



Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 05:33 pm GMT

PDB ID : 7NBU
EMDB ID : EMD-12261
Title : Structure of the HigB1 toxin mutant K95A from Mycobacterium tuberculosis (Rv1955) and its target, the cspA mRNA, on the E. coli Ribosome.
Authors : Giudice, E.; Mansour, M.; Chat, S.; D'Urso, G.; Gillet, R.; Genevoux, P.
Deposited on : 2021-01-27
Resolution : 3.11 Å(reported)
Based on initial model : 7K00

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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

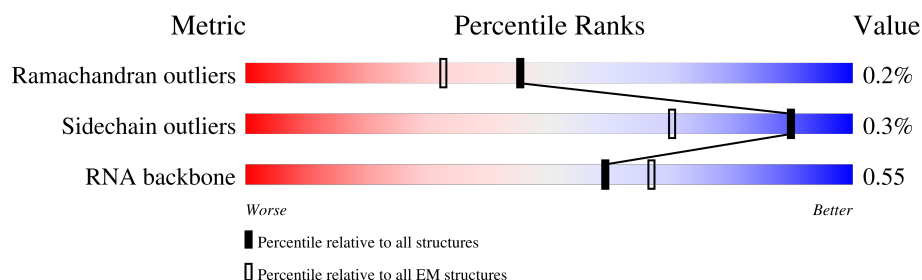
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.11 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	1539	
2	B	224	
3	C	206	
4	D	205	
5	E	156	
6	F	103	
7	G	153	
8	H	129	

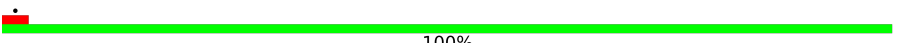
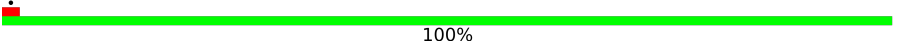
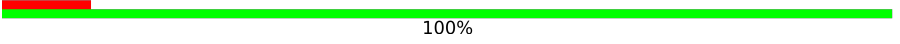
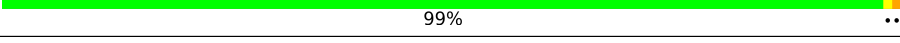
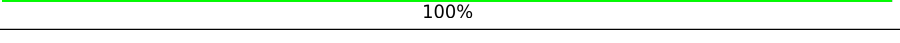
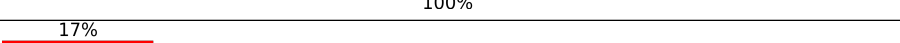
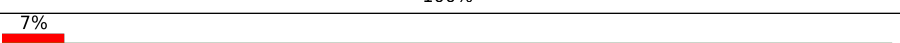

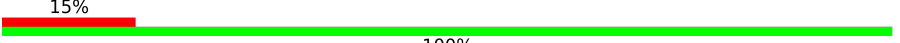
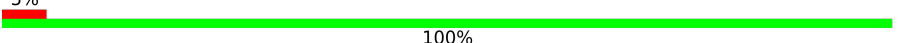
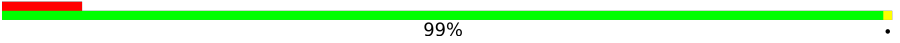
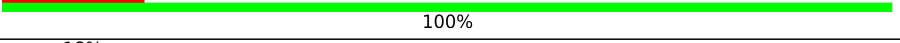
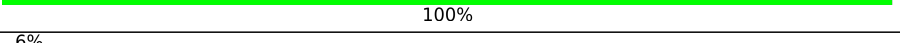
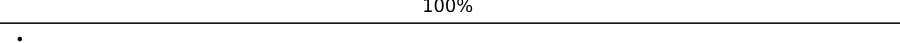
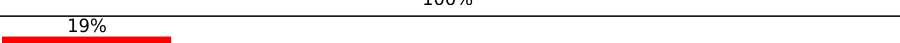


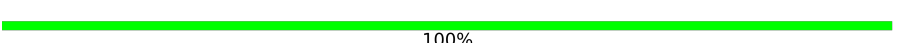
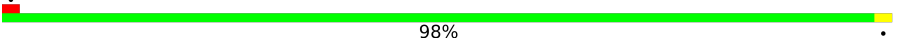
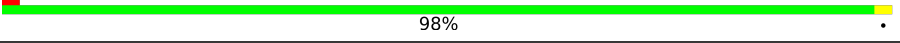
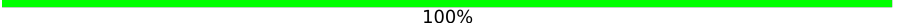


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Mol	Chain	Length	Quality of chain
9	I	127	24% 99%
10	J	98	44% 99%
11	K	117	7% 99%
12	L	123	. 98%
13	M	115	27% 100%
14	N	100	13% 100%
15	O	88	11% 100%
16	P	81	15% 100%
17	Q	79	11% 100%
18	R	66	21% 100%
19	S	84	23% 100%
20	T	86	12% 99%
21	U	70	41% 100%
22	V	77	. 78% 21%
23	W	2	50% 50% 50%
24	X	10	40% 40% 60%
25	Y	121	29% 96%
26	a	2904	8% 79% 20%
27	b	120	6% 85% 15%
28	c	271	. 100%
29	d	209	5% 100%
30	e	201	17% 99%
31	f	177	21% 99%
32	g	176	39% 98%
33	h	41	39% 100%

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Mol	Chain	Length	Quality of chain
34	i	142	 100%
35	j	123	 100%
36	k	144	 100%
37	l	148	 99% ..
38	Z	54	 100%
39	m	118	 100%
40	n	116	 100%
41	o	114	 100%
42	p	117	 100%
43	q	103	 100%
44	r	110	 100%
45	s	93	 99% .
46	t	102	 100%
47	u	94	 100%
48	v	84	 100%
49	w	77	 100%
50	x	62	 100%
51	y	58	 100%
52	z	56	 100%
53	0	51	 100%
54	1	46	 98% .
55	2	64	 98% .
56	3	38	 100%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 144938 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1539	Total	C	N	O	P	0	0
			33023	14736	6046	10702	1539		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

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

- Molecule 22 is a RNA chain called P-site fMet-tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	77	Total	C	N	O	P	S	0	0
			1643	733	297	535	77	1		

- Molecule 23 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 24 is a RNA chain called cspA mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	10	Total	C	N	O	P	0	0
			211	95	38	68	10		

- Molecule 25 is a protein called Probable endoribonuclease HigB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	121	Total	C	N	O	S	0	0
			992	645	180	165	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	95	ALA	LYS	engineered mutation	UNP P9WJA5
Y	126	LEU	-	expression tag	UNP P9WJA5
Y	127	GLU	-	expression tag	UNP P9WJA5

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	2900	Total	C	N	O	P	0	0
			62275	27789	11458	20128	2900		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16,50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	148	Total	C	N	O	S	0	0
			1179	735	237	196	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	81	4D4	-	linker	UNP P0ADY7
l	82	MS6	-	linker	UNP P0ADY7

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Z	54	Total	C	N	O	S	0	0
			418	274	67	75	2		

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	t	102	Total	C	N	O		
			779	492	146	141	0	0

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	v	84	Total	C	N	O	S	
			634	391	129	113	1	0

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	y	58	Total	C	N	O	S	
			449	281	87	79	2	0

- Molecule 52 is a protein called 50S ribosomal protein L32.

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

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms		AltConf
57	A	71	Total	Mg	0
			71	71	
57	a	234	Total	Mg	0
			234	234	
57	b	2	Total	Mg	0
			2	2	
57	c	3	Total	Mg	0
			3	3	
57	d	1	Total	Mg	0
			1	1	
57	m	1	Total	Mg	0
			1	1	
57	z	1	Total	Mg	0
			1	1	

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



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

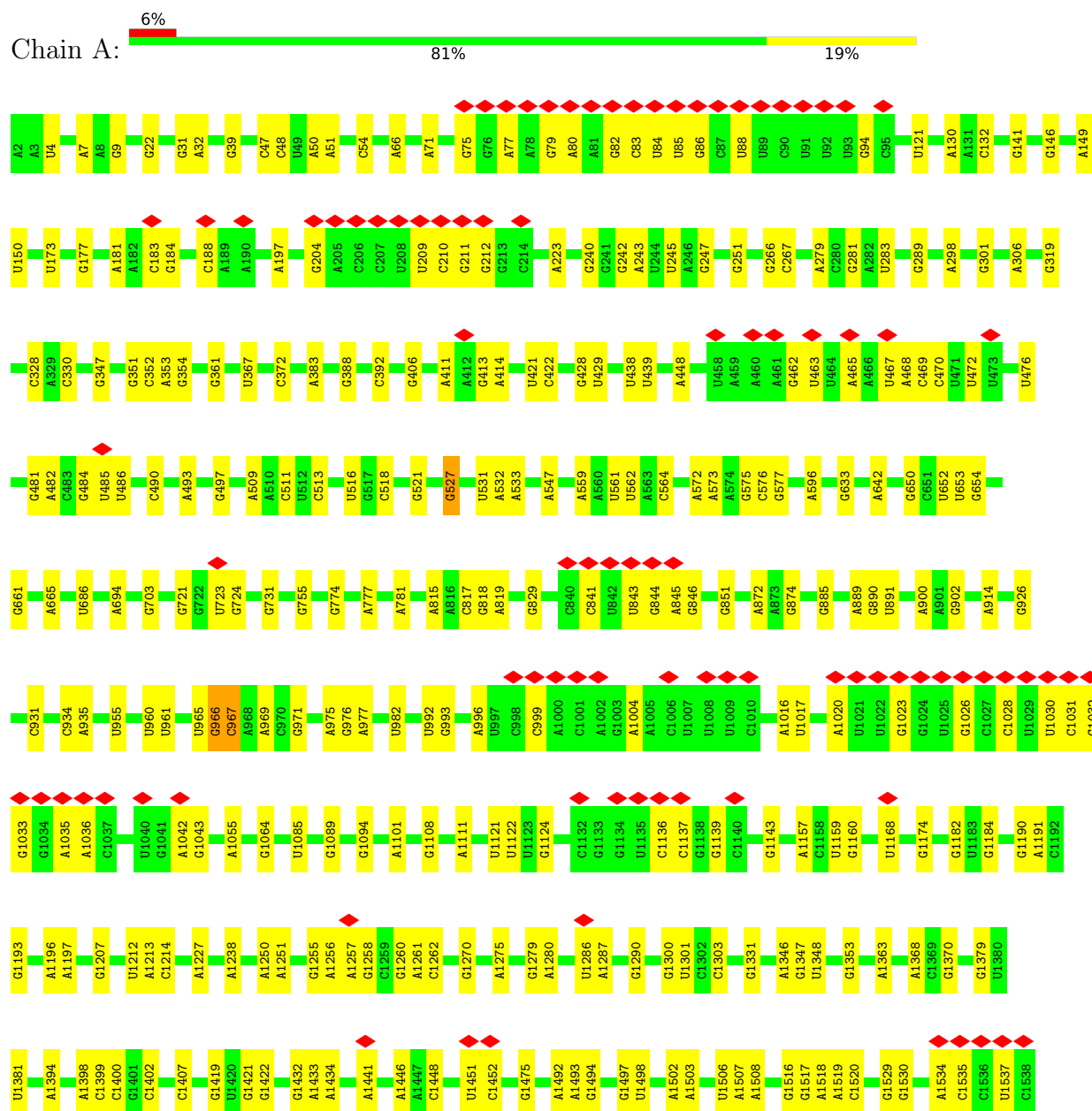
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	1	1	Total	Zn	0
			1	1	
59	3	1	Total	Zn	0
			1	1	

3 Residue-property plots

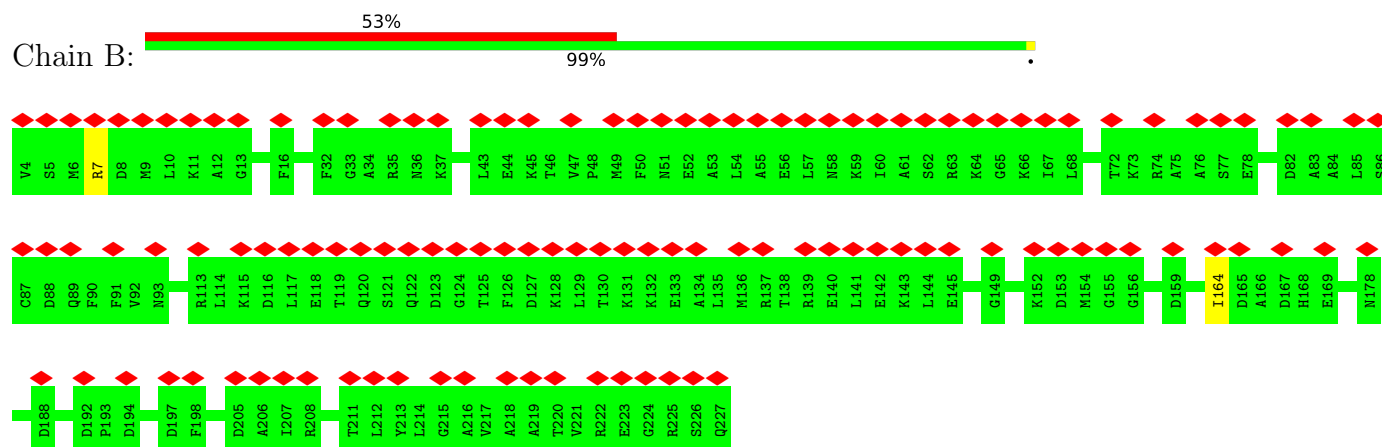
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S ribosomal RNA

