	81 (94%)	5 (6%)	20	53
22	P	99/100 (99%)	92 (93%)	7 (7%)	14	44
23	Q	89/90 (99%)	81 (91%)	8 (9%)	9	33
24	R	84/84 (100%)	79 (94%)	5 (6%)	19	51
25	S	93/93 (100%)	85 (91%)	8 (9%)	10	35
26	T	81/84 (96%)	79 (98%)	2 (2%)	47	77
27	U	84/85 (99%)	79 (94%)	5 (6%)	19	51
28	V	78/78 (100%)	73 (94%)	5 (6%)	17	49
29	W	58/63 (92%)	56 (97%)	2 (3%)	37	70
30	X	67/68 (98%)	64 (96%)	3 (4%)	27	62
31	Y	54/55 (98%)	51 (94%)	3 (6%)	21	54
32	Z	48/49 (98%)	45 (94%)	3 (6%)	18	49
33	a	59/62 (95%)	54 (92%)	5 (8%)	10	36
34	b	47/48 (98%)	44 (94%)	3 (6%)	17	49
35	c	47/49 (96%)	45 (96%)	2 (4%)	29	64
36	d	38/38 (100%)	35 (92%)	3 (8%)	12	39
37	e	51/52 (98%)	48 (94%)	3 (6%)	19	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	f	34/34 (100%)	31 (91%)	3 (9%)	10	34
39	g	187/199 (94%)	182 (97%)	5 (3%)	44	75
40	h	171/190 (90%)	160 (94%)	11 (6%)	17	49
41	i	172/173 (99%)	163 (95%)	9 (5%)	23	57
42	j	119/126 (94%)	105 (88%)	14 (12%)	5	21
43	k	91/116 (78%)	84 (92%)	7 (8%)	13	40
44	l	125/147 (85%)	113 (90%)	12 (10%)	8	30
45	m	104/105 (99%)	100 (96%)	4 (4%)	33	67
46	n	105/107 (98%)	98 (93%)	7 (7%)	16	47
47	o	86/90 (96%)	77 (90%)	9 (10%)	7	25
48	p	90/99 (91%)	83 (92%)	7 (8%)	12	40
49	q	102/103 (99%)	93 (91%)	9 (9%)	10	34
50	r	94/96 (98%)	84 (89%)	10 (11%)	6	25
51	s	83/84 (99%)	77 (93%)	6 (7%)	14	43
52	t	76/77 (99%)	65 (86%)	11 (14%)	3	14
53	u	65/65 (100%)	59 (91%)	6 (9%)	9	32
54	v	74/78 (95%)	70 (95%)	4 (5%)	22	55
55	w	57/65 (88%)	55 (96%)	2 (4%)	36	69
56	x	72/79 (91%)	68 (94%)	4 (6%)	21	54
57	y	65/66 (98%)	58 (89%)	7 (11%)	6	24
58	z	60/61 (98%)	58 (97%)	2 (3%)	38	71
All	All	5217/5423 (96%)	4837 (93%)	380 (7%)	18	42

All (380) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	1	MET
6	6	31	LYS
7	7	4	ILE
7	7	27	TYR
7	7	42	GLU
7	7	60	ARG
7	7	71	ASP
7	7	83	LEU
7	7	86	LEU

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Mol	Chain	Res	Type
7	7	95	THR
7	7	106	LEU
7	7	107	GLU
7	7	124	ASP
7	7	127	ASP
7	7	140	GLU
7	7	149	GLU
7	7	159	ARG
7	7	164	GLU
7	7	186	ASP
7	7	195	GLU
7	7	234	ILE
7	7	245	ARG
7	7	256	ARG
7	7	265	HIS
7	7	299	GLU
7	7	300	MET
7	7	303	LYS
7	7	311	GLU
7	7	312	ASP
7	7	317	ILE
7	7	337	ARG
7	7	362	LYS
7	7	365	LEU
8	B	52	ARG
8	B	130	LEU
8	B	156	ARG
8	B	189	ARG
8	B	195	VAL
8	B	202	LEU
8	B	203	ARG
8	B	204	VAL
8	B	205	LEU
8	B	242	LYS
8	B	252	THR
8	B	258	ARG
9	C	13	ARG
9	C	32	ASN
9	C	43	ASP
9	C	77	ARG
9	C	118	PHE
10	D	7	ASP

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Mol	Chain	Res	Type
10	D	21	ARG
10	D	22	ASP
10	D	40	ARG
10	D	57	LYS
10	D	69	ARG
10	D	73	ILE
10	D	77	ILE
10	D	88	ARG
10	D	108	ILE
10	D	109	LEU
10	D	111	GLU
10	D	122	GLU
10	D	149	ILE
10	D	184	ASP
11	E	6	ASP
11	E	17	MET
11	E	40	VAL
11	E	47	LYS
11	E	57	LEU
11	E	80	ARG
11	E	115	ARG
11	E	117	LEU
11	E	123	ASP
11	E	133	ARG
11	E	140	GLU
11	E	152	LEU
12	F	25	THR
12	F	32	GLU
12	F	95	ARG
12	F	110	SER
12	F	141	ILE
12	F	155	GLU
12	F	166	ASP
12	F	176	LYS
13	G	1	MET
13	G	11	ASN
13	G	12	LEU
13	G	17	ASP
13	G	41	LYS
13	G	51	ARG
13	G	66	ASN
13	G	72	ILE

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Mol	Chain	Res	Type
13	G	101	ASP
13	G	114	GLU
13	G	129	GLU
14	H	3	LEU
14	H	34	THR
14	H	54	VAL
14	H	57	ASN
14	H	65	GLU
14	H	74	ASP
14	H	80	THR
14	H	86	MET
14	H	94	ARG
14	H	107	GLU
14	H	109	LYS
14	H	117	LEU
14	H	123	ILE
15	I	8	VAL
15	I	10	LEU
15	I	11	GLN
15	I	20	SER
15	I	38	CYS
15	I	41	PHE
15	I	42	ASN
15	I	46	ASP
15	I	67	THR
15	I	78	LEU
15	I	81	LYS
15	I	135	MET
15	I	137	LEU
16	J	1	MET
16	J	30	THR
16	J	35	ARG
16	J	57	LEU
16	J	108	MET
16	J	123	LYS
16	J	129	GLU
16	J	142	ILE
17	K	18	ARG
17	K	35	VAL
17	K	41	ILE
17	K	58	LEU
17	K	67	LYS

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Mol	Chain	Res	Type
17	K	99	ILE
17	K	111	LYS
18	L	4	ASN
18	L	30	THR
18	L	40	SER
18	L	48	ARG
18	L	67	THR
18	L	78	ARG
18	L	84	LYS
18	L	115	GLU
19	M	16	ARG
19	M	18	ARG
19	M	78	LEU
19	M	80	VAL
19	M	100	LYS
19	M	106	ASP
19	M	110	GLU
19	M	115	GLU
20	N	2	ARG
20	N	20	MET
20	N	51	LEU
20	N	63	ARG
20	N	65	LEU
20	N	69	ARG
21	O	13	ARG
21	O	19	GLN
21	O	47	VAL
21	O	48	LEU
21	O	116	GLN
22	P	26	VAL
22	P	80	VAL
22	P	88	ARG
22	P	104	THR
22	P	111	LYS
22	P	113	ARG
22	P	114	LEU
23	Q	11	ARG
23	Q	18	LEU
23	Q	20	GLN
23	Q	51	ARG
23	Q	52	GLN
23	Q	59	GLN

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Mol	Chain	Res	Type
23	Q	91	ASP
23	Q	117	LEU
24	R	10	LYS
24	R	39	LEU
24	R	48	LYS
24	R	79	ARG
24	R	86	GLN
25	S	19	LEU
25	S	41	LYS
25	S	67	ASP
25	S	69	LEU
25	S	83	LYS
25	S	97	LEU
25	S	109	ASP
25	S	110	ARG
26	T	1	MET
26	T	89	GLU
27	U	7	ARG
27	U	9	ASP
27	U	46	GLN
27	U	52	LEU
27	U	72	ILE
28	V	1	MET
28	V	34	LYS
28	V	40	ILE
28	V	41	GLU
28	V	45	ASP
29	W	11	ARG
29	W	70	GLU
30	X	44	LYS
30	X	48	THR
30	X	60	ASP
31	Y	7	ARG
31	Y	57	LEU
31	Y	58	ASN
32	Z	10	THR
32	Z	19	LYS
32	Z	45	ARG
33	a	37	CYS
33	a	40	CYS
33	a	43	PHE
33	a	47	LYS

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Mol	Chain	Res	Type
33	a	59	ARG
34	b	12	LYS
34	b	40	ARG
34	b	55	ILE
35	c	5	ILE
35	c	32	GLU
36	d	22	MET
36	d	25	LYS
36	d	42	LEU
37	e	30	ARG
37	e	31	HIS
37	e	55	LEU
38	f	3	VAL
38	f	26	ILE
38	f	37	GLN
39	g	23	TRP
39	g	105	LYS
39	g	129	LEU
39	g	132	LYS
39	g	220	THR
40	h	14	ILE
40	h	35	SER
40	h	89	LYS
40	h	154	SER
40	h	164	ARG
40	h	165	THR
40	h	172	ARG
40	h	175	LEU
40	h	178	LEU
40	h	185	ASN
40	h	200	VAL
41	i	47	ARG
41	i	58	LYS
41	i	95	GLU
41	i	104	ARG
41	i	116	GLN
41	i	138	SER
41	i	143	VAL
41	i	197	GLU
41	i	206	LYS
42	j	15	LEU
42	j	18	VAL

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Mol	Chain	Res	Type
42	j	46	VAL
42	j	60	ILE
42	j	65	GLU
42	j	93	ARG
42	j	114	VAL
42	j	115	LEU
42	j	120	VAL
42	j	123	VAL
42	j	138	ARG
42	j	141	ILE
42	j	142	ASP
42	j	146	ASN
43	k	7	VAL
43	k	16	GLU
43	k	24	ARG
43	k	38	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	50	LEU
44	l	79	ARG
44	l	80	VAL
44	l	109	ARG
44	l	123	GLU
44	l	130	ASN
44	l	146	GLU
45	m	3	MET
45	m	77	ARG
45	m	96	MET
45	m	121	LEU
46	n	12	ARG
46	n	41	ARG
46	n	57	MET
46	n	63	LEU
46	n	98	LEU
46	n	118	LEU
46	n	123	ARG

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Mol	Chain	Res	Type
47	o	5	ARG
47	o	6	ILE
47	o	7	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
48	p	13	ARG
48	p	14	LYS
48	p	15	GLN
48	p	37	ARG
48	p	76	GLU
48	p	100	LEU
48	p	107	ILE
49	q	5	ASN
49	q	24	LEU
49	q	40	THR
49	q	43	LYS
49	q	44	LYS
49	q	47	SER
49	q	62	GLU
49	q	64	THR
49	q	102	LEU
50	r	11	ASP
50	r	16	VAL
50	r	25	VAL
50	r	29	ARG
50	r	59	GLU
50	r	89	LEU
50	r	92	ARG
50	r	93	ARG
50	r	96	PRO
50	r	104	THR
51	s	45	VAL
51	s	46	LEU
51	s	52	PRO
51	s	89	MET
51	s	92	GLU
51	s	100	SER
52	t	22	THR