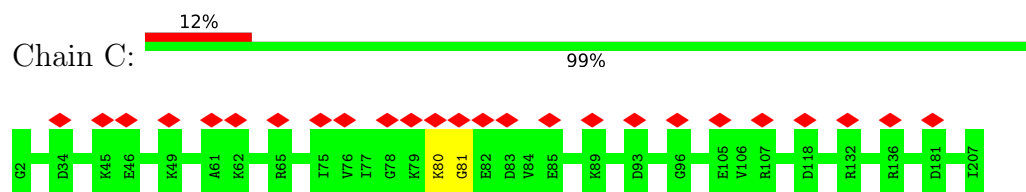




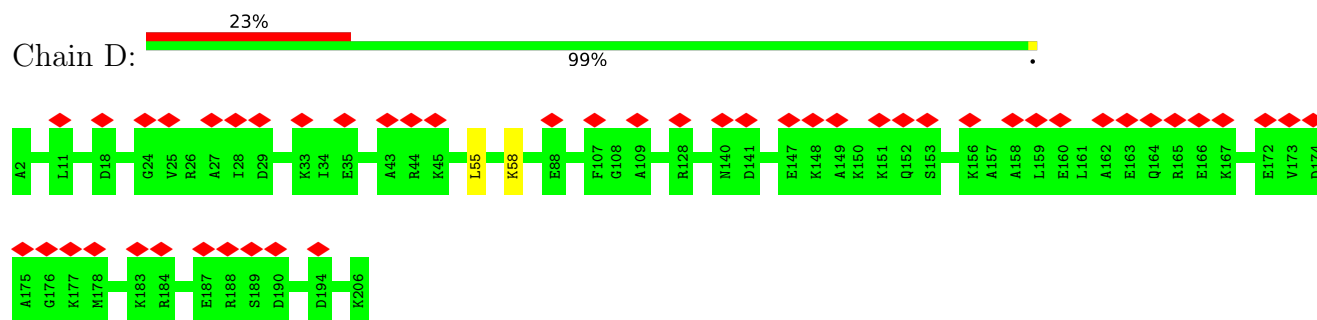
• Molecule 2: 30S ribosomal protein S2



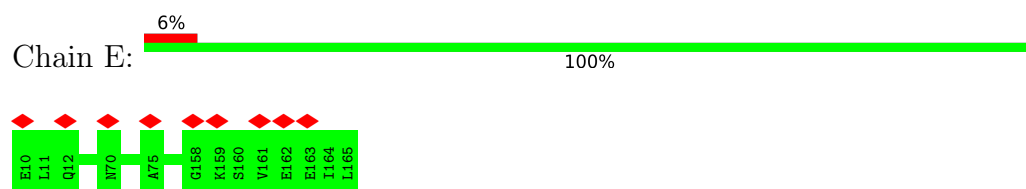
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

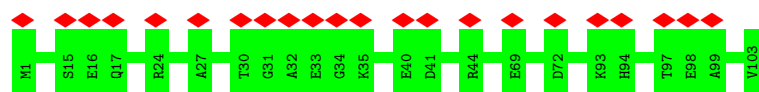


• Molecule 5: 30S ribosomal protein S5

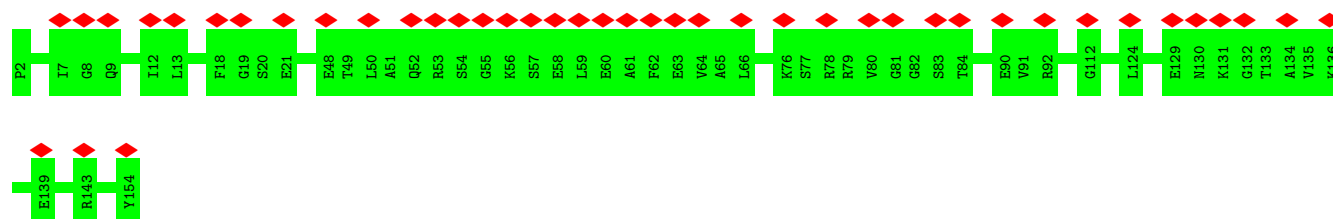


• Molecule 6: 30S ribosomal protein S6

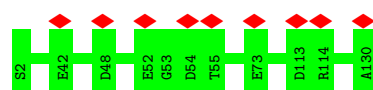




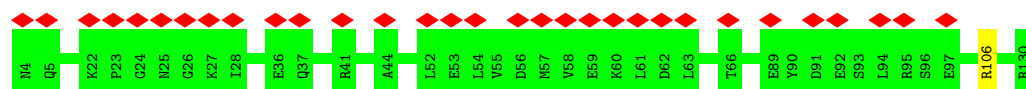
- Molecule 7: 30S ribosomal protein S7



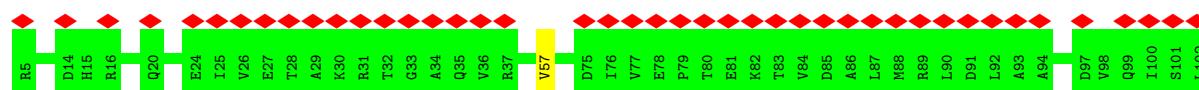
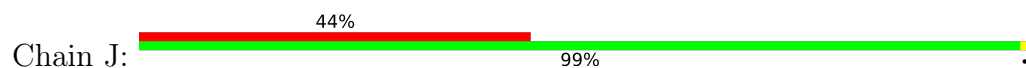
- Molecule 8: 30S ribosomal protein S8



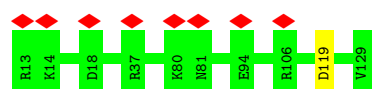
- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10

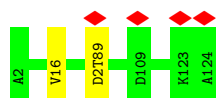


- Molecule 11: 30S ribosomal protein S11

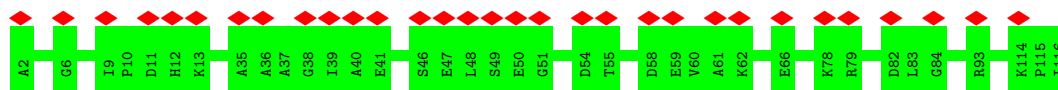


- Molecule 12: 30S ribosomal protein S12

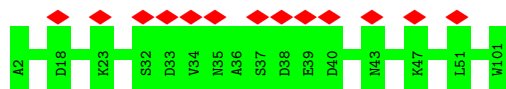




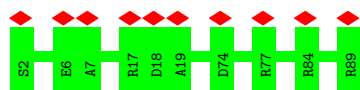
- Molecule 13: 30S ribosomal protein S13



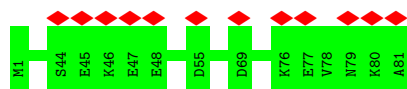
- Molecule 14: 30S ribosomal protein S14



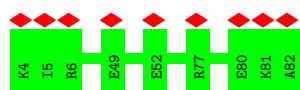
- Molecule 15: 30S ribosomal protein S15



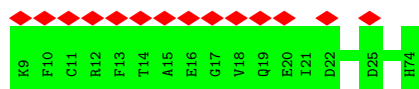
- Molecule 16: 30S ribosomal protein S16



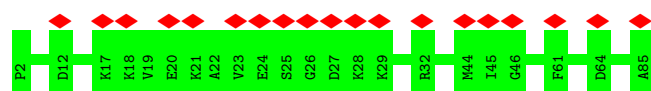
- Molecule 17: 30S ribosomal protein S17



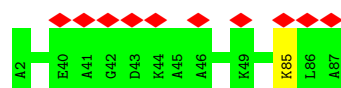
- Molecule 18: 30S ribosomal protein S18



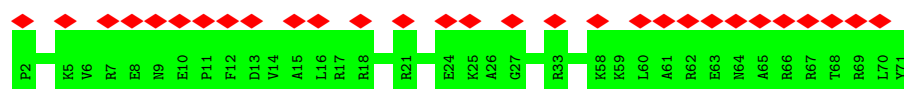
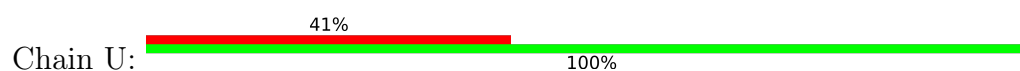
- Molecule 19: 30S ribosomal protein S19



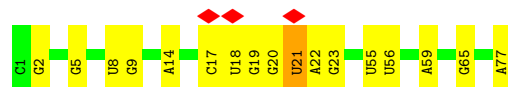
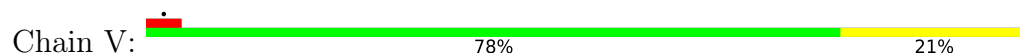
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



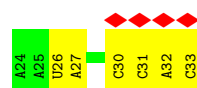
- Molecule 22: P-site fMet-tRNA(fMet)



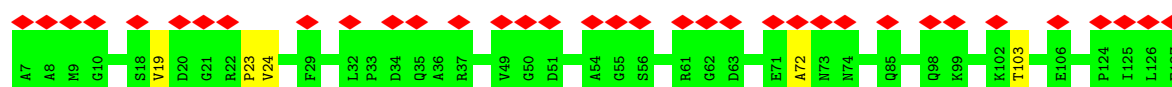
- Molecule 23: E-site tRNA



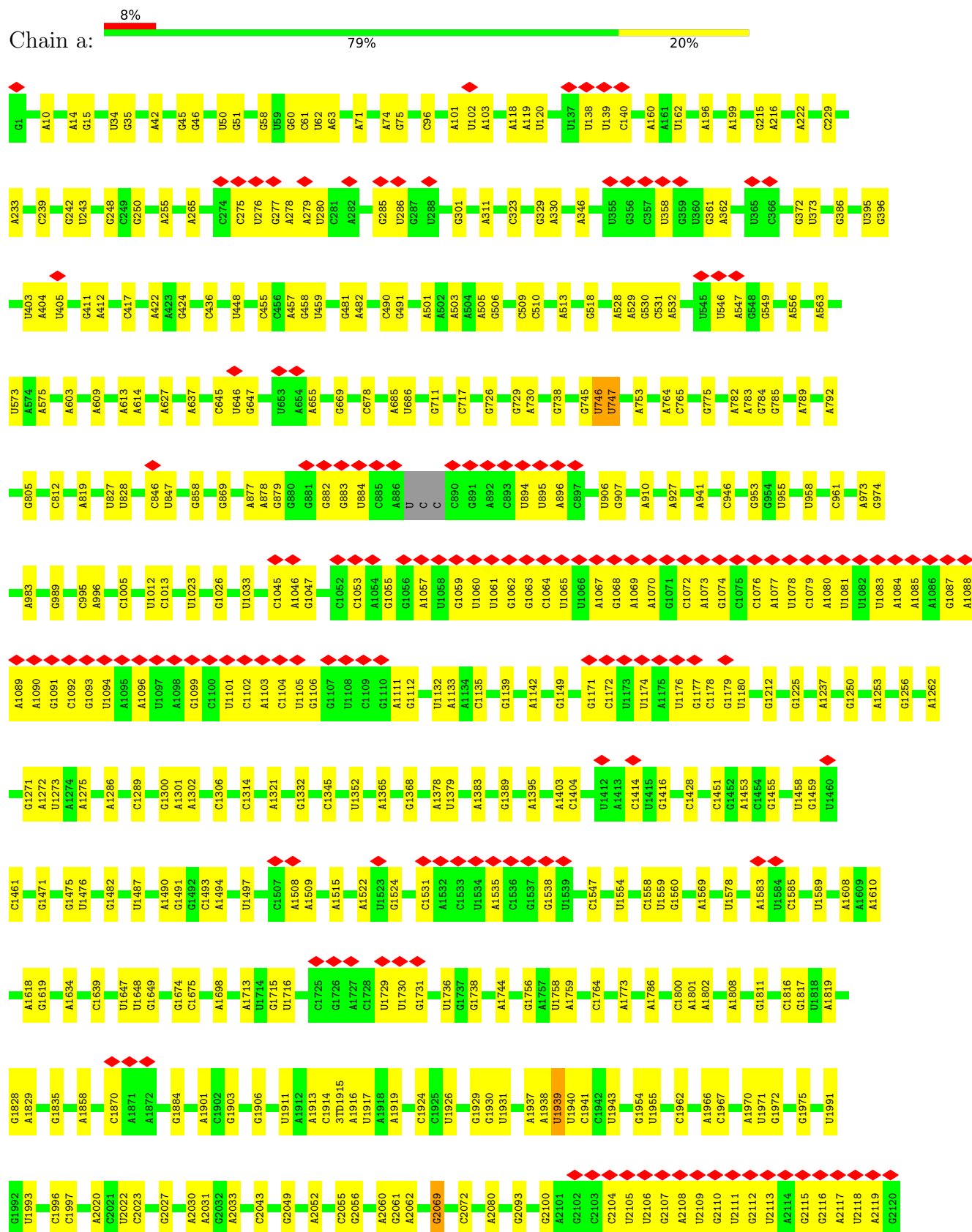
- Molecule 24: cspA mRNA

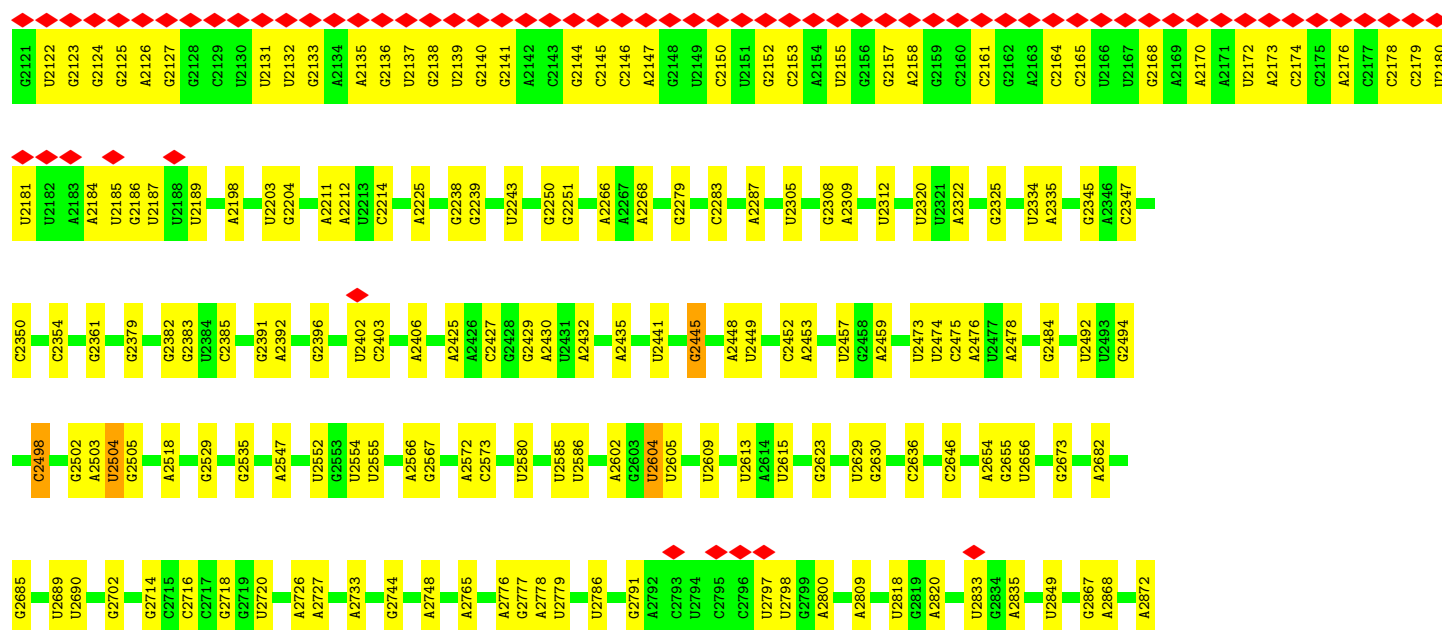


- Molecule 25: Probable endoribonuclease HigB1

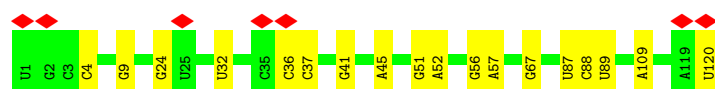
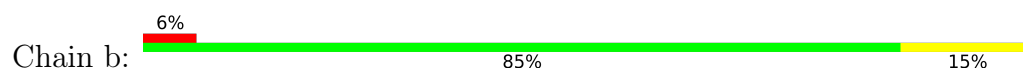