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Mol	Chain	Res	Type
52	t	39	LEU
52	t	40	GLN
52	t	61	SER
52	t	64	ARG
52	t	66	LEU
52	t	67	LEU
52	t	70	LEU
52	t	80	GLN
52	t	84	ARG
52	t	85	LEU
53	u	1	MET
53	u	6	LEU
53	u	18	GLN
53	u	19	VAL
53	u	50	THR
53	u	77	GLU
54	v	33	ILE
54	v	53	CYS
54	v	67	LEU
54	v	75	LEU
55	w	71	THR
55	w	74	HIS
56	x	21	LYS
56	x	33	THR
56	x	49	ILE
56	x	79	THR
57	y	6	SER
57	y	10	ARG
57	y	15	GLU
57	y	43	ASP
57	y	48	GLN
57	y	54	MET
57	y	64	LYS
58	z	4	ILE
58	z	67	ARG

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2898/2904 (99%)	556 (19%)	81 (2%)
2	2	1528/1534 (99%)	295 (19%)	37 (2%)
3	3	119/120 (99%)	15 (12%)	0
4	4	4/18 (22%)	1 (25%)	0
5	5	73/78 (93%)	23 (31%)	9 (12%)
All	All	4622/4654 (99%)	890 (19%)	127 (2%)

All (890) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	14	A
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	62	U
1	1	63	A
1	1	71	A
1	1	74	A
1	1	75	G
1	1	83	A
1	1	84	A
1	1	85	G
1	1	99	U
1	1	101	A
1	1	102	U
1	1	110	G
1	1	118	A
1	1	119	A
1	1	120	U
1	1	122	G
1	1	131	A
1	1	138	U
1	1	139	U
1	1	140	C
1	1	141	G
1	1	142	A
1	1	144	A
1	1	149	A

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Mol	Chain	Res	Type
1	1	163	C
1	1	165	A
1	1	181	A
1	1	196	A
1	1	200	U
1	1	215	G
1	1	216	A
1	1	221	A
1	1	222	A
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	310	A
1	1	311	A
1	1	327	G
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	386	G
1	1	396	G
1	1	405	U
1	1	411	G
1	1	412	A
1	1	424	G
1	1	435	C
1	1	451	U
1	1	456	C
1	1	457	A
1	1	477	A

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Mol	Chain	Res	Type
1	1	480	A
1	1	481	G
1	1	491	G
1	1	501	A
1	1	503	A
1	1	504	A
1	1	505	A
1	1	508	A
1	1	509	C
1	1	531	C
1	1	532	A
1	1	533	G
1	1	543	G
1	1	546	U
1	1	547	A
1	1	549	G
1	1	551	G
1	1	563	A
1	1	569	U
1	1	573	U
1	1	574	A
1	1	575	A
1	1	586	A
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	651	G
1	1	654	A
1	1	655	A
1	1	668	A
1	1	686	U
1	1	696	G
1	1	710	U
1	1	717	C

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Mol	Chain	Res	Type
1	1	724	U
1	1	730	A
1	1	738	G
1	1	746	PSU
1	1	747	5MU
1	1	757	G
1	1	764	A
1	1	765	C
1	1	775	G
1	1	776	G
1	1	782	A
1	1	783	A
1	1	784	G
1	1	785	G
1	1	788	A
1	1	789	A
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	845	A
1	1	846	U
1	1	858	G
1	1	859	G
1	1	869	G
1	1	878	A
1	1	881	G
1	1	884	U
1	1	885	C
1	1	887	A
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	910	A
1	1	914	G
1	1	915	C
1	1	931	U

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Mol	Chain	Res	Type
1	1	933	A
1	1	940	G
1	1	941	A
1	1	945	A
1	1	946	C
1	1	953	G
1	1	961	C
1	1	974	G
1	1	983	A
1	1	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	1023	U
1	1	1026	G
1	1	1033	U
1	1	1040	A
1	1	1043	C
1	1	1045	C
1	1	1046	A
1	1	1047	G
1	1	1050	A
1	1	1055	G
1	1	1060	U
1	1	1061	U
1	1	1063	G
1	1	1064	C
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1069	A
1	1	1070	A
1	1	1073	A
1	1	1074	G
1	1	1083	U
1	1	1084	A
1	1	1087	G

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Mol	Chain	Res	Type
1	1	1088	A
1	1	1090	A
1	1	1107	G
1	1	1111	A
1	1	1112	G
1	1	1119	U
1	1	1122	G
1	1	1128	G
1	1	1129	A
1	1	1130	U
1	1	1132	U
1	1	1134	A
1	1	1135	C
1	1	1142	A
1	1	1169	A
1	1	1170	C
1	1	1171	G
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	1236	G
1	1	1238	G
1	1	1248	G
1	1	1253	A
1	1	1256	G
1	1	1265	A
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	1302	A
1	1	1321	A
1	1	1345	C
1	1	1352	U

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Mol	Chain	Res	Type
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	1405	U
1	1	1406	U
1	1	1407	G
1	1	1408	G
1	1	1409	U
1	1	1414	C
1	1	1416	G
1	1	1417	C
1	1	1420	A
1	1	1428	C
1	1	1434	A
1	1	1452	G
1	1	1453	A
1	1	1455	G
1	1	1458	U
1	1	1460	U
1	1	1478	G
1	1	1482	G
1	1	1483	G
1	1	1490	A
1	1	1493	C
1	1	1497	U
1	1	1503	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1529	G
1	1	1534	U
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1554	U
1	1	1558	C
1	1	1559	U

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Mol	Chain	Res	Type
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	1592	C
1	1	1593	A
1	1	1594	U
1	1	1595	C
1	1	1596	A
1	1	1597	A
1	1	1608	A
1	1	1609	A
1	1	1610	A
1	1	1613	G
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	1677	A
1	1	1703	G
1	1	1713	A
1	1	1714	U
1	1	1715	G
1	1	1718	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1742	U
1	1	1750	G
1	1	1755	A
1	1	1758	U
1	1	1761	C
1	1	1764	C

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Mol	Chain	Res	Type
1	1	1773	A
1	1	1791	A
1	1	1800	C
1	1	1801	A
1	1	1808	A
1	1	1811	G
1	1	1816	C
1	1	1829	A
1	1	1833	C
1	1	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	1917	PSU
1	1	1918	A
1	1	1919	A
1	1	1929	G
1	1	1930	G
1	1	1931	U
1	1	1936	A
1	1	1938	A
1	1	1939	5MU
1	1	1955	U
1	1	1960	A
1	1	1963	U
1	1	1965	C
1	1	1966	A
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G

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Mol	Chain	Res	Type
1	1	1987	A
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2022	U
1	1	2023	C
1	1	2026	U
1	1	2031	A
1	1	2033	A
1	1	2043	C
1	1	2051	A
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2063	C
1	1	2069	G7M
1	1	2097	A
1	1	2099	U
1	1	2100	G
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	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

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Mol	Chain	Res	Type
1	1	2133	G
1	1	2134	A
1	1	2139	U
1	1	2141	G
1	1	2146	C
1	1	2147	A
1	1	2154	A
1	1	2157	G
1	1	2158	A
1	1	2159	G
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2169	A
1	1	2171	A
1	1	2172	U
1	1	2178	C
1	1	2182	U
1	1	2183	A
1	1	2185	U
1	1	2188	U
1	1	2190	G
1	1	2194	U
1	1	2197	U
1	1	2198	A
1	1	2203	U
1	1	2204	G
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	2245	U
1	1	2246	G
1	1	2250	G
1	1	2251	OMG
1	1	2252	G
1	1	2268	A

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Mol	Chain	Res	Type
1	1	2278	A
1	1	2283	C
1	1	2287	A
1	1	2294	G
1	1	2297	A
1	1	2305	U
1	1	2308	G
1	1	2309	A
1	1	2315	G
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2335	A
1	1	2336	A
1	1	2347	C
1	1	2350	C
1	1	2361	G
1	1	2372	U
1	1	2376	A
1	1	2383	G
1	1	2385	C
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2410	G
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	2441	U
1	1	2445	2MG
1	1	2448	A
1	1	2470	G
1	1	2474	U
1	1	2476	A
1	1	2478	A
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	2512	C
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2525	G
1	1	2529	G
1	1	2535	G
1	1	2547	A
1	1	2552	OMU
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2573	C
1	1	2574	G
1	1	2585	U
1	1	2586	U
1	1	2603	G
1	1	2609	U
1	1	2610	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	2726	A
1	1	2744	G
1	1	2748	A
1	1	2757	A
1	1	2762	C
1	1	2777	G
1	1	2778	A
1	1	2791	G
1	1	2793	C
1	1	2796	U
1	1	2797	U

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Mol	Chain	Res	Type
1	1	2798	U
1	1	2799	A
1	1	2801	G
1	1	2818	U
1	1	2820	A
1	1	2821	A
1	1	2825	G
1	1	2849	U
1	1	2859	G
1	1	2861	U
1	1	2867	G
1	1	2872	A
1	1	2879	A
1	1	2880	C
1	1	2883	A
1	1	2884	U
1	1	2885	G
1	1	2891	U
1	1	2902	C
2	2	4	U
2	2	5	U
2	2	6	G
2	2	9	G
2	2	19	A
2	2	22	G
2	2	29	U
2	2	32	A
2	2	39	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	69	G
2	2	70	U
2	2	71	A
2	2	72	A
2	2	74	A
2	2	76	G
2	2	81	A
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	120	A
2	2	121	U
2	2	131	A
2	2	141	G
2	2	144	G
2	2	148	G
2	2	149	A
2	2	160	A
2	2	164	G
2	2	173	U
2	2	181	A
2	2	182	A
2	2	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	216	U
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	279	A
2	2	289	G
2	2	306	A
2	2	316	C

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Mol	Chain	Res	Type
2	2	321	A
2	2	328	C
2	2	329	A
2	2	332	G
2	2	340	U
2	2	347	G
2	2	352	C
2	2	354	G
2	2	367	U
2	2	372	C
2	2	373	A
2	2	376	G
2	2	384	G
2	2	388	G
2	2	389	A
2	2	392	C
2	2	397	A
2	2	406	G
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	429	U
2	2	446	G
2	2	451	A
2	2	457	G
2	2	458	U
2	2	460	A
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	469	C
2	2	478	A
2	2	479	U
2	2	480	U
2	2	481	G
2	2	484	G
2	2	485	U
2	2	486	U

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Mol	Chain	Res	Type
2	2	495	A
2	2	511	C
2	2	516	PSU
2	2	517	G
2	2	518	C
2	2	521	G
2	2	526	C
2	2	531	U
2	2	532	A
2	2	533	A
2	2	547	A
2	2	559	A
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	587	G
2	2	588	G
2	2	596	A
2	2	628	G
2	2	633	G
2	2	642	A
2	2	649	A
2	2	650	G
2	2	653	U
2	2	656	G
2	2	665	A
2	2	687	A
2	2	700	G
2	2	702	A
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	747	A
2	2	748	G
2	2	755	G
2	2	777	A
2	2	793	U
2	2	794	A

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Mol	Chain	Res	Type
2	2	815	A
2	2	817	C
2	2	828	U
2	2	841	C
2	2	844	G
2	2	845	A
2	2	849	G
2	2	874	G
2	2	887	G
2	2	902	G
2	2	914	A
2	2	916	U
2	2	926	G
2	2	928	G
2	2	934	C
2	2	935	A
2	2	936	C
2	2	960	U
2	2	961	U
2	2	966	2MG
2	2	967	5MC
2	2	969	A
2	2	972	C
2	2	975	A
2	2	976	G
2	2	977	A
2	2	987	G
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	1005	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

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Mol	Chain	Res	Type
2	2	1030	U
2	2	1031	C
2	2	1037	C
2	2	1042	A
2	2	1043	G
2	2	1044	A
2	2	1046	A
2	2	1065	U
2	2	1085	U
2	2	1086	U
2	2	1092	A
2	2	1094	G
2	2	1095	U
2	2	1099	G
2	2	1101	A
2	2	1124	G
2	2	1133	G
2	2	1135	U
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1142	G
2	2	1143	G
2	2	1145	A
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1158	C
2	2	1159	U
2	2	1167	A
2	2	1171	A
2	2	1174	G
2	2	1175	G
2	2	1176	A
2	2	1184	G
2	2	1187	G
2	2	1196	A
2	2	1197	A
2	2	1211	U
2	2	1212	U