• Molecule 26: 23S ribosomal RNA

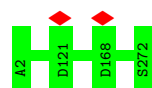




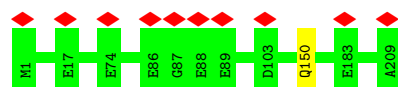
• Molecule 27: 5S ribosomal RNA



• Molecule 28: 50S ribosomal protein L2

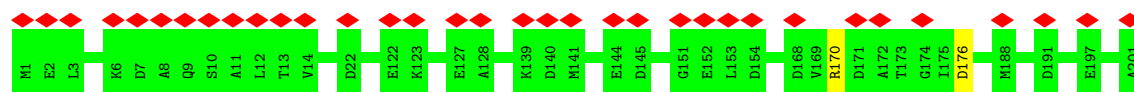


• Molecule 29: 50S ribosomal protein L3

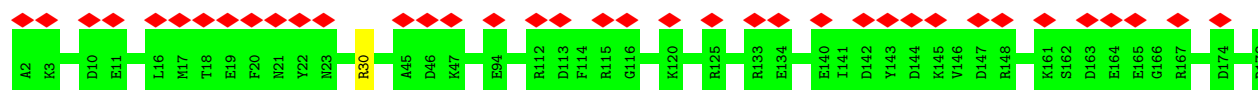


• Molecule 30: 50S ribosomal protein L4

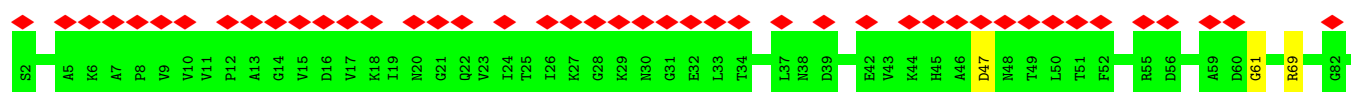
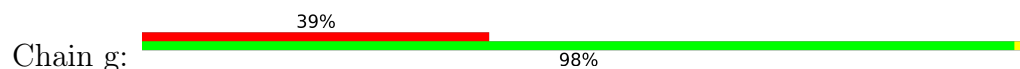




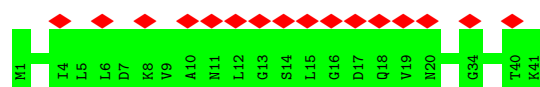
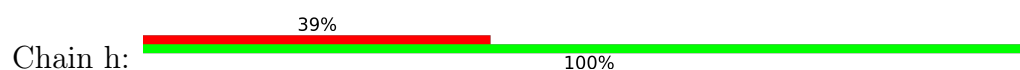
- Molecule 31: 50S ribosomal protein L5



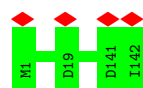
- Molecule 32: 50S ribosomal protein L6



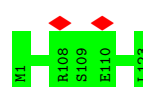
- Molecule 33: 50S ribosomal protein L9



- Molecule 34: 50S ribosomal protein L13

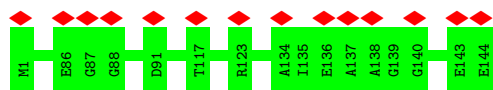


- Molecule 35: 50S ribosomal protein L14

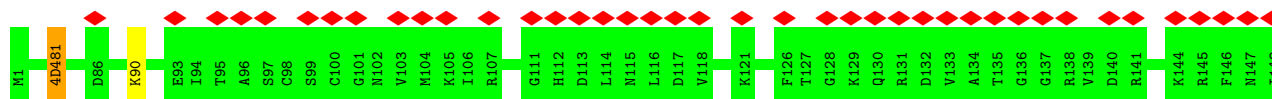


- Molecule 36: 50S ribosomal protein L15





- Molecule 37: 50S ribosomal protein L16, 50S ribosomal protein L31



- Molecule 38: 50S ribosomal protein L16

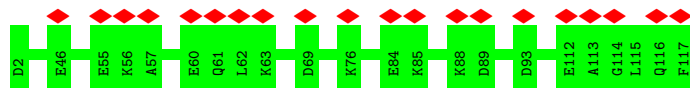


- Molecule 39: 50S ribosomal protein L17

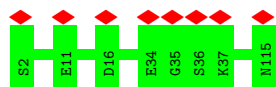


There are no outlier residues recorded for this chain.

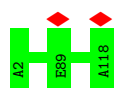
- Molecule 40: 50S ribosomal protein L18



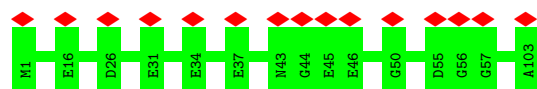
- Molecule 41: 50S ribosomal protein L19



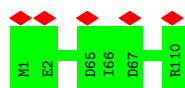
- Molecule 42: 50S ribosomal protein L20



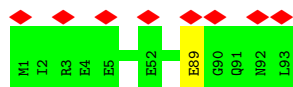
- Molecule 43: 50S ribosomal protein L21



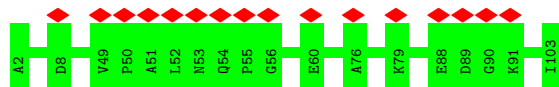
- Molecule 44: 50S ribosomal protein L22



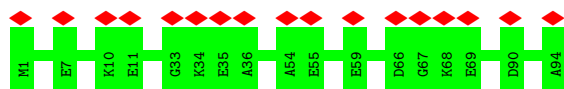
- Molecule 45: 50S ribosomal protein L23



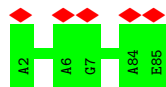
- Molecule 46: 50S ribosomal protein L24



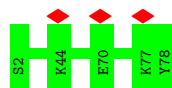
- Molecule 47: 50S ribosomal protein L25



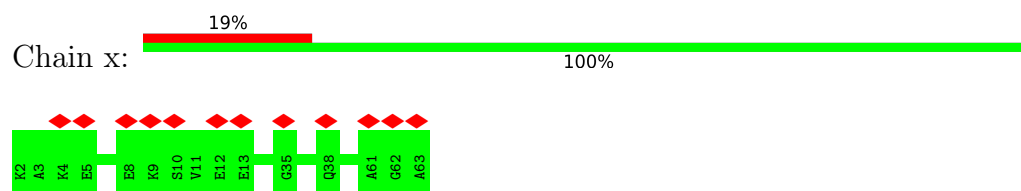
- Molecule 48: 50S ribosomal protein L27



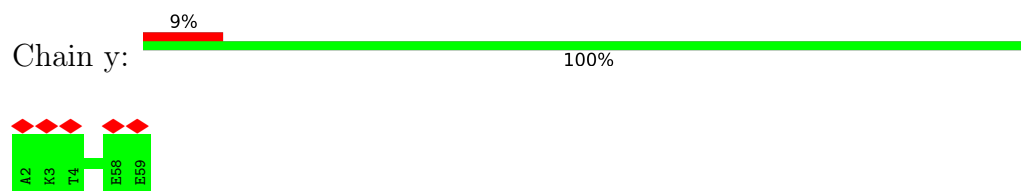
- Molecule 49: 50S ribosomal protein L28



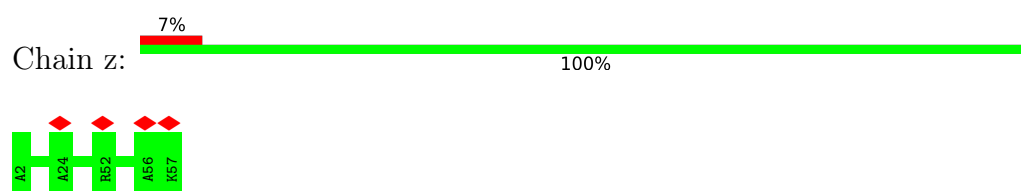
- Molecule 50: 50S ribosomal protein L29



- Molecule 51: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L32

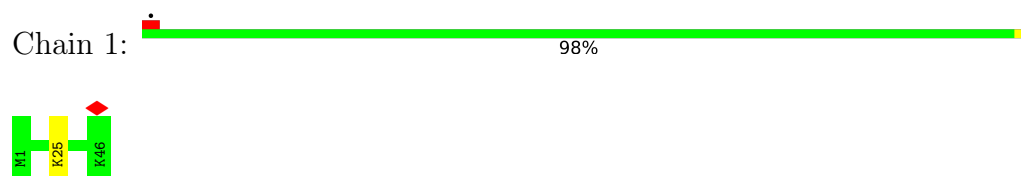


- Molecule 53: 50S ribosomal protein L33

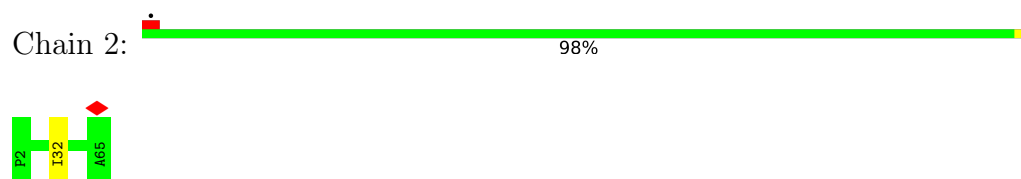


There are no outlier residues recorded for this chain.

- Molecule 54: 50S ribosomal protein L34



- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13877	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	120000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	19.049	Depositor
Minimum map value	-4.324	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	457.216, 457.216, 457.216	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.893, 0.893, 0.893	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, 4OC, OMG, OMC, 2MA, ZN, PSU, D2T, 1MG, OMU, UR3, MS6, 2MG, G7M, 6MZ, MG, 5MU, H2U, 4D4, MEQ, 5MC, 4SU, 3TD, IAS, MA6

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.66	0/36693	0.82	0/57234
2	B	0.32	0/1784	0.47	0/2403
3	C	0.34	0/1651	0.46	0/2225
4	D	0.37	0/1665	0.47	0/2227
5	E	0.37	0/1165	0.48	0/1568
6	F	0.38	0/858	0.50	0/1160
7	G	0.29	0/1219	0.43	0/1635
8	H	0.37	0/989	0.50	0/1326
9	I	0.35	0/1034	0.48	0/1375
10	J	0.33	0/796	0.54	0/1077
11	K	0.38	0/884	0.48	0/1191
12	L	0.36	0/960	0.50	0/1286
13	M	0.32	0/900	0.51	0/1204
14	N	0.34	0/817	0.44	0/1088
15	O	0.33	0/722	0.44	0/964
16	P	0.37	0/653	0.49	0/877
17	Q	0.36	0/650	0.48	0/871
18	R	0.38	0/553	0.49	0/742
19	S	0.33	0/685	0.49	0/922
20	T	0.31	0/676	0.43	0/895
21	U	0.30	0/597	0.43	0/792
22	V	0.52	0/1746	0.81	0/2721
23	W	0.37	0/46	0.73	0/69
24	X	0.48	0/235	0.87	0/363
25	Y	0.40	0/1020	0.58	0/1377
26	a	0.76	0/69174	0.82	0/107911
27	b	0.62	0/2872	0.80	0/4478
28	c	0.41	0/2121	0.50	0/2852
29	d	0.42	0/1576	0.51	0/2119
30	e	0.41	0/1571	0.49	0/2113
31	f	0.34	0/1434	0.47	0/1926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.33	0/1343	0.49	0/1816
33	h	0.33	0/306	0.60	0/413
34	i	0.41	0/1152	0.47	0/1551
35	j	0.39	0/955	0.51	0/1279
36	k	0.38	0/1062	0.52	0/1413
37	l	0.36	0/1178	0.49	0/1569
38	Z	0.41	0/426	0.49	0/573
39	m	0.40	0/958	0.47	0/1281
40	n	0.37	0/902	0.46	0/1209
41	o	0.39	0/929	0.49	0/1242
42	p	0.46	0/960	0.43	0/1278
43	q	0.42	0/829	0.51	0/1107
44	r	0.37	0/864	0.50	0/1156
45	s	0.38	0/744	0.48	0/994
46	t	0.37	0/787	0.50	0/1051
47	u	0.37	0/766	0.49	0/1025
48	v	0.40	0/642	0.45	0/848
49	w	0.39	0/635	0.47	0/848
50	x	0.31	0/502	0.43	0/667
51	y	0.37	0/453	0.54	0/605
52	z	0.39	0/450	0.46	0/599
53	0	0.37	0/424	0.48	0/565
54	1	0.39	0/380	0.48	0/498
55	2	0.41	0/513	0.53	0/676
56	3	0.37	0/303	0.46	0/397
All	All	0.64	0/156209	0.75	0/233651

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

Mol	Chain	#Chirality outliers	#Planarity outliers
37	l	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	1	81	4D4	Mainchain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	222/224 (99%)	200 (90%)	21 (10%)	1 (0%)	25	56
3	C	204/206 (99%)	191 (94%)	11 (5%)	2 (1%)	13	40
4	D	203/205 (99%)	194 (96%)	9 (4%)	0	100	100
5	E	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
6	F	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
7	G	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
8	H	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
9	I	125/127 (98%)	121 (97%)	4 (3%)	0	100	100
10	J	96/98 (98%)	89 (93%)	6 (6%)	1 (1%)	13	40
11	K	113/117 (97%)	105 (93%)	8 (7%)	0	100	100
12	L	120/123 (98%)	108 (90%)	11 (9%)	1 (1%)	16	46
13	M	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
14	N	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
15	O	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
16	P	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
17	Q	77/79 (98%)	73 (95%)	4 (5%)	0	100	100
18	R	64/66 (97%)	62 (97%)	2 (3%)	0	100	100
19	S	82/84 (98%)	77 (94%)	5 (6%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
21	U	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
25	Y	119/121 (98%)	99 (83%)	18 (15%)	2 (2%)	7	29
28	c	269/271 (99%)	258 (96%)	11 (4%)	0	100	100
29	d	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
30	e	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
31	f	175/177 (99%)	158 (90%)	17 (10%)	0	100	100
32	g	174/176 (99%)	158 (91%)	14 (8%)	2 (1%)	12	37
33	h	39/41 (95%)	34 (87%)	5 (13%)	0	100	100
34	i	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
35	j	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
36	k	142/144 (99%)	132 (93%)	10 (7%)	0	100	100
37	l	143/148 (97%)	131 (92%)	12 (8%)	0	100	100
38	Z	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
39	m	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
40	n	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
41	o	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
42	p	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
43	q	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
44	r	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
45	s	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	12	37
46	t	100/102 (98%)	83 (83%)	17 (17%)	0	100	100
47	u	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
48	v	82/84 (98%)	74 (90%)	8 (10%)	0	100	100
49	w	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
50	x	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
51	y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
52	z	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
53	0	49/51 (96%)	49 (100%)	0	0	100	100
54	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
55	2	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	8	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
All	All	5613/5720 (98%)	5275 (94%)	327 (6%)	11 (0%)	45	73

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	164	ILE
12	L	16	VAL
32	g	47	ASP
32	g	61	GLY
10	J	57	VAL
25	Y	72	ALA
45	s	89	GLU
3	C	80	LYS
25	Y	23	PRO
55	2	32	ILE
3	C	81	GLY

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	
2	B	186/186 (100%)	185 (100%)	1 (0%)	86	92
3	C	170/170 (100%)	170 (100%)	0	100	100
4	D	172/172 (100%)	170 (99%)	2 (1%)	67	82
5	E	119/119 (100%)	119 (100%)	0	100	100
6	F	90/90 (100%)	90 (100%)	0	100	100
7	G	126/126 (100%)	126 (100%)	0	100	100
8	H	104/104 (100%)	104 (100%)	0	100	100
9	I	105/105 (100%)	104 (99%)	1 (1%)	73	85
10	J	86/86 (100%)	86 (100%)	0	100	100
11	K	89/89 (100%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	102/102 (100%)	102 (100%)	0	100	100
13	M	93/93 (100%)	93 (100%)	0	100	100
14	N	83/83 (100%)	83 (100%)	0	100	100
15	O	76/76 (100%)	76 (100%)	0	100	100
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	73/73 (100%)	73 (100%)	0	100	100
18	R	57/57 (100%)	57 (100%)	0	100	100
19	S	72/72 (100%)	72 (100%)	0	100	100
20	T	65/65 (100%)	64 (98%)	1 (2%)	60	78
21	U	60/60 (100%)	60 (100%)	0	100	100
25	Y	100/100 (100%)	97 (97%)	3 (3%)	36	62
28	c	216/216 (100%)	216 (100%)	0	100	100
29	d	163/163 (100%)	163 (100%)	0	100	100
30	e	165/165 (100%)	163 (99%)	2 (1%)	67	82
31	f	148/148 (100%)	147 (99%)	1 (1%)	81	90
32	g	137/137 (100%)	135 (98%)	2 (2%)	60	78
33	h	32/32 (100%)	32 (100%)	0	100	100
34	i	116/116 (100%)	116 (100%)	0	100	100
35	j	104/104 (100%)	104 (100%)	0	100	100
36	k	103/103 (100%)	103 (100%)	0	100	100
37	l	123/123 (100%)	122 (99%)	1 (1%)	79	89
38	Z	43/43 (100%)	43 (100%)	0	100	100
39	m	98/98 (100%)	98 (100%)	0	100	100
40	n	86/86 (100%)	86 (100%)	0	100	100
41	o	99/99 (100%)	99 (100%)	0	100	100
42	p	89/89 (100%)	89 (100%)	0	100	100
43	q	84/84 (100%)	84 (100%)	0	100	100
44	r	93/93 (100%)	93 (100%)	0	100	100
45	s	80/80 (100%)	80 (100%)	0	100	100
46	t	83/83 (100%)	83 (100%)	0	100	100
47	u	78/78 (100%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	v	62/62 (100%)	62 (100%)	0	100	100
49	w	67/67 (100%)	67 (100%)	0	100	100
50	x	54/54 (100%)	54 (100%)	0	100	100
51	y	48/48 (100%)	48 (100%)	0	100	100
52	z	47/47 (100%)	47 (100%)	0	100	100
53	0	46/46 (100%)	46 (100%)	0	100	100
54	1	38/38 (100%)	37 (97%)	1 (3%)	41	66
55	2	51/51 (100%)	51 (100%)	0	100	100
56	3	34/34 (100%)	34 (100%)	0	100	100
All	All	4680/4680 (100%)	4665 (100%)	15 (0%)	90	95

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	ARG
4	D	55	LEU
4	D	58	LYS
9	I	106	ARG
20	T	85	LYS
25	Y	19	VAL
25	Y	24	VAL
25	Y	103	THR
30	e	170	ARG
30	e	176	ASP
31	f	30	ARG
32	g	69	ARG
32	g	175	LYS
37	l	90	LYS
54	1	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	39	HIS
9	I	5	GLN
9	I	37	GLN
28	c	53	HIS
29	d	36	GLN

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Mol	Chain	Res	Type
29	d	49	GLN
32	g	38	ASN
55	2	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1535/1539 (99%)	277 (18%)	20 (1%)
22	V	76/77 (98%)	13 (17%)	1 (1%)
23	W	1/2 (50%)	1 (100%)	0
24	X	9/10 (90%)	6 (66%)	0
26	a	2894/2904 (99%)	578 (19%)	0
27	b	119/120 (99%)	18 (15%)	0
All	All	4634/4652 (99%)	893 (19%)	21 (0%)

All (893) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	7	A
1	A	9	G
1	A	22	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	66	A
1	A	71	A
1	A	75	G
1	A	77	A
1	A	79	G
1	A	80	A
1	A	82	G
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G

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Mol	Chain	Res	Type
1	A	88	U
1	A	94	G
1	A	121	U
1	A	130	A
1	A	132	C
1	A	141	G
1	A	146	G
1	A	149	A
1	A	150	U
1	A	173	U
1	A	177	G
1	A	181	A
1	A	183	C
1	A	184	G
1	A	188	C
1	A	197	A
1	A	204	G
1	A	209	U
1	A	210	C
1	A	211	G
1	A	212	G
1	A	223	A
1	A	240	G
1	A	243	A
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	279	A
1	A	281	G
1	A	283	U
1	A	289	G
1	A	298	A
1	A	301	G
1	A	306	A
1	A	319	G
1	A	328	C
1	A	330	C
1	A	347	G
1	A	351	G
1	A	352	C

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Mol	Chain	Res	Type
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	383	A
1	A	388	G
1	A	392	C
1	A	406	G
1	A	411	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	429	U
1	A	439	U
1	A	448	A
1	A	462	G
1	A	463	U
1	A	465	A
1	A	467	U
1	A	468	A
1	A	469	C
1	A	470	C
1	A	472	U
1	A	476	U
1	A	482	A
1	A	484	G
1	A	485	U
1	A	486	U
1	A	493	A
1	A	497	G
1	A	509	A
1	A	511	C
1	A	513	C
1	A	518	C
1	A	521	G
1	A	527	G7M
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A

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Mol	Chain	Res	Type
1	A	562	U
1	A	564	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	C
1	A	577	G
1	A	596	A
1	A	633	G
1	A	642	A
1	A	650	G
1	A	653	U
1	A	654	G
1	A	661	G
1	A	665	A
1	A	686	U
1	A	694	A
1	A	703	G
1	A	721	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	755	G
1	A	777	A
1	A	781	A
1	A	815	A
1	A	817	C
1	A	819	A
1	A	829	G
1	A	841	C
1	A	843	U
1	A	844	G
1	A	845	A
1	A	846	G
1	A	851	G
1	A	872	A
1	A	874	G
1	A	885	G
1	A	889	A
1	A	890	G
1	A	891	U
1	A	900	A

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Mol	Chain	Res	Type
1	A	902	G
1	A	914	A
1	A	926	G
1	A	931	C
1	A	934	C
1	A	935	A
1	A	955	U
1	A	960	U
1	A	961	U
1	A	965	U
1	A	966	2MG
1	A	967	5MC
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	992	U
1	A	993	G
1	A	996	A
1	A	999	C
1	A	1004	A
1	A	1016	A
1	A	1017	U
1	A	1020	A
1	A	1023	G
1	A	1026	G
1	A	1028	C
1	A	1030	U
1	A	1031	C
1	A	1032	G
1	A	1033	G
1	A	1035	A
1	A	1036	A
1	A	1042	A
1	A	1043	G
1	A	1055	A
1	A	1064	G
1	A	1085	U
1	A	1089	G
1	A	1094	G

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Mol	Chain	Res	Type
1	A	1101	A
1	A	1108	G
1	A	1121	U
1	A	1122	U
1	A	1124	G
1	A	1136	C
1	A	1137	C
1	A	1139	G
1	A	1143	G
1	A	1157	A
1	A	1159	U
1	A	1160	G
1	A	1168	U
1	A	1174	G
1	A	1182	G
1	A	1184	G
1	A	1191	A
1	A	1193	G
1	A	1196	A
1	A	1197	A
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1238	A
1	A	1250	A
1	A	1251	A
1	A	1255	G
1	A	1256	A
1	A	1257	A
1	A	1258	G
1	A	1260	G
1	A	1261	A
1	A	1262	C
1	A	1270	G
1	A	1275	A
1	A	1279	G
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1290	G
1	A	1300	G

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Mol	Chain	Res	Type
1	A	1301	U
1	A	1303	C
1	A	1331	G
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1363	A
1	A	1368	A
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1394	A
1	A	1398	A
1	A	1399	C
1	A	1400	C
1	A	1419	G
1	A	1421	G
1	A	1422	G
1	A	1432	G
1	A	1433	A
1	A	1434	A
1	A	1441	A
1	A	1446	A
1	A	1448	C
1	A	1451	U
1	A	1452	C
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1502	A
1	A	1503	A
1	A	1506	U
1	A	1507	A
1	A	1508	A
1	A	1517	G
1	A	1520	C
1	A	1529	G
1	A	1530	G
1	A	1534	A
1	A	1535	C

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Mol	Chain	Res	Type
1	A	1537	U
1	A	1540	U
22	V	2	G
22	V	5	G
22	V	9	G
22	V	14	A
22	V	17	C
22	V	18	U
22	V	19	G
22	V	21	H2U
22	V	22	A
22	V	23	G
22	V	59	A
22	V	65	G
22	V	77	A
23	W	77	A
24	X	26	U
24	X	27	A
24	X	30	C
24	X	31	C
24	X	32	A
24	X	33	C
26	a	10	A
26	a	14	A
26	a	15	G
26	a	34	U
26	a	35	G
26	a	42	A
26	a	45	G
26	a	46	G
26	a	50	U
26	a	51	G
26	a	58	G
26	a	60	G
26	a	61	C
26	a	62	U
26	a	63	A
26	a	71	A
26	a	74	A
26	a	75	G
26	a	96	C
26	a	101	A

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Mol	Chain	Res	Type
26	a	102	U
26	a	103	A
26	a	118	A
26	a	119	A
26	a	120	U
26	a	138	U
26	a	139	U
26	a	140	C
26	a	160	A
26	a	162	U
26	a	196	A
26	a	199	A
26	a	215	G
26	a	216	A
26	a	222	A
26	a	229	C
26	a	233	A
26	a	239	C
26	a	242	G
26	a	243	U
26	a	248	G
26	a	250	G
26	a	255	A
26	a	265	A
26	a	275	C
26	a	276	U
26	a	277	G
26	a	278	A
26	a	279	A
26	a	280	U
26	a	285	G
26	a	286	U
26	a	301	G
26	a	311	A
26	a	323	C
26	a	329	G
26	a	330	A
26	a	346	A
26	a	358	U
26	a	361	G
26	a	362	A
26	a	372	G

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Mol	Chain	Res	Type
26	a	373	U
26	a	386	G
26	a	395	U
26	a	396	G
26	a	403	U
26	a	404	A
26	a	405	U
26	a	411	G
26	a	412	A
26	a	417	C
26	a	422	A
26	a	424	G
26	a	436	C
26	a	448	U
26	a	455	C
26	a	457	A
26	a	458	G
26	a	459	U
26	a	481	G
26	a	482	A
26	a	490	C
26	a	491	G
26	a	501	A
26	a	503	A
26	a	505	A
26	a	506	G
26	a	509	C
26	a	510	C
26	a	513	A
26	a	518	G
26	a	528	A
26	a	529	A
26	a	530	G
26	a	531	C
26	a	532	A
26	a	546	U
26	a	547	A
26	a	549	G
26	a	556	A
26	a	563	A
26	a	573	U
26	a	575	A

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Mol	Chain	Res	Type
26	a	603	A
26	a	609	A
26	a	613	A
26	a	614	A
26	a	627	A
26	a	637	A
26	a	645	C
26	a	646	U
26	a	647	G
26	a	655	A
26	a	669	G
26	a	678	C
26	a	685	A
26	a	686	U
26	a	711	G
26	a	717	C
26	a	726	G
26	a	729	G
26	a	730	A
26	a	738	G
26	a	746	PSU
26	a	747	5MU
26	a	753	A
26	a	764	A
26	a	765	C
26	a	775	G
26	a	782	A
26	a	783	A
26	a	784	G
26	a	785	G
26	a	789	A
26	a	792	A
26	a	805	G
26	a	812	C
26	a	819	A
26	a	827	U
26	a	828	U
26	a	846	C
26	a	847	U
26	a	858	G
26	a	869	G
26	a	877	A