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Mol	Chain	Res	Type
2	2	1213	A
2	2	1214	C
2	2	1215	G
2	2	1227	A
2	2	1238	A
2	2	1239	A
2	2	1242	G
2	2	1257	A
2	2	1260	G
2	2	1275	A
2	2	1276	G
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
2	2	1312	G
2	2	1317	C
2	2	1320	C
2	2	1323	G
2	2	1329	A
2	2	1332	A
2	2	1334	G
2	2	1338	G
2	2	1340	A
2	2	1346	A
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	1383	C
2	2	1396	A
2	2	1397	C

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Mol	Chain	Res	Type
2	2	1404	C
2	2	1408	A
2	2	1419	G
2	2	1429	A
2	2	1441	A
2	2	1446	A
2	2	1447	A
2	2	1448	C
2	2	1452	C
2	2	1453	G
2	2	1487	G
2	2	1493	A
2	2	1494	G
2	2	1497	G
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1529	G
2	2	1530	G
2	2	1534	A
3	3	2	G
3	3	13	G
3	3	16	G
3	3	17	C
3	3	35	C
3	3	36	C
3	3	45	A
3	3	56	G
3	3	64	G
3	3	66	A
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	109	A
4	4	15	A
5	5	5	G
5	5	8	4SU
5	5	13	A
5	5	15	C
5	5	16	C
5	5	17	U

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Mol	Chain	Res	Type
5	5	18	G
5	5	19	G
5	5	20	H2U
5	5	21	A
5	5	22	G
5	5	25	C
5	5	31	G
5	5	37	A
5	5	47	U
5	5	48	C
5	5	49	G
5	5	55	PSU
5	5	57	A
5	5	59	A
5	5	69	C
5	5	74	C
5	5	75	C

All (127) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	33	C
1	1	62	U
1	1	70	G
1	1	71	A
1	1	101	A
1	1	125	A
1	1	138	U
1	1	140	C
1	1	196	A
1	1	199	A
1	1	271	G
1	1	310	A
1	1	404	A
1	1	446	G
1	1	503	A
1	1	532	A
1	1	545	U
1	1	546	U
1	1	685	A
1	1	748	G
1	1	764	A

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Mol	Chain	Res	Type
1	1	776	G
1	1	784	G
1	1	883	G
1	1	884	U
1	1	892	A
1	1	894	U
1	1	896	A
1	1	984	A
1	1	1045	C
1	1	1060	U
1	1	1064	C
1	1	1067	A
1	1	1069	A
1	1	1070	A
1	1	1111	A
1	1	1128	G
1	1	1173	U
1	1	1174	U
1	1	1300	G
1	1	1320	C
1	1	1344	U
1	1	1379	U
1	1	1395	A
1	1	1405	U
1	1	1407	G
1	1	1408	G
1	1	1490	A
1	1	1509	A
1	1	1584	U
1	1	1596	A
1	1	1608	A
1	1	1647	U
1	1	1784	A
1	1	1912	A
1	1	1913	A
1	1	1918	A
1	1	1962	5MC
1	1	2062	A
1	1	2146	C
1	1	2162	G
1	1	2193	G
1	1	2197	U

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Mol	Chain	Res	Type
1	1	2198	A
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	2425	A
1	1	2447	G
1	1	2573	C
1	1	2585	U
1	1	2602	A
1	1	2610	C
1	1	2756	U
1	1	2797	U
1	1	2798	U
1	1	2873	A
2	2	5	U
2	2	70	U
2	2	121	U
2	2	147	G
2	2	148	G
2	2	181	A
2	2	183	C
2	2	197	A
2	2	209	U
2	2	421	U
2	2	428	G
2	2	481	G
2	2	496	A
2	2	587	G
2	2	641	U
2	2	701	U
2	2	793	U
2	2	873	A
2	2	961	U
2	2	966	2MG
2	2	967	5MC
2	2	974	A
2	2	991	U
2	2	992	U

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Mol	Chain	Res	Type
2	2	1129	C
2	2	1145	A
2	2	1196	A
2	2	1211	U
2	2	1213	A
2	2	1214	C
2	2	1277	C
2	2	1299	A
2	2	1319	A
2	2	1363	A
2	2	1396	A
2	2	1447	A
2	2	1516	2MG
5	5	14	G
5	5	15	C
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 ⓘ

41 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	1911	1	18,21,22	1.65	5 (27%)	22,30,33	2.13	4 (18%)
1	OMG	1	2251	1,5	18,26,27	1.11	1 (5%)	19,38,41	1.29	4 (21%)
1	OMU	1	2552	59,1	19,22,23	0.56	0	26,31,34	0.77	1 (3%)
1	6MZ	1	2030	1	18,25,26	1.00	1 (5%)	16,36,39	2.05	4 (25%)
5	PSU	5	55	5	18,21,22	1.83	1 (5%)	22,30,33	1.55	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MA	1	2503	59,1	17,25,26	1.12	3 (17%)	17,37,40	2.95	6 (35%)
49	0TD	q	89	49	7,9,10	6.74	5 (71%)	6,11,13	4.11	2 (33%)
1	2MG	1	1835	1	18,26,27	1.21	3 (16%)	16,38,41	1.61	3 (18%)
2	PSU	2	516	59,2	18,21,22	1.57	1 (5%)	22,30,33	1.61	2 (9%)
1	PSU	1	2504	1	18,21,22	2.04	1 (5%)	22,30,33	1.58	3 (13%)
1	OMC	1	2498	59,1	19,22,23	0.98	1 (5%)	26,31,34	1.79	3 (11%)
5	H2U	5	20	5	18,21,22	0.65	0	21,30,33	1.88	4 (19%)
1	PSU	1	2605	1	18,21,22	2.10	1 (5%)	22,30,33	1.70	3 (13%)
1	5MU	1	1939	1	19,22,23	1.50	3 (15%)	28,32,35	2.32	6 (21%)
2	UR3	2	1498	2	19,22,23	1.39	2 (10%)	26,32,35	1.99	6 (23%)
1	5MC	1	1962	1	18,22,23	0.86	1 (5%)	26,32,35	1.07	1 (3%)
7	MEQ	7	252	7	8,9,10	0.49	0	5,10,12	2.02	2 (40%)
2	2MG	2	966	2	18,26,27	1.20	3 (16%)	16,38,41	2.11	4 (25%)
1	3TD	1	1915	1	18,22,23	0.71	0	22,32,35	1.48	4 (18%)
1	G7M	1	2069	1	20,26,27	1.52	1 (5%)	17,39,42	2.36	4 (23%)
1	PSU	1	746	59,1	18,21,22	2.12	1 (5%)	22,30,33	2.15	3 (13%)
5	5MU	5	54	5	19,22,23	0.63	0	28,32,35	1.00	2 (7%)
5	8AN	5	76	5,60	19,24,25	0.66	0	13,35,38	1.00	1 (7%)
2	7MG	2	527	2	22,26,27	2.06	5 (22%)	29,39,42	2.79	9 (31%)
2	2MG	2	1207	2	18,26,27	1.74	3 (16%)	16,38,41	1.47	4 (25%)
2	2MG	2	1516	2	18,26,27	1.22	3 (16%)	16,38,41	1.55	3 (18%)
2	5MC	2	1407	2	18,22,23	0.50	0	26,32,35	0.77	0
1	PSU	1	2580	1	18,21,22	1.75	1 (5%)	22,30,33	1.56	3 (13%)
1	PSU	1	2457	59,1	18,21,22	1.97	1 (5%)	22,30,33	1.56	3 (13%)
1	PSU	1	1917	1	18,21,22	1.57	5 (27%)	22,30,33	2.08	4 (18%)
1	1MG	1	745	1	18,26,27	1.61	2 (11%)	19,39,42	2.03	4 (21%)
5	4SU	5	8	5	18,21,22	1.63	4 (22%)	26,30,33	2.63	6 (23%)
2	5MC	2	967	2	18,22,23	0.83	1 (5%)	26,32,35	1.35	1 (3%)
2	4OC	2	1402	2	20,23,24	1.18	2 (10%)	26,32,35	1.12	2 (7%)
2	MA6	2	1518	2	19,26,27	0.58	0	18,38,41	0.78	0
1	6MZ	1	1618	1	18,25,26	0.92	1 (5%)	16,36,39	1.68	3 (18%)
1	5MU	1	747	1	19,22,23	0.73	1 (5%)	28,32,35	0.99	3 (10%)
2	MA6	2	1519	2	19,26,27	0.67	0	18,38,41	0.89	1 (5%)
1	2MG	1	2445	1	18,26,27	1.31	3 (16%)	16,38,41	1.51	3 (18%)
5	4OC	5	32	5	20,23,24	0.55	0	26,32,35	1.29	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1	955	1	18,21,22	1.93	1 (5%)	22,30,33	1.69	4 (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	1911	1	-	1/7/25/26	0/2/2/2
1	OMG	1	2251	1,5	-	0/5/27/28	0/3/3/3
1	OMU	1	2552	59,1	-	2/9/27/28	0/2/2/2
1	6MZ	1	2030	1	-	2/5/27/28	0/3/3/3
5	PSU	5	55	5	-	3/7/25/26	0/2/2/2
1	2MA	1	2503	59,1	-	1/3/25/26	0/3/3/3
49	0TD	q	89	49	-	2/7/12/14	-
1	2MG	1	1835	1	-	0/5/27/28	0/3/3/3
2	PSU	2	516	59,2	-	2/7/25/26	0/2/2/2
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
1	OMC	1	2498	59,1	-	2/9/27/28	0/2/2/2
5	H2U	5	20	5	-	4/7/38/39	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	1	1939	1	-	2/7/25/26	0/2/2/2
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	2/7/25/26	0/2/2/2
7	MEQ	7	252	7	-	2/8/9/11	-
2	2MG	2	966	2	-	4/5/27/28	0/3/3/3
1	3TD	1	1915	1	-	2/7/25/26	0/2/2/2
1	G7M	1	2069	1	-	2/3/25/26	0/3/3/3
1	PSU	1	746	59,1	-	1/7/25/26	0/2/2/2
5	5MU	5	54	5	-	0/7/25/26	0/2/2/2
5	8AN	5	76	5,60	-	1/3/25/26	0/3/3/3
2	7MG	2	527	2	-	1/7/37/38	0/3/3/3
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2457	59,1	-	0/7/25/26	0/2/2/2
1	PSU	1	1917	1	-	2/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	4SU	5	8	5	-	3/7/25/26	0/2/2/2
2	5MC	2	967	2	-	4/7/25/26	0/2/2/2
2	4OC	2	1402	2	-	0/9/29/30	0/2/2/2
2	MA6	2	1518	2	-	0/7/29/30	0/3/3/3
1	6MZ	1	1618	1	-	4/5/27/28	0/3/3/3
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	6/7/29/30	0/3/3/3
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
5	4OC	5	32	5	-	0/9/29/30	0/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2