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Mol	Chain	Res	Type
26	a	878	A
26	a	879	G
26	a	882	G
26	a	883	G
26	a	884	U
26	a	894	U
26	a	895	U
26	a	896	A
26	a	906	U
26	a	907	G
26	a	910	A
26	a	927	A
26	a	941	A
26	a	946	C
26	a	953	G
26	a	958	U
26	a	961	C
26	a	973	A
26	a	974	G
26	a	983	A
26	a	989	G
26	a	995	C
26	a	996	A
26	a	1005	C
26	a	1012	U
26	a	1013	C
26	a	1023	U
26	a	1026	G
26	a	1033	U
26	a	1045	C
26	a	1046	A
26	a	1047	G
26	a	1053	C
26	a	1055	G
26	a	1057	A
26	a	1059	G
26	a	1060	U
26	a	1061	U
26	a	1062	G
26	a	1063	G
26	a	1064	C
26	a	1065	U

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Mol	Chain	Res	Type
26	a	1067	A
26	a	1068	G
26	a	1069	A
26	a	1070	A
26	a	1072	C
26	a	1073	A
26	a	1074	G
26	a	1076	C
26	a	1077	A
26	a	1078	U
26	a	1079	C
26	a	1080	A
26	a	1081	U
26	a	1083	U
26	a	1084	A
26	a	1085	A
26	a	1087	G
26	a	1088	A
26	a	1089	A
26	a	1090	A
26	a	1091	G
26	a	1092	C
26	a	1093	G
26	a	1094	U
26	a	1096	A
26	a	1099	G
26	a	1101	U
26	a	1102	C
26	a	1103	A
26	a	1104	C
26	a	1105	U
26	a	1106	G
26	a	1111	A
26	a	1112	G
26	a	1132	U
26	a	1133	A
26	a	1135	C
26	a	1139	G
26	a	1142	A
26	a	1149	G
26	a	1171	G
26	a	1172	C

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Mol	Chain	Res	Type
26	a	1174	U
26	a	1176	U
26	a	1177	G
26	a	1178	C
26	a	1179	G
26	a	1180	U
26	a	1212	G
26	a	1225	G
26	a	1237	A
26	a	1250	G
26	a	1253	A
26	a	1256	G
26	a	1262	A
26	a	1271	G
26	a	1272	A
26	a	1273	U
26	a	1275	A
26	a	1286	A
26	a	1289	C
26	a	1300	G
26	a	1301	A
26	a	1302	A
26	a	1306	C
26	a	1314	C
26	a	1321	A
26	a	1332	G
26	a	1345	C
26	a	1352	U
26	a	1365	A
26	a	1368	G
26	a	1378	A
26	a	1379	U
26	a	1383	A
26	a	1389	G
26	a	1395	A
26	a	1403	A
26	a	1404	C
26	a	1414	C
26	a	1416	G
26	a	1428	C
26	a	1451	C
26	a	1453	A

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Mol	Chain	Res	Type
26	a	1455	G
26	a	1458	U
26	a	1459	G
26	a	1461	C
26	a	1471	G
26	a	1475	G
26	a	1476	U
26	a	1482	G
26	a	1487	U
26	a	1490	A
26	a	1491	G
26	a	1493	C
26	a	1494	A
26	a	1497	U
26	a	1508	A
26	a	1509	A
26	a	1515	A
26	a	1522	A
26	a	1524	G
26	a	1531	C
26	a	1535	A
26	a	1538	G
26	a	1547	C
26	a	1554	U
26	a	1558	C
26	a	1559	U
26	a	1560	G
26	a	1569	A
26	a	1578	U
26	a	1583	A
26	a	1585	C
26	a	1589	U
26	a	1608	A
26	a	1610	A
26	a	1619	G
26	a	1634	A
26	a	1639	C
26	a	1647	U
26	a	1648	U
26	a	1649	G
26	a	1674	G
26	a	1675	C

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Mol	Chain	Res	Type
26	a	1698	A
26	a	1713	A
26	a	1715	G
26	a	1716	U
26	a	1729	U
26	a	1730	U
26	a	1731	G
26	a	1736	U
26	a	1738	G
26	a	1744	A
26	a	1756	G
26	a	1758	U
26	a	1759	A
26	a	1764	C
26	a	1773	A
26	a	1786	A
26	a	1800	C
26	a	1801	A
26	a	1802	A
26	a	1808	A
26	a	1811	G
26	a	1816	C
26	a	1817	G
26	a	1819	A
26	a	1828	G
26	a	1829	A
26	a	1858	A
26	a	1870	C
26	a	1884	G
26	a	1901	A
26	a	1903	G
26	a	1906	G
26	a	1913	A
26	a	1914	C
26	a	1916	A
26	a	1919	A
26	a	1924	C
26	a	1926	U
26	a	1929	G
26	a	1930	G
26	a	1931	U
26	a	1937	A

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Mol	Chain	Res	Type
26	a	1938	A
26	a	1939	5MU
26	a	1940	U
26	a	1941	C
26	a	1943	U
26	a	1954	G
26	a	1955	U
26	a	1966	A
26	a	1967	C
26	a	1970	A
26	a	1971	U
26	a	1972	G
26	a	1975	G
26	a	1991	U
26	a	1993	U
26	a	1996	C
26	a	1997	C
26	a	2020	A
26	a	2022	U
26	a	2023	C
26	a	2027	G
26	a	2031	A
26	a	2033	A
26	a	2043	C
26	a	2049	G
26	a	2052	A
26	a	2055	C
26	a	2056	G
26	a	2060	A
26	a	2061	G
26	a	2062	A
26	a	2069	G7M
26	a	2072	C
26	a	2080	A
26	a	2093	G
26	a	2100	G
26	a	2104	C
26	a	2105	U
26	a	2106	U
26	a	2107	G
26	a	2108	A
26	a	2109	U

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Mol	Chain	Res	Type
26	a	2110	G
26	a	2111	U
26	a	2112	G
26	a	2113	U
26	a	2115	G
26	a	2116	G
26	a	2117	A
26	a	2118	U
26	a	2119	A
26	a	2122	U
26	a	2123	G
26	a	2124	G
26	a	2125	G
26	a	2126	A
26	a	2127	G
26	a	2131	U
26	a	2132	U
26	a	2133	G
26	a	2135	A
26	a	2136	G
26	a	2137	U
26	a	2138	G
26	a	2139	U
26	a	2140	G
26	a	2141	G
26	a	2144	G
26	a	2145	C
26	a	2146	C
26	a	2147	A
26	a	2150	C
26	a	2152	G
26	a	2153	C
26	a	2155	U
26	a	2157	G
26	a	2158	A
26	a	2161	C
26	a	2164	C
26	a	2165	C
26	a	2168	G
26	a	2170	A
26	a	2172	U
26	a	2173	A

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Mol	Chain	Res	Type
26	a	2174	C
26	a	2176	A
26	a	2178	C
26	a	2179	C
26	a	2180	U
26	a	2181	U
26	a	2184	A
26	a	2185	U
26	a	2186	G
26	a	2187	U
26	a	2189	U
26	a	2198	A
26	a	2203	U
26	a	2204	G
26	a	2211	A
26	a	2212	A
26	a	2214	C
26	a	2225	A
26	a	2238	G
26	a	2239	G
26	a	2243	U
26	a	2250	G
26	a	2266	A
26	a	2268	A
26	a	2279	G
26	a	2283	C
26	a	2287	A
26	a	2305	U
26	a	2308	G
26	a	2309	A
26	a	2312	U
26	a	2320	U
26	a	2322	A
26	a	2325	G
26	a	2334	U
26	a	2335	A
26	a	2345	G
26	a	2347	C
26	a	2350	C
26	a	2354	C
26	a	2361	G
26	a	2379	G

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Mol	Chain	Res	Type
26	a	2382	G
26	a	2383	G
26	a	2385	C
26	a	2391	G
26	a	2392	A
26	a	2396	G
26	a	2402	U
26	a	2403	C
26	a	2406	A
26	a	2425	A
26	a	2427	C
26	a	2429	G
26	a	2430	A
26	a	2432	A
26	a	2435	A
26	a	2441	U
26	a	2445	2MG
26	a	2448	A
26	a	2452	C
26	a	2453	A
26	a	2459	A
26	a	2473	U
26	a	2474	U
26	a	2475	C
26	a	2476	A
26	a	2478	A
26	a	2484	G
26	a	2492	U
26	a	2494	G
26	a	2498	OMC
26	a	2502	G
26	a	2504	PSU
26	a	2505	G
26	a	2518	A
26	a	2529	G
26	a	2535	G
26	a	2547	A
26	a	2554	U
26	a	2555	U
26	a	2566	A
26	a	2567	G
26	a	2572	A

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Mol	Chain	Res	Type
26	a	2573	C
26	a	2585	U
26	a	2586	U
26	a	2602	A
26	a	2604	PSU
26	a	2609	U
26	a	2613	U
26	a	2615	U
26	a	2623	G
26	a	2629	U
26	a	2630	G
26	a	2636	C
26	a	2646	C
26	a	2654	A
26	a	2655	G
26	a	2656	U
26	a	2673	G
26	a	2682	A
26	a	2685	G
26	a	2689	U
26	a	2690	U
26	a	2702	G
26	a	2714	G
26	a	2716	C
26	a	2718	G
26	a	2720	U
26	a	2726	A
26	a	2727	A
26	a	2733	A
26	a	2744	G
26	a	2748	A
26	a	2765	A
26	a	2776	A
26	a	2777	G
26	a	2778	A
26	a	2779	U
26	a	2786	U
26	a	2791	G
26	a	2797	U
26	a	2798	U
26	a	2800	A
26	a	2809	A

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Mol	Chain	Res	Type
26	a	2818	U
26	a	2820	A
26	a	2833	U
26	a	2835	A
26	a	2849	U
26	a	2867	G
26	a	2868	A
26	a	2872	A
26	a	2873	A
26	a	2880	C
26	a	2884	U
26	a	2891	U
27	b	4	C
27	b	9	G
27	b	24	G
27	b	32	U
27	b	36	C
27	b	37	C
27	b	41	G
27	b	45	A
27	b	51	G
27	b	52	A
27	b	56	G
27	b	57	A
27	b	67	G
27	b	87	U
27	b	88	C
27	b	89	U
27	b	109	A
27	b	120	U

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	242	G
1	A	361	G
1	A	413	G
1	A	428	G
1	A	438	U
1	A	481	G
1	A	490	C
1	A	561	U

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Mol	Chain	Res	Type
1	A	652	U
1	A	774	G
1	A	818	G
1	A	890	G
1	A	1111	A
1	A	1190	G
1	A	1256	A
1	A	1300	G
1	A	1347	G
1	A	1399	C
1	A	1432	G
1	A	1475	G
22	V	20	G

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

43 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
26	2MG	a	1835	26	18,26,27	1.07	1 (5%)	16,38,41	1.14	2 (12%)
26	OMC	a	2498	57,26	19,22,23	3.13	8 (42%)	26,31,34	0.71	0
1	4OC	A	1402	1	20,23,24	3.02	8 (40%)	26,32,35	0.92	2 (7%)
26	PSU	a	746	26	18,21,22	1.33	2 (11%)	22,30,33	1.97	4 (18%)
1	5MC	A	967	1	18,22,23	3.58	7 (38%)	26,32,35	1.04	1 (3%)
26	2MG	a	2445	26	18,26,27	1.16	1 (5%)	16,38,41	1.32	3 (18%)
22	5MU	V	55	22	19,22,23	1.46	6 (31%)	28,32,35	1.74	7 (25%)
26	3TD	a	1915	26	18,22,23	4.33	7 (38%)	22,32,35	1.73	4 (18%)
1	5MC	A	1407	1	18,22,23	3.51	7 (38%)	26,32,35	1.01	1 (3%)
11	IAS	K	119	11	6,7,8	1.11	0	6,8,10	1.38	1 (16%)
22	H2U	V	21	22	18,21,22	2.92	5 (27%)	21,30,33	1.98	5 (23%)
26	H2U	a	2449	26	18,21,22	2.69	5 (27%)	21,30,33	2.11	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	4D4	l	81	37	9,11,12	1.91	2 (22%)	8,13,15	1.86	2 (25%)
12	D2T	L	89	12	7,9,10	1.36	0	6,11,13	2.59	4 (66%)
26	PSU	a	2457	26	18,21,22	1.56	3 (16%)	22,30,33	1.93	5 (22%)
26	PSU	a	955	26	18,21,22	1.10	2 (11%)	22,30,33	1.86	4 (18%)
1	PSU	A	516	1,57	18,21,22	1.50	3 (16%)	22,30,33	1.97	3 (13%)
22	PSU	V	56	22	18,21,22	1.46	3 (16%)	22,30,33	1.81	3 (13%)
26	PSU	a	1911	26	18,21,22	1.09	2 (11%)	22,30,33	1.89	5 (22%)
26	6MZ	a	2030	26	18,25,26	1.97	3 (16%)	16,36,39	2.19	4 (25%)
26	2MA	a	2503	57,26	17,25,26	1.10	1 (5%)	17,37,40	1.25	3 (17%)
1	G7M	A	527	1	20,26,27	1.24	2 (10%)	17,39,42	0.75	0
26	6MZ	a	1618	26	18,25,26	1.94	3 (16%)	16,36,39	2.25	4 (25%)
26	5MU	a	1939	26	19,22,23	1.50	6 (31%)	28,32,35	2.16	8 (28%)
26	G7M	a	2069	26	20,26,27	1.25	2 (10%)	17,39,42	0.97	1 (5%)
1	2MG	A	1516	1	18,26,27	1.16	2 (11%)	16,38,41	1.24	1 (6%)
29	MEQ	d	150	29	8,9,10	0.95	0	5,10,12	1.14	1 (20%)
26	PSU	a	2604	26	18,21,22	1.44	2 (11%)	22,30,33	2.00	4 (18%)
26	PSU	a	2605	26	18,21,22	1.44	3 (16%)	22,30,33	1.89	4 (18%)
1	2MG	A	966	1	18,26,27	1.09	1 (5%)	16,38,41	1.44	3 (18%)
26	PSU	a	1917	26	18,21,22	1.54	3 (16%)	22,30,33	1.93	5 (22%)
26	5MU	a	747	26	19,22,23	1.49	4 (21%)	28,32,35	2.13	10 (35%)
26	OMU	a	2552	57,26	19,22,23	2.80	8 (42%)	26,31,34	1.82	4 (15%)
26	5MC	a	1962	26	18,22,23	3.53	7 (38%)	26,32,35	1.11	1 (3%)
26	PSU	a	2580	26	18,21,22	1.45	2 (11%)	22,30,33	2.06	4 (18%)
26	OMG	a	2251	26,22	18,26,27	1.10	2 (11%)	19,38,41	1.07	2 (10%)
26	1MG	a	745	26	18,26,27	0.90	0	19,39,42	1.32	4 (21%)
1	UR3	A	1498	1	19,22,23	2.78	7 (36%)	26,32,35	1.40	2 (7%)
26	PSU	a	2504	26	18,21,22	1.54	2 (11%)	22,30,33	2.02	5 (22%)
1	2MG	A	1207	1	18,26,27	1.18	2 (11%)	16,38,41	1.20	2 (12%)
1	MA6	A	1518	1	18,26,27	1.22	3 (16%)	19,38,41	2.20	7 (36%)
22	4SU	V	8	22	18,21,22	3.71	7 (38%)	26,30,33	2.35	6 (23%)
1	MA6	A	1519	1	18,26,27	1.22	3 (16%)	19,38,41	1.83	7 (36%)