All (67) 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	746	PSU	C2'-C1'	-8.78	1.42	1.53
1	1	2605	PSU	C2'-C1'	-8.55	1.42	1.53
1	1	2504	PSU	C2'-C1'	-8.42	1.42	1.53
1	1	2457	PSU	C2'-C1'	-7.98	1.43	1.53
1	1	955	PSU	C2'-C1'	-7.69	1.43	1.53
5	5	55	PSU	C2'-C1'	-7.56	1.43	1.53
1	1	2580	PSU	C2'-C1'	-6.99	1.44	1.53
2	2	516	PSU	C2'-C1'	-6.32	1.45	1.53
1	1	2069	G7M	C2'-C1'	-5.48	1.45	1.53
2	2	527	7MG	C4-N9	-5.38	1.31	1.37
5	5	8	4SU	C4-S4	-4.91	1.59	1.68
1	1	745	1MG	C2'-C1'	-4.85	1.46	1.53
2	2	527	7MG	C5-N7	-4.60	1.30	1.35
2	2	1207	2MG	C6-N1	-4.16	1.31	1.37
2	2	527	7MG	C6-N1	-3.77	1.31	1.38
2	2	1207	2MG	C2'-C1'	-3.61	1.48	1.53
1	1	1939	5MU	C4-N3	-3.56	1.32	1.38
1	1	1911	PSU	C4-N3	-3.53	1.32	1.38
1	1	1917	PSU	C4-N3	-3.49	1.32	1.38
1	1	2251	OMG	C6-N1	-3.49	1.32	1.37
1	1	2498	OMC	C3'-C2'	-3.20	1.45	1.52
49	q	89	0TD	CA-N	-3.17	1.37	1.47
1	1	1939	5MU	C2-N3	-3.14	1.32	1.38
1	1	2030	6MZ	C2'-C1'	-3.07	1.49	1.53
1	1	1939	5MU	C6-N1	-3.00	1.32	1.38
1	1	1835	2MG	C5-C6	-2.93	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1207	2MG	C2-N1	-2.92	1.32	1.36
1	1	2445	2MG	C5-C6	-2.91	1.41	1.47
2	2	1516	2MG	C5-C6	-2.83	1.41	1.47
1	1	745	1MG	C5-C6	-2.83	1.39	1.47
1	1	1911	PSU	C2-N3	-2.83	1.32	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
1	1	1911	PSU	C2'-C1'	-2.68	1.50	1.53
1	1	1917	PSU	C2-N3	-2.68	1.32	1.37
49	q	89	0TD	CB-CG	-2.68	1.47	1.52
2	2	527	7MG	C8-N9	-2.67	1.44	1.46
1	1	1917	PSU	C2-N1	-2.67	1.33	1.36
2	2	1498	UR3	C5-C4	-2.66	1.37	1.43
2	2	966	2MG	C6-N1	2.64	1.41	1.37
1	1	1911	PSU	C2-N1	-2.58	1.33	1.36
2	2	1498	UR3	C6-N1	-2.56	1.31	1.38
49	q	89	0TD	CSB-SB	-2.53	1.74	1.79
1	1	1962	5MC	C2'-C1'	-2.53	1.45	1.53
1	1	1618	6MZ	C2'-C1'	-2.52	1.49	1.53
1	1	2445	2MG	C5-C4	-2.49	1.36	1.43
2	2	1516	2MG	C6-N1	2.45	1.41	1.37
2	2	527	7MG	C2-N1	-2.43	1.31	1.37
1	1	2445	2MG	C6-N1	2.42	1.41	1.37
1	1	1835	2MG	C6-N1	2.36	1.41	1.37
1	1	1911	PSU	C6-C5	2.36	1.38	1.35
5	5	8	4SU	C2-N1	2.34	1.42	1.38
2	2	967	5MC	C2'-C1'	-2.33	1.46	1.53
2	2	1402	4OC	C6-N1	-2.30	1.32	1.38
1	1	747	5MU	C2'-C1'	-2.30	1.46	1.53
2	2	1516	2MG	C5-C4	-2.30	1.37	1.43
1	1	1835	2MG	C5-C4	-2.28	1.37	1.43
2	2	966	2MG	C5-C4	-2.24	1.37	1.43
1	1	1917	PSU	C2'-C1'	-2.18	1.50	1.53
5	5	8	4SU	C5-C4	-2.18	1.39	1.42
1	1	2503	2MA	C8-N7	-2.06	1.31	1.35
1	1	2503	2MA	C5-C4	-2.05	1.37	1.43
1	1	2503	2MA	C2'-C3'	-2.04	1.47	1.53
5	5	8	4SU	C4-N3	-2.03	1.35	1.37
1	1	1917	PSU	C6-N1	-2.02	1.32	1.36
2	2	1402	4OC	C2-N3	-2.01	1.32	1.36

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	527	7MG	N9-C4-N3	8.99	138.91	125.47
1	1	746	PSU	C3'-C2'-C1'	7.92	110.86	101.64
5	5	8	4SU	C5-C4-N3	7.58	121.72	114.69
49	q	89	0TD	CB-CA-N	-7.52	93.08	109.10
1	1	2503	2MA	C3'-C2'-C1'	-7.36	89.89	100.98
5	5	8	4SU	C4-N3-C2	-6.87	120.67	127.34
2	2	1498	UR3	C4-N3-C2	-6.64	118.31	124.56
1	1	1911	PSU	N1-C2-N3	6.38	122.35	115.13
49	q	89	0TD	CSB-SB-CB	6.19	113.63	102.44
1	1	1917	PSU	N1-C2-N3	6.09	122.03	115.13
2	2	966	2MG	O3'-C3'-C4'	6.06	128.58	111.05
1	1	2498	OMC	O3'-C3'-C2'	6.00	128.22	111.17
2	2	527	7MG	C5-C4-N3	-5.90	116.89	128.13
1	1	2498	OMC	O2'-C2'-C1'	5.85	120.50	109.08
1	1	1939	5MU	C4-N3-C2	-5.81	119.83	127.35
2	2	527	7MG	N9-C8-N7	-5.58	95.39	103.38
2	2	516	PSU	O2'-C2'-C3'	5.47	129.52	111.82
1	1	1939	5MU	C5-C4-N3	5.40	119.92	115.31
2	2	967	5MC	O3'-C3'-C2'	5.28	128.91	111.82
1	1	745	1MG	C3'-C2'-C1'	5.25	108.88	100.98
1	1	1939	5MU	N3-C2-N1	5.23	121.84	114.89
5	5	8	4SU	C5-C4-S4	-5.18	117.79	124.47
5	5	55	PSU	O2'-C2'-C3'	5.13	128.40	111.82
1	1	2030	6MZ	C3'-C2'-C1'	-5.10	93.30	100.98
1	1	1618	6MZ	O3'-C3'-C4'	5.05	125.66	111.05
1	1	955	PSU	O2'-C2'-C3'	5.02	128.06	111.82
1	1	2504	PSU	O2'-C2'-C3'	5.00	128.01	111.82
1	1	2069	G7M	O2'-C2'-C3'	4.95	127.85	111.82
1	1	2457	PSU	O2'-C2'-C3'	4.89	127.64	111.82
1	1	2069	G7M	O2'-C2'-C1'	4.88	128.88	110.85
1	1	2503	2MA	O3'-C3'-C4'	4.82	124.98	111.05
2	2	527	7MG	C2-N3-C4	4.81	120.88	112.30
1	1	2503	2MA	O3'-C3'-C2'	4.80	127.36	111.82
1	1	745	1MG	O3'-C3'-C2'	4.78	127.28	111.82
5	5	20	H2U	O2'-C2'-C3'	4.73	127.13	111.82
1	1	2580	PSU	O2'-C2'-C3'	4.71	127.04	111.82
5	5	32	4OC	O3'-C3'-C2'	4.67	124.43	111.17
1	1	2605	PSU	O2'-C2'-C3'	4.66	126.88	111.82
1	1	2069	G7M	C3'-C2'-C1'	-4.59	94.06	100.98
1	1	746	PSU	O2'-C2'-C3'	4.56	126.56	111.82
1	1	1939	5MU	C5-C6-N1	-4.56	118.65	123.34
1	1	2503	2MA	O2'-C2'-C1'	4.40	127.12	110.85
5	5	20	H2U	O3'-C3'-C2'	4.29	125.71	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2605	PSU	O2'-C2'-C1'	4.27	121.41	111.23
1	1	1915	3TD	C5'-C4'-C3'	-4.25	99.24	115.18
1	1	955	PSU	O2'-C2'-C1'	4.25	121.37	111.23
1	1	1917	PSU	C4-N3-C2	-4.24	120.23	126.34
1	1	1939	5MU	O4-C4-C5	-4.23	120.00	124.90
1	1	1911	PSU	C4-N3-C2	-4.22	120.26	126.34
1	1	2445	2MG	O3'-C3'-C2'	4.20	125.41	111.82
5	5	20	H2U	O3'-C3'-C4'	4.15	123.06	111.05
1	1	2580	PSU	O2'-C2'-C1'	4.00	120.76	111.23
5	5	55	PSU	O2'-C2'-C1'	3.97	120.71	111.23
1	1	2457	PSU	O2'-C2'-C1'	3.85	120.42	111.23
2	2	1498	UR3	O2-C2-N3	-3.82	115.96	121.34
2	2	1516	2MG	O3'-C3'-C4'	3.79	122.00	111.05
1	1	2504	PSU	O2'-C2'-C1'	3.76	120.20	111.23
1	1	2030	6MZ	O3'-C3'-C4'	3.71	121.77	111.05
1	1	1835	2MG	O3'-C3'-C2'	3.70	123.80	111.82
1	1	1835	2MG	O3'-C3'-C4'	3.67	121.66	111.05
2	2	1516	2MG	O3'-C3'-C2'	3.66	123.67	111.82
2	2	966	2MG	C2'-C3'-C4'	-3.62	95.61	102.64
2	2	516	PSU	O2'-C2'-C1'	3.53	119.66	111.23
1	1	745	1MG	O3'-C3'-C4'	3.48	121.11	111.05
1	1	1917	PSU	O2-C2-N1	-3.47	118.97	122.79
5	5	8	4SU	N3-C2-N1	3.45	119.47	114.89
7	7	252	MEQ	CG-CD-NE2	3.42	121.04	116.29
1	1	2503	2MA	O2'-C2'-C3'	3.39	122.78	111.82
5	5	20	H2U	O2'-C2'-C1'	3.35	121.23	110.02
1	1	1911	PSU	O2-C2-N1	-3.35	119.11	122.79
1	1	2030	6MZ	O3'-C3'-C2'	3.34	122.63	111.82
1	1	1962	5MC	O3'-C3'-C4'	3.33	120.69	111.05
1	1	2503	2MA	O4'-C1'-C2'	3.31	111.77	106.93
1	1	1939	5MU	O2-C2-N1	-3.22	118.50	122.79
1	1	1917	PSU	C3'-C2'-C1'	3.19	105.35	101.64
1	1	1915	3TD	O2'-C2'-C1'	-3.15	103.72	111.23
1	1	1618	6MZ	C2-N1-C6	3.11	119.26	116.59
1	1	2030	6MZ	C2-N1-C6	3.06	119.22	116.59
1	1	2605	PSU	C2'-C3'-C4'	-3.05	96.71	102.64
1	1	745	1MG	O2'-C2'-C3'	3.03	121.63	111.82
2	2	966	2MG	O3'-C3'-C2'	2.98	121.47	111.82
1	1	746	PSU	O2'-C2'-C1'	2.98	118.34	111.23
2	2	1207	2MG	C5-C6-N1	2.98	119.21	113.95
2	2	1498	UR3	O4'-C1'-C2'	-2.97	100.17	106.64
1	1	2069	G7M	C2'-C3'-C4'	-2.96	96.89	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	527	7MG	O4'-C4'-C3'	-2.89	99.39	105.11
1	1	955	PSU	C2'-C3'-C4'	-2.88	97.04	102.64
1	1	1911	PSU	C3'-C2'-C1'	2.84	104.95	101.64
5	5	8	4SU	C1'-N1-C2	2.81	122.67	117.57
1	1	1835	2MG	C3'-C2'-C1'	2.81	105.20	100.98
5	5	32	4OC	O3'-C3'-C4'	2.78	119.10	111.05
5	5	8	4SU	C6-C5-C4	-2.76	117.56	119.95
1	1	2251	OMG	C5-C6-N1	2.69	118.70	113.95
1	1	2580	PSU	C3'-C2'-C1'	2.68	104.76	101.64
2	2	527	7MG	C5-C6-N1	2.66	115.68	110.99
1	1	2445	2MG	O3'-C3'-C4'	2.62	118.62	111.05
2	2	1498	UR3	C1'-N1-C2	2.59	121.37	116.99
2	2	1402	4OC	O4'-C4'-C3'	-2.58	100.00	105.11
1	1	2504	PSU	C2'-C3'-C4'	-2.57	97.65	102.64
1	1	2457	PSU	C2'-C3'-C4'	-2.57	97.65	102.64
5	5	54	5MU	C2'-C1'-N1	2.42	120.06	113.22
2	2	1402	4OC	O2-C2-N3	-2.41	118.42	122.33
2	2	527	7MG	O4'-C1'-N9	2.40	112.57	109.30
2	2	1207	2MG	CM2-N2-C2	-2.37	118.62	123.86
1	1	2445	2MG	C3'-C2'-C1'	2.26	104.38	100.98
2	2	1207	2MG	O2'-C2'-C1'	-2.26	102.52	110.85
5	5	76	8AN	C2'-C3'-C4'	2.24	105.81	102.68
2	2	1519	MA6	C2'-C3'-C4'	-2.20	98.36	102.64
2	2	966	2MG	C3'-C2'-C1'	2.20	104.29	100.98
7	7	252	MEQ	OE1-CD-CG	-2.20	118.00	122.02
1	1	2251	OMG	C8-N7-C5	2.19	107.17	102.99
1	1	1915	3TD	O4'-C4'-C5'	-2.18	102.20	109.37
1	1	2251	OMG	O6-C6-C5	-2.15	120.17	124.37
1	1	747	5MU	C2'-C1'-N1	2.15	119.30	113.22
1	1	747	5MU	N3-C2-N1	2.15	117.74	114.89
1	1	2552	OMU	N3-C2-N1	2.14	117.74	114.89
2	2	1498	UR3	C3U-N3-C2	2.14	121.07	117.31
1	1	1915	3TD	C3'-C2'-C1'	2.14	104.13	101.64
2	2	527	7MG	O6-C6-C5	-2.13	122.31	127.54
5	5	54	5MU	N3-C2-N1	2.12	117.70	114.89
1	1	2498	OMC	O3'-C3'-C4'	2.11	117.15	111.05
1	1	747	5MU	C4-N3-C2	-2.10	124.63	127.35
5	5	55	PSU	C3'-C2'-C1'	2.07	104.05	101.64
1	1	955	PSU	C3'-C2'-C1'	-2.06	99.24	101.64
2	2	1516	2MG	C3'-C2'-C1'	2.06	104.08	100.98
1	1	1618	6MZ	C3'-C2'-C1'	-2.03	97.92	100.98
2	2	1498	UR3	O3'-C3'-C4'	-2.03	105.18	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2251	OMG	O2'-C2'-C1'	-2.01	105.10	109.09
2	2	527	7MG	O2'-C2'-C1'	-2.01	103.32	110.02
2	2	1207	2MG	C8-N7-C5	2.00	106.80	102.99