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
26	2MG	a	1835	26	-	2/5/27/28	0/3/3/3
26	OMC	a	2498	57,26	-	2/9/27/28	0/2/2/2
1	4OC	A	1402	1	-	1/9/29/30	0/2/2/2
26	PSU	a	746	26	-	2/7/25/26	0/2/2/2
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2
26	2MG	a	2445	26	-	2/5/27/28	0/3/3/3
22	5MU	V	55	22	-	0/7/25/26	0/2/2/2
26	3TD	a	1915	26	-	6/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
11	IAS	K	119	11	-	2/7/7/8	-
22	H2U	V	21	22	-	7/7/38/39	0/2/2/2
26	H2U	a	2449	26	-	0/7/38/39	0/2/2/2
37	4D4	l	81	37	-	2/11/12/14	-
12	D2T	L	89	12	-	3/7/12/14	-
26	PSU	a	2457	26	-	0/7/25/26	0/2/2/2
26	PSU	a	955	26	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1,57	-	0/7/25/26	0/2/2/2
22	PSU	V	56	22	-	0/7/25/26	0/2/2/2
26	PSU	a	1911	26	-	0/7/25/26	0/2/2/2
26	6MZ	a	2030	26	-	2/5/27/28	0/3/3/3
26	2MA	a	2503	57,26	-	1/3/25/26	0/3/3/3
1	G7M	A	527	1	-	1/3/25/26	0/3/3/3
26	6MZ	a	1618	26	-	4/5/27/28	0/3/3/3
26	5MU	a	1939	26	-	2/7/25/26	0/2/2/2
26	G7M	a	2069	26	-	2/3/25/26	0/3/3/3
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
29	MEQ	d	150	29	-	2/8/9/11	-
26	PSU	a	2604	26	-	2/7/25/26	0/2/2/2
26	PSU	a	2605	26	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	0/5/27/28	0/3/3/3
26	PSU	a	1917	26	-	0/7/25/26	0/2/2/2
26	5MU	a	747	26	-	1/7/25/26	0/2/2/2
26	OMU	a	2552	57,26	-	3/9/27/28	0/2/2/2
26	5MC	a	1962	26	-	2/7/25/26	0/2/2/2
26	PSU	a	2580	26	-	1/7/25/26	0/2/2/2
26	OMG	a	2251	26,22	-	1/5/27/28	0/3/3/3
26	1MG	a	745	26	-	0/3/25/26	0/3/3/3
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
26	PSU	a	2504	26	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	1207	1	-	2/5/27/28	0/3/3/3
1	MA6	A	1518	1	-	2/7/29/30	0/3/3/3
22	4SU	V	8	22	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	5/7/29/30	0/3/3/3

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	1915	3TD	C6-C5	12.38	1.49	1.35
1	A	1407	5MC	C6-C5	9.32	1.49	1.34
22	V	21	H2U	C2-N1	9.24	1.48	1.35
1	A	967	5MC	C6-C5	9.23	1.49	1.34
26	a	1915	3TD	C2-N1	9.15	1.49	1.37
26	a	1962	5MC	C6-C5	8.95	1.49	1.34
22	V	8	4SU	C4-N3	8.34	1.46	1.37
26	a	2449	H2U	C2-N1	8.07	1.47	1.35
22	V	8	4SU	C2-N3	7.11	1.50	1.38
1	A	1402	4OC	C4-N3	6.70	1.44	1.32
26	a	2030	6MZ	C6-N6	6.69	1.46	1.35
1	A	1498	UR3	C2-N1	6.63	1.48	1.38
26	a	1618	6MZ	C6-N6	6.61	1.45	1.35
22	V	8	4SU	C2-N1	6.50	1.48	1.38
26	a	1962	5MC	C4-N3	6.39	1.44	1.34
1	A	967	5MC	C4-N3	6.28	1.44	1.34
1	A	967	5MC	C2-N3	6.25	1.49	1.36
26	a	1962	5MC	C2-N3	6.24	1.49	1.36
26	a	2498	OMC	C6-C5	6.24	1.49	1.35
26	a	2498	OMC	C2-N3	6.19	1.48	1.36
1	A	1402	4OC	C6-C5	6.16	1.49	1.35
26	a	2498	OMC	C4-N4	6.13	1.48	1.33
1	A	1407	5MC	C2-N3	6.02	1.48	1.36
22	V	21	H2U	C2-N3	5.96	1.48	1.38
1	A	1407	5MC	C4-N3	5.89	1.44	1.34
1	A	1498	UR3	C6-C5	5.87	1.48	1.35
26	a	2552	OMU	C2-N1	5.84	1.47	1.38
22	V	8	4SU	C6-C5	5.77	1.48	1.35
1	A	1402	4OC	C2-N3	5.72	1.47	1.36
26	a	2552	OMU	C2-N3	5.67	1.48	1.38
26	a	1915	3TD	C6-N1	5.66	1.45	1.36
26	a	2449	H2U	C2-N3	5.49	1.47	1.38
26	a	1915	3TD	C5'-C4'	-5.21	1.35	1.51
1	A	1498	UR3	C2-N3	5.10	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	2498	OMC	C4-N3	5.01	1.44	1.34
37	l	81	4D4	CZ-NE	4.77	1.42	1.33
26	a	2552	OMU	O2-C2	-4.76	1.14	1.23
26	a	2552	OMU	C6-C5	4.57	1.45	1.35
1	A	967	5MC	C6-N1	4.52	1.45	1.38
22	V	21	H2U	C4-N3	4.52	1.45	1.37
1	A	1407	5MC	C6-N1	4.52	1.45	1.38
26	a	1915	3TD	C2-N3	4.51	1.48	1.38
1	A	1407	5MC	C4-N4	4.40	1.45	1.34
1	A	967	5MC	C4-N4	4.40	1.45	1.34
26	a	1962	5MC	C4-N4	4.38	1.45	1.34
26	a	1962	5MC	C6-N1	4.36	1.45	1.38
22	V	8	4SU	C4-S4	-4.35	1.60	1.68
1	A	1402	4OC	C4-N4	4.30	1.44	1.35
22	V	8	4SU	C5-C4	4.30	1.48	1.42
26	a	2498	OMC	C2-N1	4.24	1.49	1.40
26	a	2504	PSU	C6-C5	4.07	1.40	1.35
26	a	2449	H2U	C4-N3	4.03	1.44	1.37
1	A	527	G7M	C5-C4	3.93	1.46	1.39
26	a	1962	5MC	C2-N1	3.90	1.48	1.40
1	A	967	5MC	C2-N1	3.85	1.48	1.40
26	a	2069	G7M	C5-C4	3.81	1.46	1.39
1	A	1402	4OC	C5-C4	3.78	1.48	1.40
1	A	1402	4OC	C2-N1	3.77	1.48	1.40
26	a	2605	PSU	C6-C5	3.71	1.39	1.35
26	a	2552	OMU	O4-C4	-3.70	1.17	1.24
22	V	56	PSU	C6-C5	3.70	1.39	1.35
26	a	2457	PSU	C6-C5	3.64	1.39	1.35
1	A	1407	5MC	C2-N1	3.60	1.47	1.40
1	A	516	PSU	C6-C5	3.52	1.39	1.35
1	A	1498	UR3	C6-N1	3.51	1.46	1.38
26	a	2604	PSU	C6-C5	3.46	1.39	1.35
26	a	1917	PSU	C6-C5	3.45	1.39	1.35
26	a	2580	PSU	C6-C5	3.36	1.39	1.35
26	a	2457	PSU	C4-N3	-3.30	1.32	1.38
26	a	2498	OMC	O2-C2	-3.21	1.17	1.23
26	a	2498	OMC	C6-N1	3.17	1.45	1.38
26	a	746	PSU	C6-C5	3.17	1.39	1.35
26	a	1911	PSU	C6-C5	3.14	1.39	1.35
1	A	1402	4OC	O2-C2	-3.12	1.17	1.23
26	a	2552	OMU	C4-N3	3.11	1.44	1.38
1	A	516	PSU	C4-N3	-3.04	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	O2-C2	-3.03	1.17	1.22
22	V	55	5MU	C4-N3	-3.03	1.33	1.38
26	a	2030	6MZ	C5-C4	-3.02	1.32	1.40
26	a	1962	5MC	O2-C2	-2.99	1.18	1.23
1	A	1407	5MC	O2-C2	-2.97	1.18	1.23
1	A	967	5MC	O2-C2	-2.95	1.18	1.23
22	V	8	4SU	C6-N1	2.93	1.45	1.38
26	a	1618	6MZ	C5-C4	-2.88	1.33	1.40
1	A	1402	4OC	C6-N1	2.88	1.44	1.38
26	a	955	PSU	C6-C5	2.86	1.38	1.35
22	V	56	PSU	C4-N3	-2.85	1.33	1.38
26	a	2605	PSU	C4-N3	-2.84	1.33	1.38
26	a	2580	PSU	C4-N3	-2.82	1.33	1.38
26	a	1917	PSU	C4-N3	-2.82	1.33	1.38
26	a	747	5MU	C2-N1	2.79	1.42	1.38
26	a	2604	PSU	C4-N3	-2.78	1.33	1.38
26	a	747	5MU	C4-N3	-2.77	1.33	1.38
26	a	1939	5MU	C4-N3	-2.68	1.33	1.38
1	A	1207	2MG	C6-N1	-2.67	1.33	1.37
1	A	1498	UR3	O4-C4	-2.66	1.17	1.23
26	a	2445	2MG	C6-N1	-2.65	1.33	1.37
22	V	55	5MU	C6-C5	2.65	1.38	1.34
26	a	1939	5MU	C6-C5	2.64	1.38	1.34
26	a	747	5MU	C6-C5	2.63	1.38	1.34
26	a	2251	OMG	C6-N1	-2.63	1.34	1.37
26	a	2449	H2U	O2-C2	-2.62	1.18	1.23
26	a	1915	3TD	O4-C4	-2.61	1.17	1.23
26	a	2504	PSU	C4-N3	-2.60	1.34	1.38
26	a	746	PSU	C4-N3	-2.60	1.34	1.38
1	A	527	G7M	C6-N1	-2.59	1.34	1.37
26	a	2552	OMU	C6-N1	2.58	1.44	1.38
1	A	966	2MG	C6-N1	-2.58	1.34	1.37
26	a	2449	H2U	O4-C4	-2.57	1.18	1.23
26	a	2069	G7M	C6-N1	-2.57	1.34	1.37
1	A	1519	MA6	C5-C4	2.56	1.47	1.40
1	A	1498	UR3	C5-C4	2.52	1.50	1.43
1	A	1516	2MG	C6-N1	-2.50	1.34	1.37
26	a	1915	3TD	C4-N3	2.49	1.45	1.40
26	a	1917	PSU	C2'-C1'	-2.49	1.50	1.53
26	a	1835	2MG	C6-N1	-2.45	1.34	1.37
1	A	1518	MA6	C5-C4	2.41	1.47	1.40
26	a	1939	5MU	C4-C5	2.39	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	55	5MU	C2-N3	-2.38	1.33	1.38
26	a	747	5MU	C4-C5	2.37	1.48	1.44
22	V	21	H2U	O2-C2	-2.35	1.18	1.23
26	a	2457	PSU	C2-N3	-2.31	1.33	1.37
1	A	1516	2MG	O4'-C1'	2.27	1.44	1.41
22	V	55	5MU	C2-N1	2.26	1.42	1.38
1	A	1519	MA6	O3'-C3'	2.25	1.48	1.43
26	a	1939	5MU	C2-N3	-2.22	1.34	1.38
26	a	2251	OMG	O4'-C1'	2.21	1.44	1.41
26	a	1939	5MU	C2-N1	2.21	1.42	1.38
37	l	81	4D4	CZ-NH1	2.17	1.43	1.34
22	V	21	H2U	O4-C4	-2.16	1.18	1.23
1	A	1518	MA6	C6-N1	2.16	1.36	1.33
1	A	1518	MA6	C2'-C1'	-2.15	1.50	1.53
26	a	955	PSU	C4-C5	-2.14	1.38	1.44
26	a	2498	OMC	C5-C4	2.14	1.47	1.42
26	a	1618	6MZ	C2-N3	2.14	1.35	1.32
26	a	1939	5MU	C6-N1	-2.12	1.34	1.38
1	A	1519	MA6	O4'-C1'	2.12	1.44	1.41
1	A	1207	2MG	O4'-C1'	2.11	1.44	1.41
26	a	2030	6MZ	C2-N3	2.10	1.35	1.32
26	a	2503	2MA	C2-N3	2.07	1.35	1.31
26	a	1911	PSU	C4-C5	-2.07	1.38	1.44
22	V	56	PSU	C2-N3	-2.06	1.34	1.37
22	V	55	5MU	C6-N1	-2.06	1.34	1.38
26	a	2552	OMU	C5-C4	2.05	1.48	1.43
22	V	55	5MU	C4-C5	2.03	1.48	1.44
26	a	2605	PSU	C2-N3	-2.03	1.34	1.37
1	A	516	PSU	C2-N3	-2.01	1.34	1.37

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	8	4SU	C4-N3-C2	-7.93	119.64	127.34
26	a	2449	H2U	C4-N3-C2	-6.97	120.01	125.79
1	A	1518	MA6	N1-C6-N6	6.69	124.10	117.06
22	V	21	H2U	C4-N3-C2	-6.58	120.33	125.79
26	a	2457	PSU	N1-C2-N3	6.39	122.37	115.13
1	A	516	PSU	N1-C2-N3	6.23	122.19	115.13
26	a	2504	PSU	N1-C2-N3	6.03	121.97	115.13
26	a	746	PSU	N1-C2-N3	6.00	121.93	115.13
26	a	2604	PSU	N1-C2-N3	5.99	121.91	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	1917	PSU	N1-C2-N3	5.96	121.89	115.13
22	V	56	PSU	N1-C2-N3	5.84	121.74	115.13
26	a	2605	PSU	N1-C2-N3	5.84	121.74	115.13
26	a	2580	PSU	N1-C2-N3	5.77	121.67	115.13
26	a	2552	OMU	C4-N3-C2	-5.66	119.11	126.58
22	V	8	4SU	C5-C4-N3	5.57	119.85	114.69
26	a	1618	6MZ	N3-C2-N1	-5.50	120.09	128.68
26	a	747	5MU	N3-C2-N1	5.47	122.16	114.89
26	a	2030	6MZ	N3-C2-N1	-5.25	120.47	128.68
26	a	1939	5MU	C4-N3-C2	-5.22	120.59	127.35
26	a	2030	6MZ	C9-N6-C6	-5.21	118.39	122.87
26	a	1939	5MU	N3-C2-N1	5.07	121.61	114.89
26	a	1915	3TD	N1-C2-N3	4.93	120.03	116.14
26	a	1618	6MZ	C9-N6-C6	-4.91	118.64	122.87
26	a	1911	PSU	C4-N3-C2	-4.86	119.34	126.34
26	a	747	5MU	C4-N3-C2	-4.83	121.09	127.35
26	a	1911	PSU	N1-C2-N3	4.80	120.56	115.13
1	A	1498	UR3	C4-N3-C2	-4.79	120.06	124.56
26	a	955	PSU	N1-C2-N3	4.74	120.50	115.13
26	a	955	PSU	C4-N3-C2	-4.69	119.58	126.34
26	a	1939	5MU	C5-C4-N3	4.57	119.21	115.31
22	V	8	4SU	C5-C4-S4	-4.42	118.77	124.47
22	V	55	5MU	N3-C2-N1	4.41	120.74	114.89
12	L	89	D2T	OD2-CG-CB	4.11	122.04	113.15
26	a	2552	OMU	N3-C2-N1	4.09	120.32	114.89
26	a	2605	PSU	C4-N3-C2	-3.74	120.95	126.34
1	A	1407	5MC	C5-C6-N1	-3.69	119.55	123.34
26	a	1939	5MU	C5-C6-N1	-3.67	119.57	123.34
26	a	2504	PSU	C4-N3-C2	-3.66	121.06	126.34
26	a	747	5MU	C5-C4-N3	3.63	118.41	115.31
22	V	8	4SU	N3-C2-N1	3.63	119.70	114.89
26	a	2552	OMU	C5-C4-N3	3.61	120.25	114.84
26	a	2449	H2U	N3-C2-N1	3.61	120.47	116.65
22	V	21	H2U	N3-C2-N1	3.59	120.45	116.65
22	V	55	5MU	C4-N3-C2	-3.59	122.70	127.35
1	A	516	PSU	C4-N3-C2	-3.56	121.20	126.34
26	a	1939	5MU	O4-C4-C5	-3.56	120.77	124.90
26	a	1915	3TD	C4-N3-C2	-3.56	120.74	124.61
26	a	746	PSU	C4-N3-C2	-3.56	121.22	126.34
26	a	2604	PSU	C4-N3-C2	-3.50	121.29	126.34
1	A	1519	MA6	C4-C5-N7	-3.49	105.76	109.40
26	a	746	PSU	O2-C2-N1	-3.46	118.98	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	966	2MG	C3'-C2'-C1'	3.43	106.14	100.98
26	a	1618	6MZ	C2-N1-C6	3.42	119.52	116.59
37	l	81	4D4	O-C-CA	-3.39	115.90	124.78
26	a	2457	PSU	C4-N3-C2	-3.38	121.46	126.34
26	a	2580	PSU	C4-N3-C2	-3.38	121.47	126.34
1	A	967	5MC	C5-C6-N1	-3.37	119.87	123.34
26	a	2580	PSU	O2-C2-N1	-3.37	119.08	122.79
26	a	2504	PSU	O2-C2-N1	-3.34	119.11	122.79
22	V	55	5MU	C5-C4-N3	3.33	118.15	115.31
22	V	56	PSU	C4-N3-C2	-3.32	121.56	126.34
1	A	1519	MA6	C9-N6-C6	-3.32	109.47	119.51
26	a	1917	PSU	C4-N3-C2	-3.30	121.58	126.34
26	a	2504	PSU	C6-C5-C4	-3.29	115.90	118.20
26	a	2604	PSU	C3'-C2'-C1'	3.28	105.45	101.64
26	a	1917	PSU	O2-C2-N1	-3.27	119.19	122.79
1	A	516	PSU	O2-C2-N1	-3.26	119.20	122.79
26	a	747	5MU	O4-C4-C5	-3.23	121.16	124.90
1	A	1518	MA6	N3-C2-N1	-3.22	123.64	128.68
26	a	1962	5MC	C5-C6-N1	-3.21	120.04	123.34
26	a	2580	PSU	C3'-C2'-C1'	3.16	105.32	101.64
26	a	2604	PSU	O2-C2-N1	-3.15	119.32	122.79
26	a	2449	H2U	C5-C4-N3	3.10	120.13	116.65
26	a	746	PSU	C3'-C2'-C1'	3.04	105.17	101.64
26	a	2605	PSU	O2-C2-N1	-3.00	119.49	122.79
26	a	1618	6MZ	C1'-N9-C4	-2.98	121.41	126.64
22	V	55	5MU	O4-C4-C5	-2.93	121.51	124.90
26	a	2030	6MZ	C2-N1-C6	2.93	119.10	116.59
26	a	2449	H2U	O2-C2-N1	-2.92	119.44	123.11
26	a	2552	OMU	O4-C4-C5	-2.90	120.06	125.16
26	a	745	1MG	C3'-C2'-C1'	2.89	105.33	100.98
1	A	1518	MA6	C3'-C2'-C1'	2.88	105.32	100.98
26	a	955	PSU	O2-C2-N1	-2.88	119.62	122.79
1	A	1519	MA6	C10-N6-C9	-2.82	107.05	116.12
1	A	1519	MA6	N3-C2-N1	-2.81	124.29	128.68
12	L	89	D2T	OD1-CG-CB	-2.80	116.59	122.44
26	a	955	PSU	C6-N1-C2	-2.77	119.85	122.68
1	A	1518	MA6	C10-N6-C6	-2.77	111.12	119.51
22	V	21	H2U	C5-C4-N3	2.76	119.75	116.65
37	l	81	4D4	NE-CZ-NH2	2.75	125.53	120.70
26	a	2030	6MZ	C1'-N9-C4	-2.75	121.81	126.64
26	a	747	5MU	C5-C6-N1	-2.75	120.51	123.34
26	a	1915	3TD	O4'-C4'-C5'	-2.74	100.36	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	2457	PSU	O2-C2-N1	-2.74	119.78	122.79
1	A	1519	MA6	C10-N6-C6	-2.71	111.30	119.51
1	A	1498	UR3	C1'-N1-C2	2.66	121.48	116.99
1	A	1518	MA6	C9-N6-C6	-2.65	111.48	119.51
22	V	56	PSU	O2-C2-N1	-2.62	119.90	122.79
26	a	2449	H2U	C5-C6-N1	2.59	120.15	111.61
22	V	21	H2U	C5-C6-N1	2.57	120.08	111.61
26	a	747	5MU	O2-C2-N3	-2.56	116.74	121.50
26	a	2605	PSU	C6-C5-C4	-2.54	116.42	118.20
1	A	966	2MG	C5-C6-N1	2.53	118.42	113.95
26	a	1917	PSU	C3'-C2'-C1'	2.53	104.58	101.64
26	a	745	1MG	C5-C6-N1	2.47	117.61	113.90
12	L	89	D2T	CB-CA-N	2.46	114.34	109.10
26	a	1911	PSU	O2-C2-N1	-2.45	120.09	122.79
26	a	2503	2MA	C3'-C2'-C1'	2.45	104.66	100.98
1	A	1207	2MG	C5-C6-N1	2.44	118.25	113.95
1	A	1516	2MG	C5-C6-N1	2.43	118.25	113.95
26	a	2251	OMG	C5-C6-N1	2.43	118.25	113.95
26	a	2069	G7M	C2'-C3'-C4'	-2.43	97.92	102.64
26	a	1915	3TD	C5'-C4'-C3'	2.42	124.24	115.18
26	a	2503	2MA	C5-C6-N1	2.41	118.17	114.02
26	a	1835	2MG	C5-C6-N1	2.40	118.19	113.95
22	V	21	H2U	O2-C2-N1	-2.38	120.12	123.11
26	a	747	5MU	C6-N1-C2	-2.37	118.90	121.30
26	a	745	1MG	C8-N7-C5	2.37	107.50	102.99
29	d	150	MEQ	CB-CG-CD	-2.34	107.81	113.04
1	A	1402	4OC	CM4-N4-C4	-2.32	117.92	122.45
22	V	8	4SU	C1'-N1-C2	2.31	121.75	117.57
22	V	55	5MU	C3'-C2'-C1'	2.30	105.80	101.43
26	a	1911	PSU	C6-N1-C2	-2.28	120.36	122.68
26	a	1917	PSU	C6-C5-C4	-2.27	116.61	118.20
26	a	2445	2MG	C5-C6-N1	2.26	117.94	113.95
26	a	747	5MU	O4'-C1'-N1	2.25	113.52	108.36
26	a	1939	5MU	O5'-C5'-C4'	2.24	116.62	108.99
26	a	2504	PSU	O3'-C3'-C4'	2.24	117.52	111.05
22	V	8	4SU	O2-C2-N1	-2.23	119.82	122.79
26	a	2503	2MA	C8-N7-C5	2.23	107.24	102.99
26	a	1939	5MU	O2-C2-N1	-2.22	119.83	122.79
26	a	745	1MG	O6-C6-C5	-2.21	120.27	124.19
1	A	966	2MG	C8-N7-C5	2.21	107.21	102.99
1	A	1207	2MG	C8-N7-C5	2.20	107.18	102.99
26	a	747	5MU	C5M-C5-C6	-2.20	119.92	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1518	MA6	C4-C5-N7	-2.19	107.11	109.40
26	a	1835	2MG	C8-N7-C5	2.19	107.16	102.99
1	A	1402	4OC	C6-C5-C4	2.18	119.63	116.96
26	a	2445	2MG	O5'-C5'-C4'	-2.17	101.61	108.99
26	a	747	5MU	C5M-C5-C4	2.17	121.15	118.77
1	A	1519	MA6	N1-C6-N6	2.16	119.33	117.06
26	a	2251	OMG	C8-N7-C5	2.12	107.03	102.99
22	V	55	5MU	C5-C6-N1	-2.11	121.17	123.34
26	a	2457	PSU	O2-C2-N3	-2.11	117.84	121.82
1	A	1519	MA6	O3'-C3'-C2'	2.09	118.58	111.82
26	a	1911	PSU	C6-C5-C4	2.08	119.65	118.20
22	V	55	5MU	O2-C2-N3	-2.08	117.63	121.50
12	L	89	D2T	O-C-CA	-2.07	119.34	124.78
1	A	1518	MA6	C10-N6-C9	-2.06	109.48	116.12
26	a	1939	5MU	C2'-C3'-C4'	2.06	106.64	102.64
26	a	2445	2MG	C8-N7-C5	2.04	106.87	102.99
11	K	119	IAS	OD1-CG-CB	-2.02	119.53	125.43
26	a	2457	PSU	C3'-C2'-C1'	2.00	103.97	101.64