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2552	OMU	O4'-C4'-C5'-O5'
2	2	966	2MG	O4'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
2	2	966	2MG	N1-C2-N2-CM2
2	2	966	2MG	N3-C2-N2-CM2
2	2	1519	MA6	O4'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C9
2	2	1519	MA6	C5-C6-N6-C10
7	7	252	MEQ	CG-CD-NE2-CE
7	7	252	MEQ	OE1-CD-NE2-CE
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'
5	5	76	8AN	C4'-C5'-O5'-P
1	1	1917	PSU	O4'-C4'-C5'-O5'
1	1	2552	OMU	C3'-C4'-C5'-O5'
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	967	5MC	C3'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
1	1	1917	PSU	C3'-C4'-C5'-O5'
2	2	516	PSU	C3'-C4'-C5'-O5'
2	2	516	PSU	O4'-C4'-C5'-O5'
5	5	20	H2U	C3'-C4'-C5'-O5'
2	2	1519	MA6	N1-C6-N6-C10
5	5	20	H2U	O4'-C1'-N1-C2
1	1	2445	2MG	O4'-C4'-C5'-O5'
1	1	2498	OMC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	5	55	PSU	O4'-C4'-C5'-O5'
1	1	2498	OMC	C3'-C4'-C5'-O5'
1	1	1618	6MZ	C5-C6-N6-C9
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2069	G7M	O4'-C4'-C5'-O5'
49	q	89	0TD	CG-CB-SB-CSB
5	5	8	4SU	O4'-C1'-N1-C6
1	1	1939	5MU	O4'-C4'-C5'-O5'
1	1	2069	G7M	C4'-C5'-O5'-P
5	5	8	4SU	O4'-C1'-N1-C2
1	1	1911	PSU	O4'-C4'-C5'-O5'
1	1	2504	PSU	O4'-C4'-C5'-O5'
5	5	8	4SU	C4'-C5'-O5'-P
2	2	527	7MG	C4'-C5'-O5'-P
1	1	1962	5MC	O4'-C1'-N1-C6
1	1	1939	5MU	C3'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
2	2	967	5MC	C2'-C1'-N1-C2
1	1	746	PSU	O4'-C1'-C5-C6
1	1	2503	2MA	O4'-C4'-C5'-O5'
2	2	1519	MA6	C4'-C5'-O5'-P
1	1	1962	5MC	O4'-C1'-N1-C2
1	1	2504	PSU	C3'-C4'-C5'-O5'
2	2	967	5MC	C4'-C5'-O5'-P
5	5	55	PSU	C4'-C5'-O5'-P

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 443 ligands modelled in this entry, 442 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	103	5	8,9,10	0.54	0	7,9,11	1.15	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	FME	5	103	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	103	FME	O-C-CA	-3.00	116.91	124.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	5	103	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](#)

There are no chain breaks in this entry.

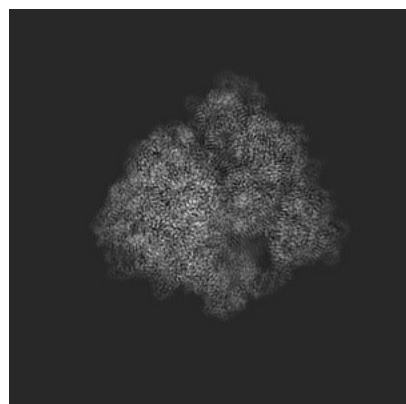
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3489. These allow visual inspection of the internal detail of the map and identification of artifacts.

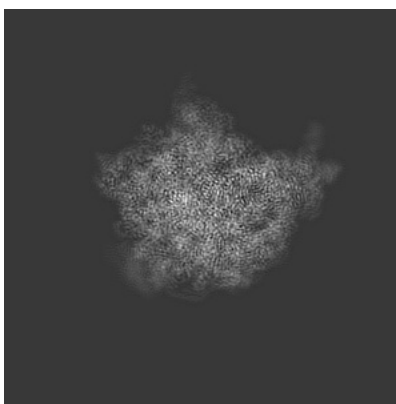
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

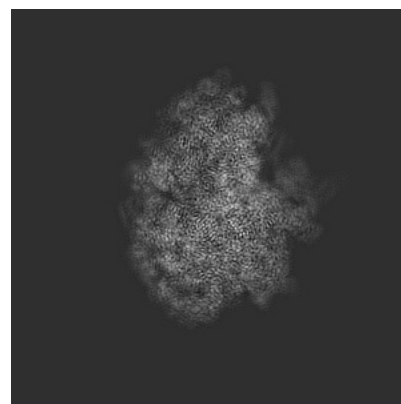
6.1.1 Primary map



X

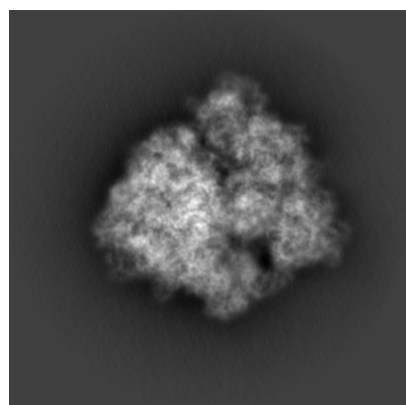


Y

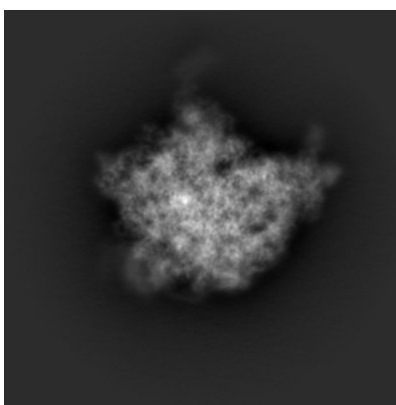


Z

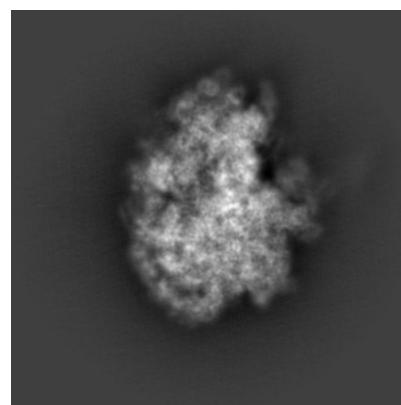
6.1.2 Raw map



X



Y

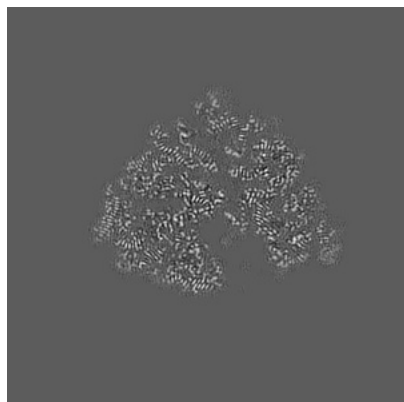


Z

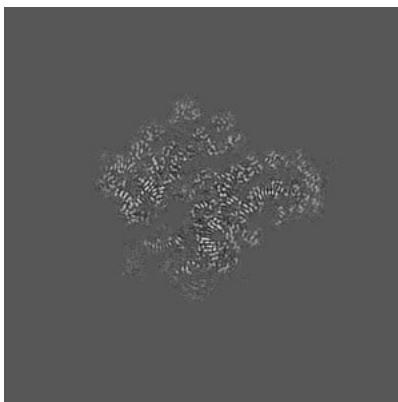
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

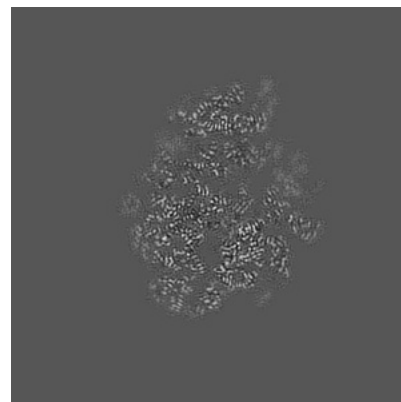
6.2.1 Primary map



X Index: 200

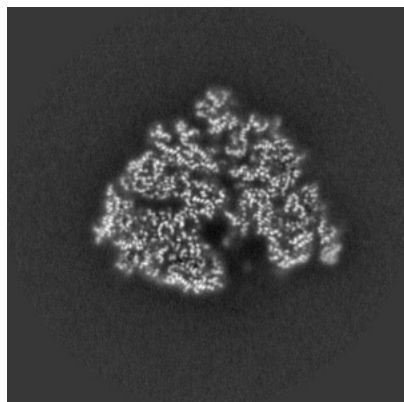


Y Index: 200

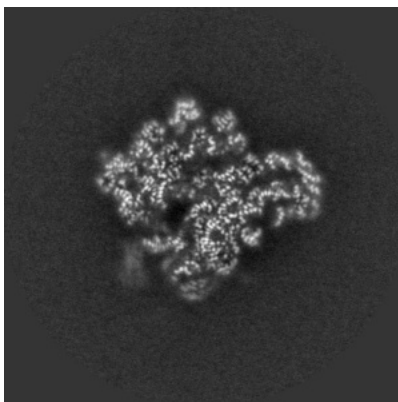


Z Index: 200

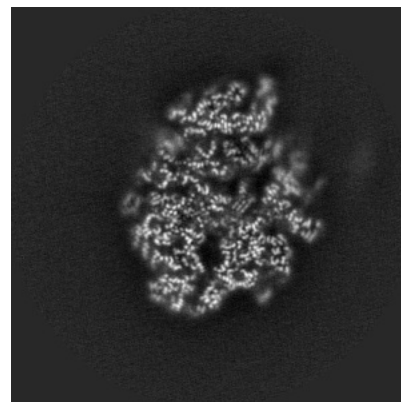
6.2.2 Raw map



X Index: 200



Y Index: 200

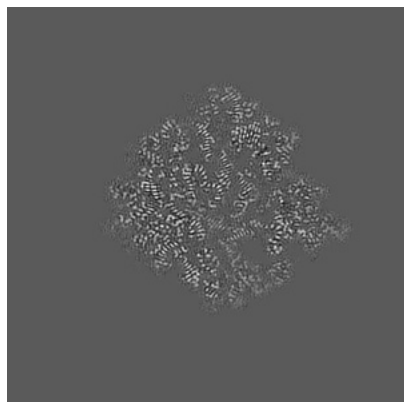


Z Index: 200

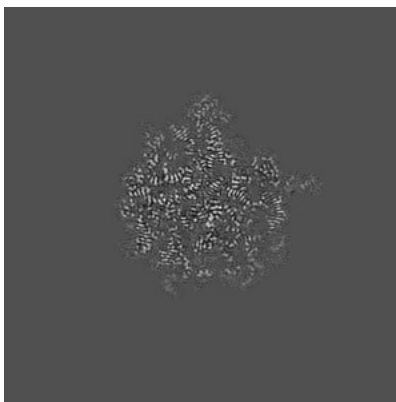
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

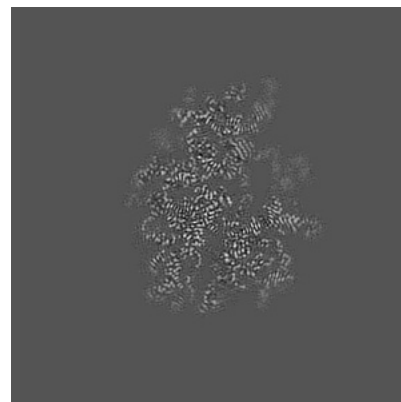
6.3.1 Primary map



X Index: 213

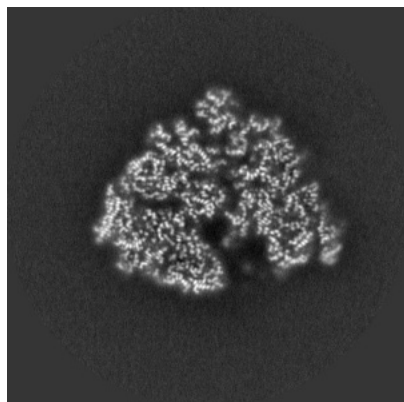


Y Index: 181

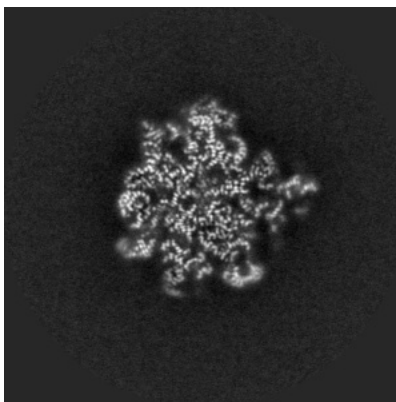


Z Index: 206

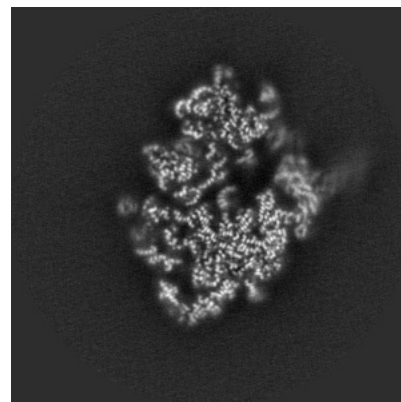
6.3.2 Raw map



X Index: 201



Y Index: 187

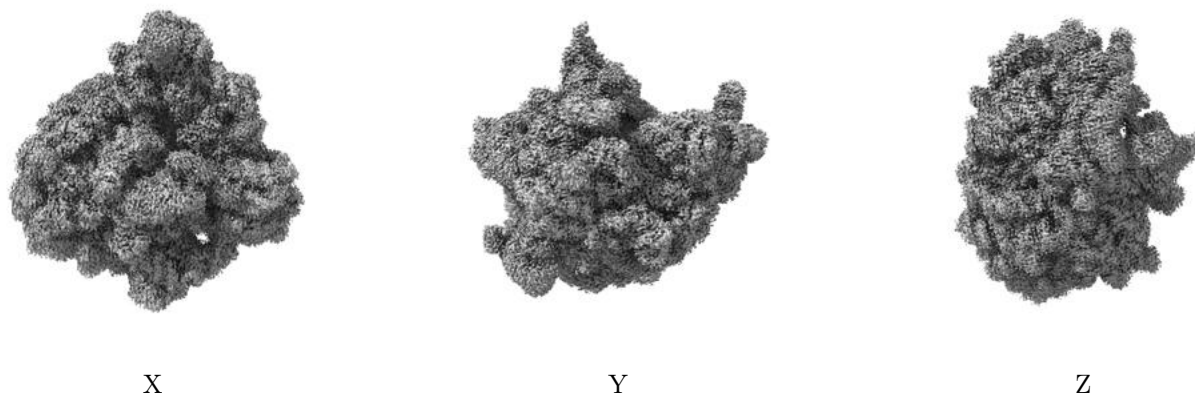


Z Index: 186

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

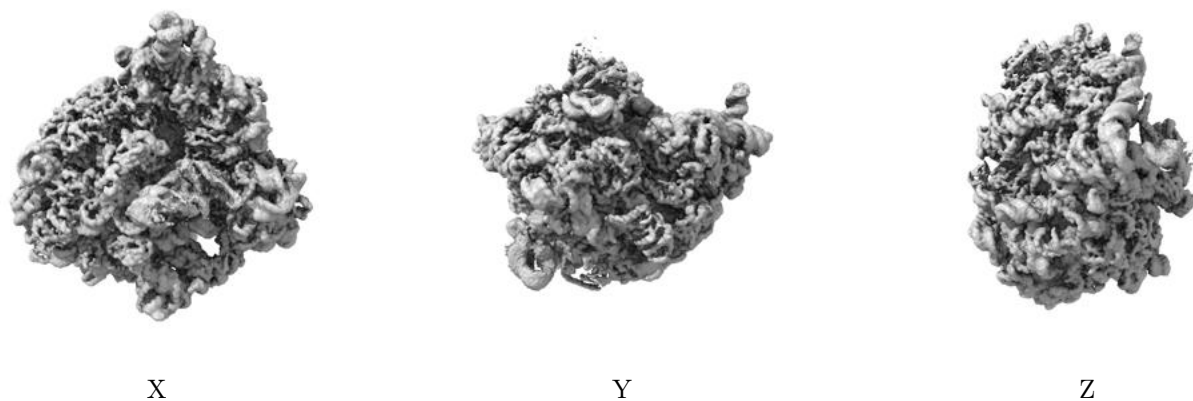
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

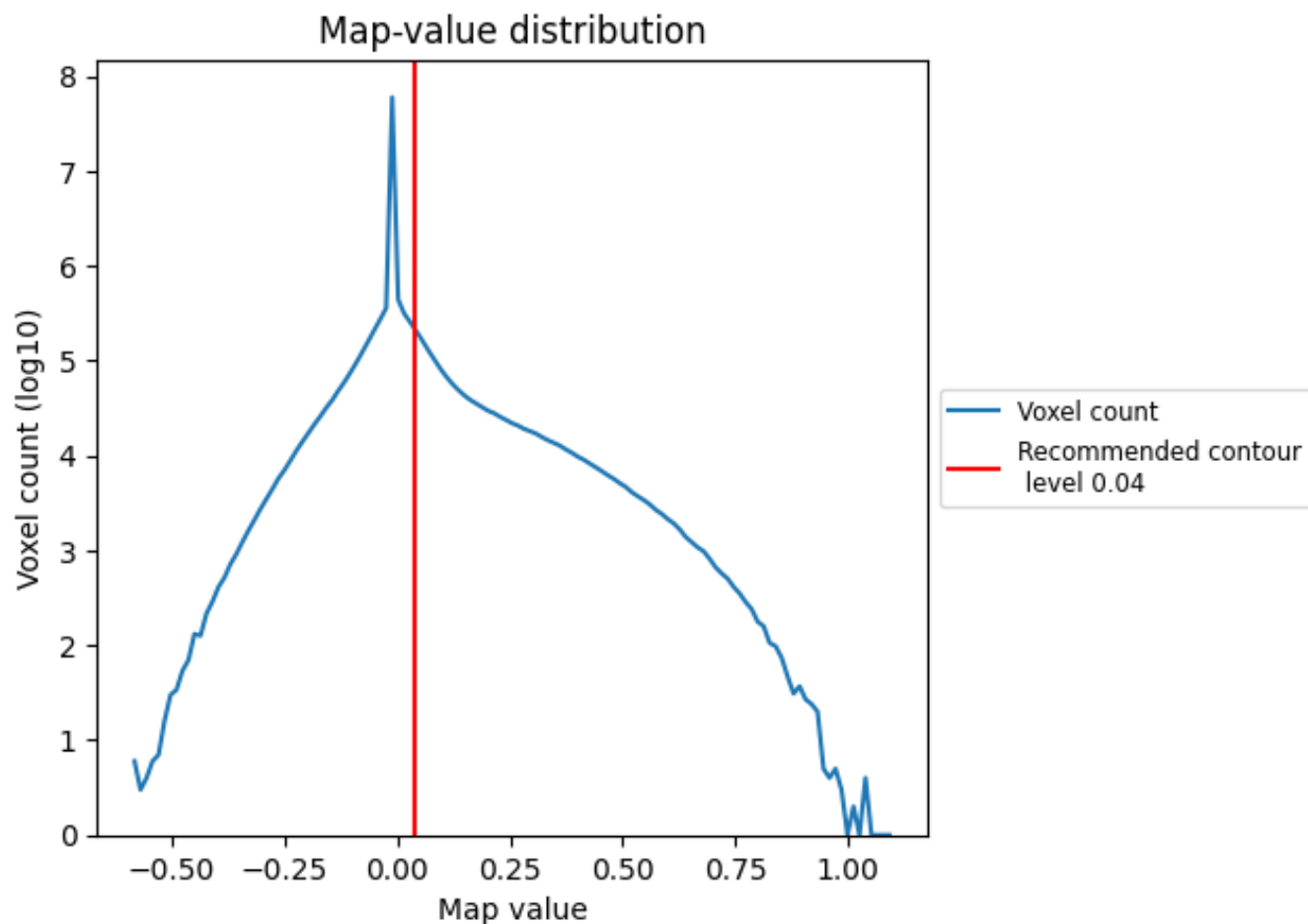
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

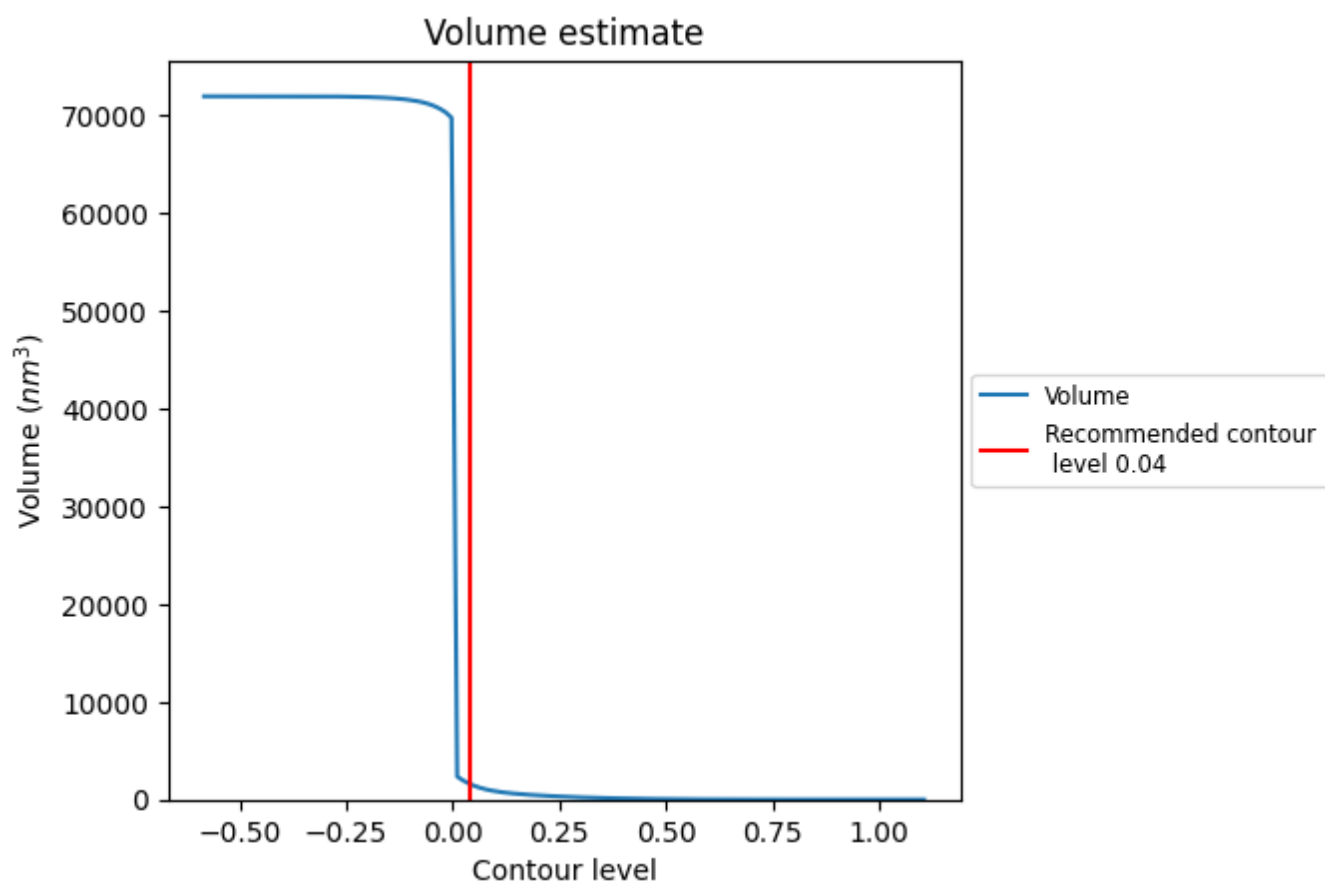
This section contains the results of statistical analysis of the map.

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.

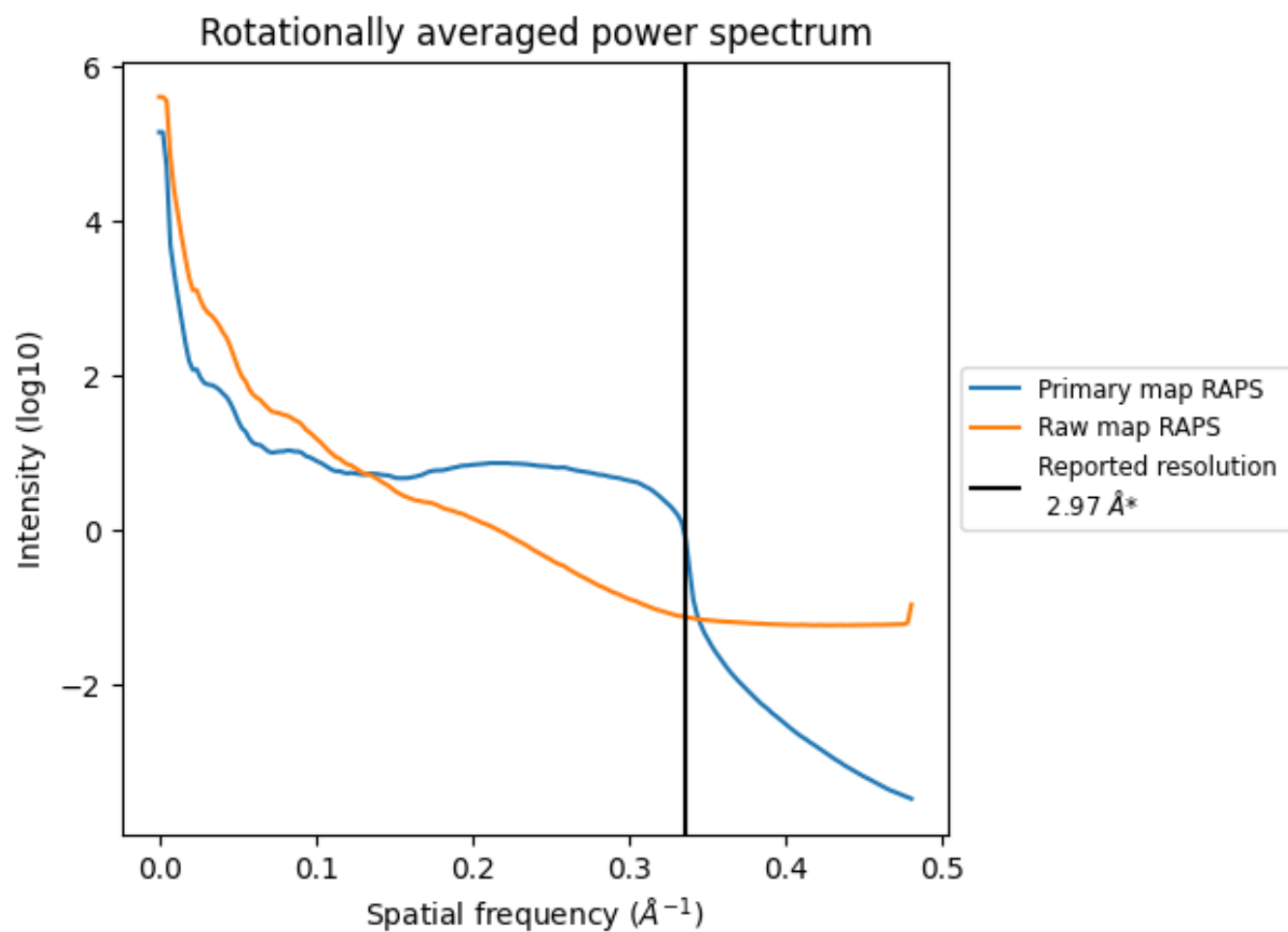
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1608 nm^3 ; this corresponds to an approximate mass of 1452 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 ⓘ

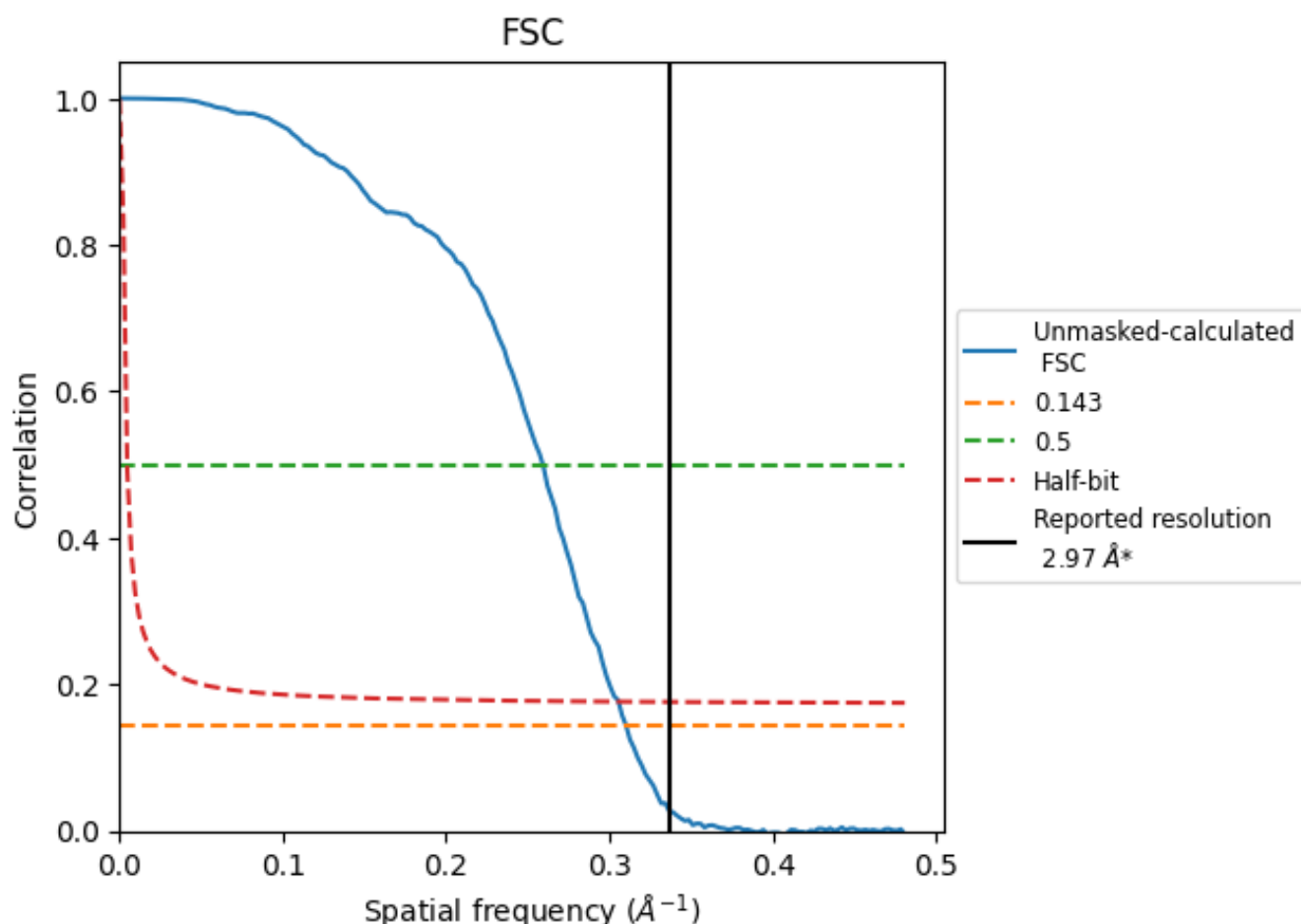


*Reported resolution corresponds to spatial frequency of 0.337 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.337 \AA^{-1}

8.2 Resolution estimates [i](#)

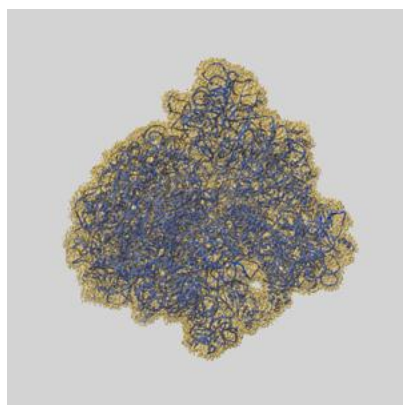
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.22	3.86	3.27

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

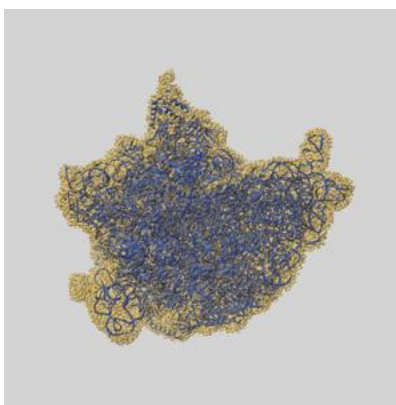
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3489 and PDB model 5MDV. Per-residue inclusion information can be found in section [3](#) on page [15](#).

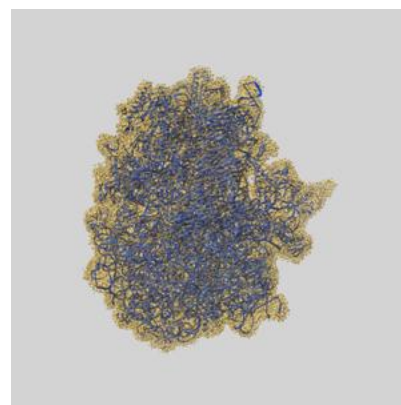
9.1 Map-model overlay [i](#)



X



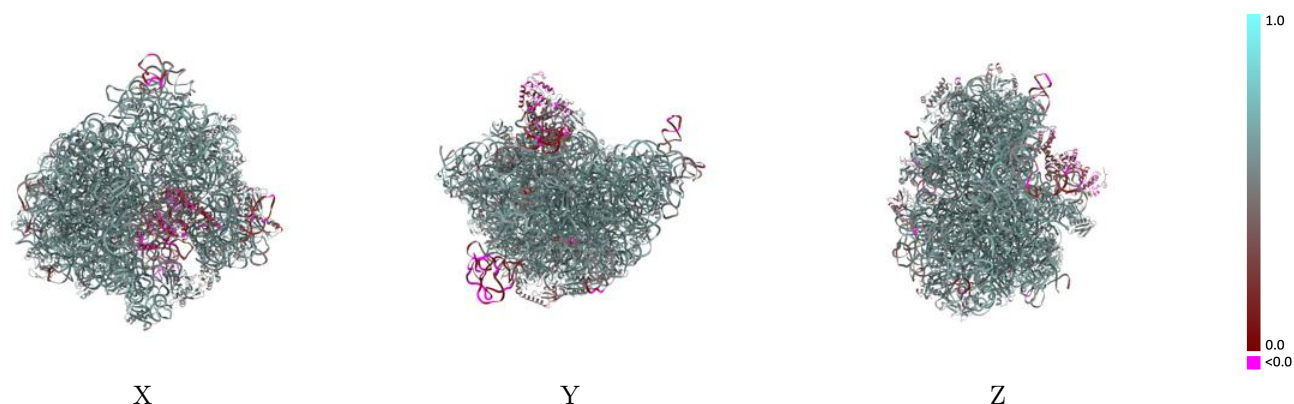
Y



Z

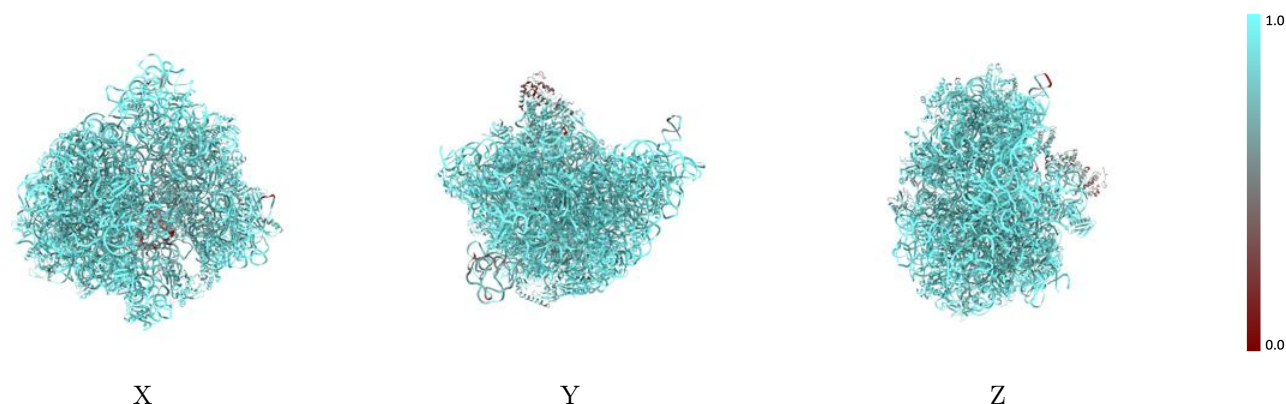
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



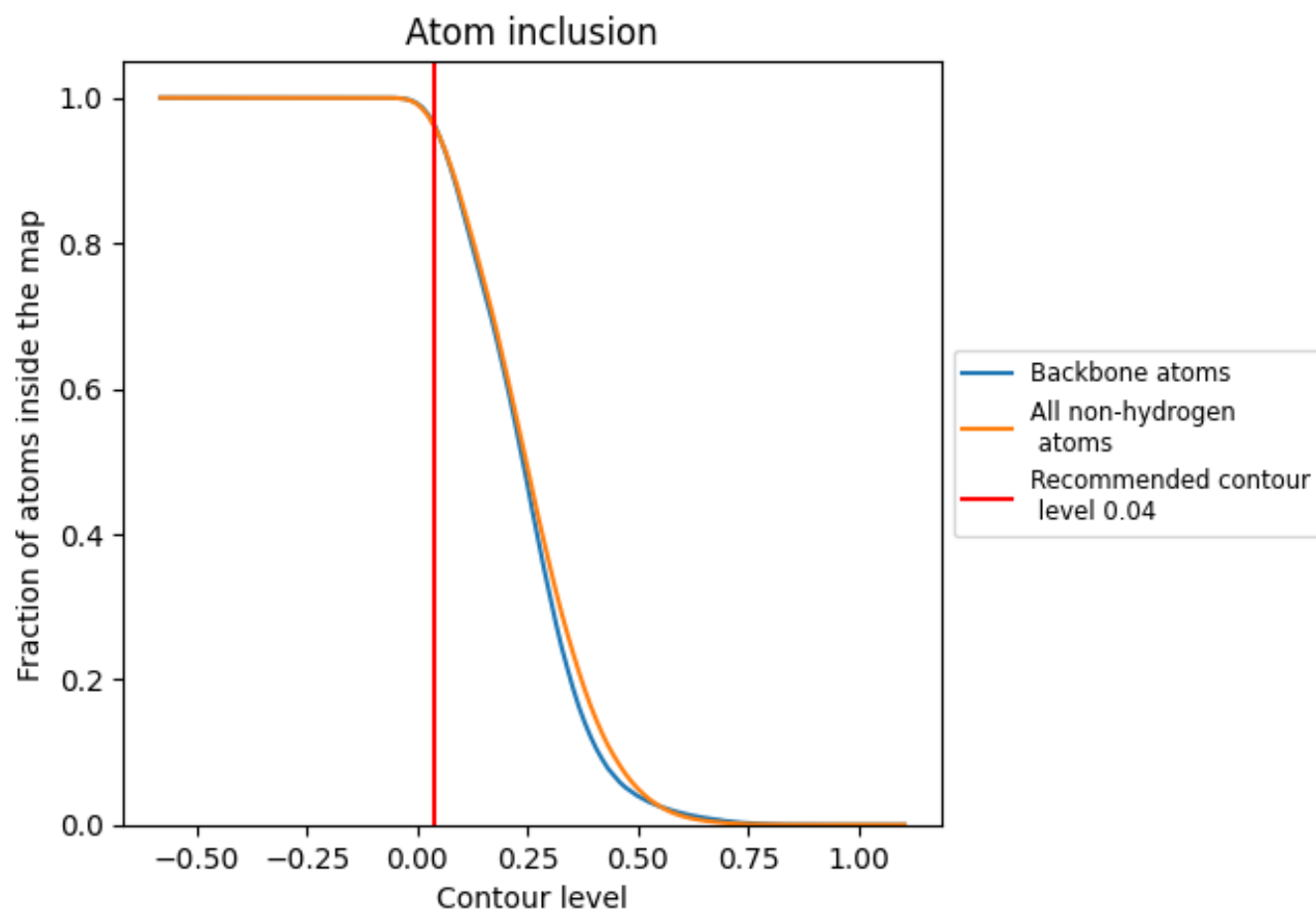
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9588	 0.5620
1	 0.9770	 0.5700
2	 0.9825	 0.5830
3	 0.9833	 0.5840
4	 1.0000	 0.6090
5	 0.9627	 0.5490
6	 0.9673	 0.5990
7	 0.8521	 0.4610
B	 0.9673	 0.6010
C	 0.9590	 0.5860
D	 0.9375	 0.5390
E	 0.9417	 0.5410
F	 0.9510	 0.5360
G	 0.7792	 0.3820
H	 0.3969	 0.0650
I	 0.5513	 0.0940
J	 0.9591	 0.5810
K	 0.9653	 0.5930
L	 0.9668	 0.5840
M	 0.9616	 0.5920
N	 0.9650	 0.5950
O	 0.9641	 0.5750
P	 0.9628	 0.5920
Q	 0.9637	 0.5860
R	 0.9674	 0.5820
S	 0.9545	 0.5800
T	 0.9397	 0.5500
U	 0.9472	 0.5460
V	 0.9363	 0.5640
W	 0.9823	 0.6060
X	 0.9700	 0.5860
Y	 0.9346	 0.5200
Z	 0.9495	 0.5720
a	 0.9082	 0.4680
b	 0.9627	 0.5980



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Chain	Atom inclusion	Q-score
c	 0.9522	 0.5730
d	 0.9577	 0.6000
e	 0.9695	 0.6020
f	 0.9693	 0.5970
g	 0.8832	 0.4880
h	 0.9535	 0.5690
i	 0.9522	 0.5780
j	 0.9566	 0.5810
k	 0.9407	 0.5440
l	 0.9229	 0.5200
m	 0.9615	 0.5830
n	 0.9530	 0.5620
o	 0.9190	 0.5130
p	 0.9484	 0.5650
q	 0.9729	 0.5970
r	 0.9447	 0.5590
s	 0.9509	 0.5710
t	 0.9565	 0.5670
u	 0.9585	 0.5820
v	 0.9478	 0.5570
w	 0.9388	 0.5650
x	 0.9629	 0.5620
y	 0.9495	 0.5690
z	 0.8730	 0.5040