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1207	2MG	N1-C2-N2-CM2
1	A	1207	2MG	N3-C2-N2-CM2
1	A	1498	UR3	O4'-C1'-N1-C6
1	A	1498	UR3	O4'-C1'-N1-C2
1	A	1518	MA6	C5-C6-N6-C9
1	A	1519	MA6	C5-C6-N6-C9
1	A	1519	MA6	C5-C6-N6-C10
1	A	1519	MA6	N1-C6-N6-C9
12	L	89	D2T	CA-CB-SB-CB1
12	L	89	D2T	SB-CB-CG-OD2
22	V	21	H2U	O4'-C4'-C5'-O5'
22	V	21	H2U	C3'-C4'-C5'-O5'
22	V	21	H2U	O4'-C1'-N1-C6
22	V	21	H2U	C2'-C1'-N1-C2
22	V	21	H2U	C2'-C1'-N1-C6
26	a	746	PSU	O4'-C1'-C5-C4
26	a	746	PSU	O4'-C1'-C5-C6
26	a	1618	6MZ	C5-C6-N6-C9
26	a	1618	6MZ	N1-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
26	a	1618	6MZ	O4'-C4'-C5'-O5'
26	a	1915	3TD	C2'-C1'-C5-C4
26	a	1915	3TD	O4'-C1'-C5-C4
26	a	1915	3TD	O4'-C1'-C5-C6
26	a	1915	3TD	C3'-C4'-C5'-O5'
26	a	1915	3TD	O4'-C4'-C5'-O5'
26	a	1939	5MU	C3'-C4'-C5'-O5'
26	a	1939	5MU	O4'-C4'-C5'-O5'
26	a	2030	6MZ	C3'-C4'-C5'-O5'
26	a	2069	G7M	O4'-C4'-C5'-O5'
26	a	2069	G7M	C3'-C4'-C5'-O5'
26	a	2251	OMG	C1'-C2'-O2'-CM2
26	a	2445	2MG	C3'-C4'-C5'-O5'
26	a	2504	PSU	O4'-C4'-C5'-O5'
26	a	2552	OMU	O4'-C1'-N1-C2
26	a	2552	OMU	O4'-C1'-N1-C6
26	a	2552	OMU	C1'-C2'-O2'-CM2
26	a	2604	PSU	C3'-C4'-C5'-O5'
26	a	2604	PSU	O4'-C4'-C5'-O5'
26	a	1618	6MZ	C3'-C4'-C5'-O5'
26	a	2498	OMC	C3'-C4'-C5'-O5'
26	a	2504	PSU	C3'-C4'-C5'-O5'
1	A	967	5MC	O4'-C4'-C5'-O5'
26	a	2030	6MZ	O4'-C4'-C5'-O5'
26	a	2498	OMC	O4'-C4'-C5'-O5'
26	a	1835	2MG	O4'-C4'-C5'-O5'
26	a	2445	2MG	O4'-C4'-C5'-O5'
29	d	150	MEQ	OE1-CD-CG-CB
29	d	150	MEQ	NE2-CD-CG-CB
26	a	1835	2MG	C3'-C4'-C5'-O5'
22	V	21	H2U	O4'-C1'-N1-C2
1	A	1518	MA6	N1-C6-N6-C9
1	A	1519	MA6	C4'-C5'-O5'-P
1	A	527	G7M	C4'-C5'-O5'-P
26	a	747	5MU	C4'-C5'-O5'-P
26	a	1915	3TD	C4'-C5'-O5'-P
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
11	K	119	IAS	CA-CB-CG-OD1
26	a	1962	5MC	C2'-C1'-N1-C6
1	A	1519	MA6	N1-C6-N6-C10
26	a	1962	5MC	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
26	a	2580	PSU	O4'-C4'-C5'-O5'
37	l	81	4D4	NE-CD-CG-CB
12	L	89	D2T	CG-CB-SB-CB1
22	V	21	H2U	C4'-C5'-O5'-P
26	a	2503	2MA	O4'-C4'-C5'-O5'
11	K	119	IAS	N-CA-CB-CG
37	l	81	4D4	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 316 ligands modelled in this entry, 315 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	FME	V	101	22	8,9,10	0.97	0	7,9,11	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	FME	V	101	22	-	5/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	V	101	FME	O1-CN-N-CA
58	V	101	FME	O-C-CA-CB
58	V	101	FME	CA-CB-CG-SD
58	V	101	FME	N-CA-CB-CG
58	V	101	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
37	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	82:MS6	C	83:MET	N	78.87

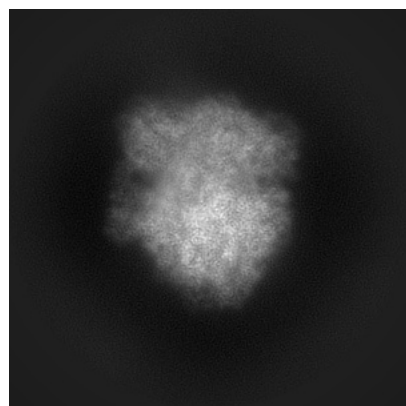
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12261. These allow visual inspection of the internal detail of the map and identification of artifacts.

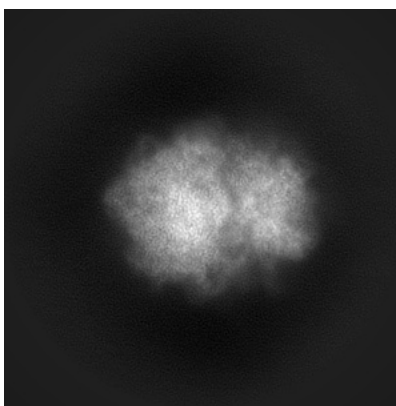
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

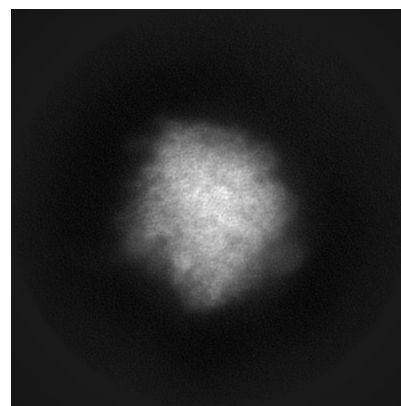
6.1.1 Primary map



X

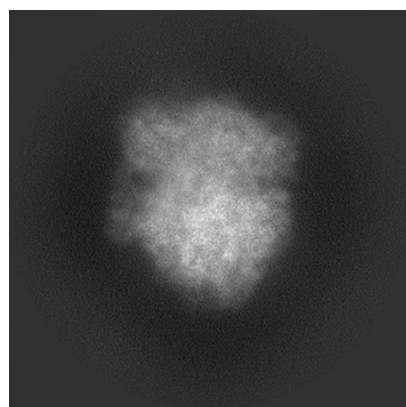


Y

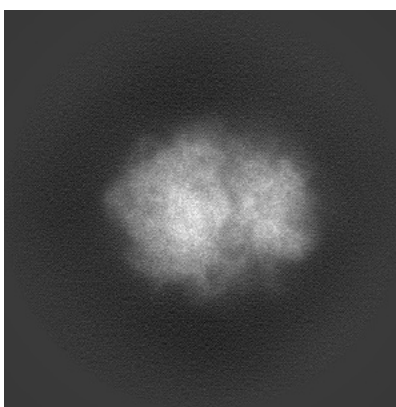


Z

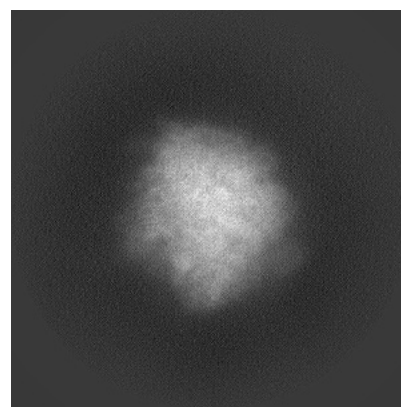
6.1.2 Raw map



X



Y

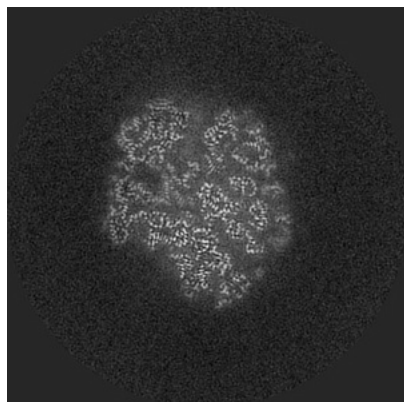


Z

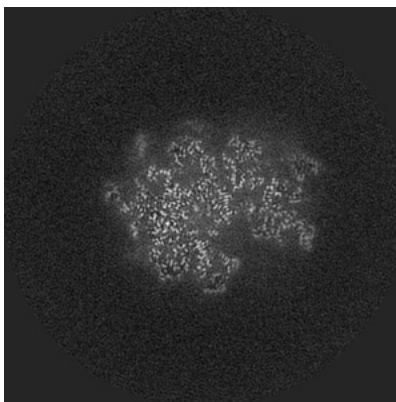
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

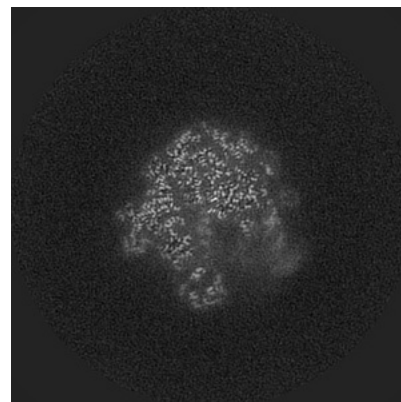
6.2.1 Primary map



X Index: 256

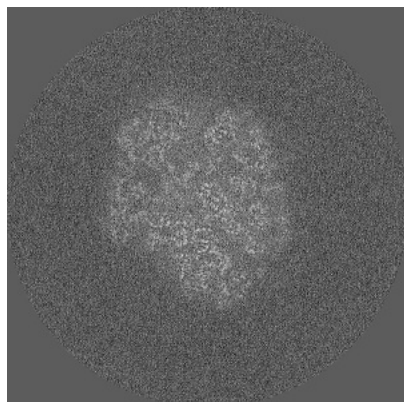


Y Index: 256

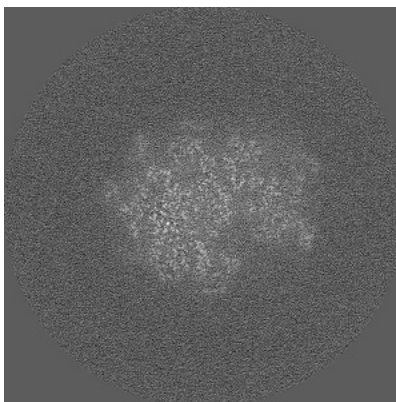


Z Index: 256

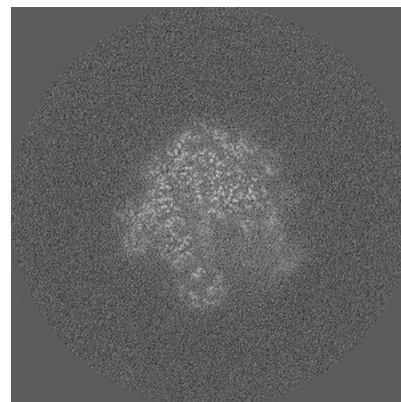
6.2.2 Raw map



X Index: 256



Y Index: 256

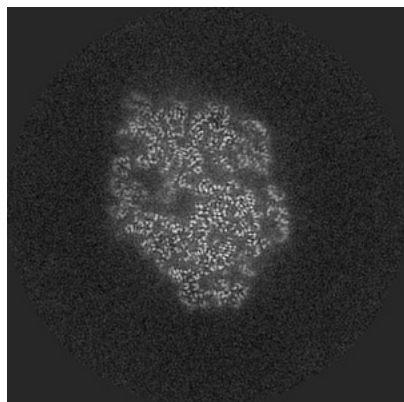


Z Index: 256

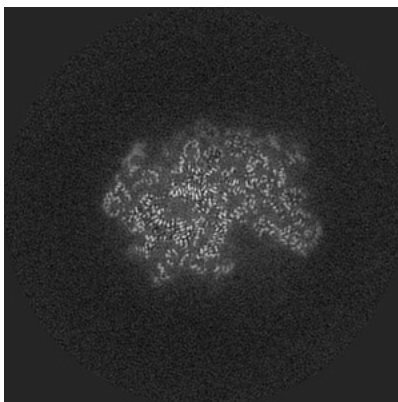
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

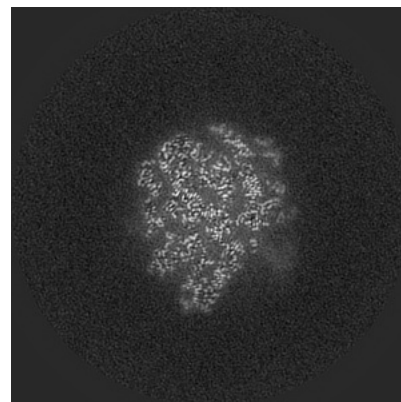
6.3.1 Primary map



X Index: 267

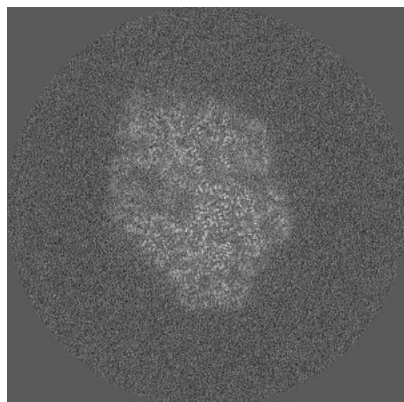


Y Index: 271

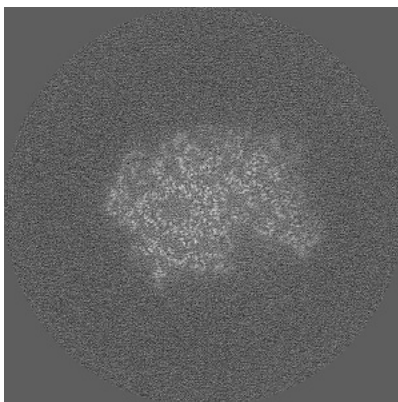


Z Index: 226

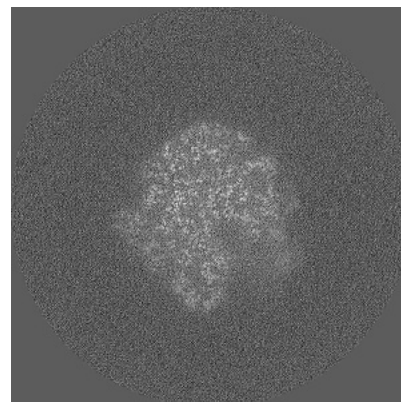
6.3.2 Raw map



X Index: 268



Y Index: 275

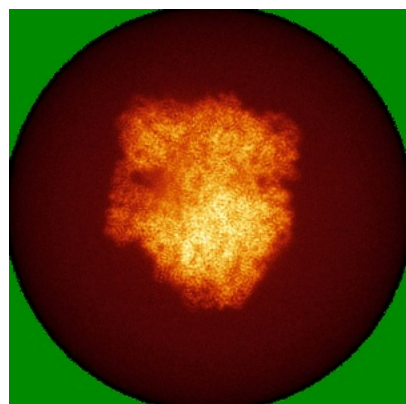


Z Index: 245

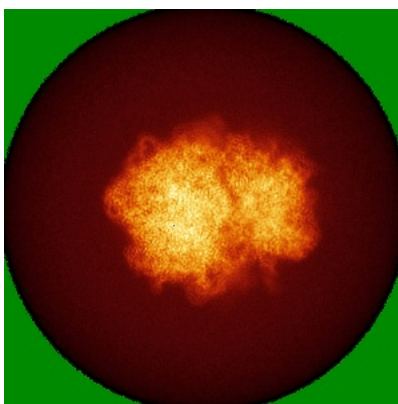
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

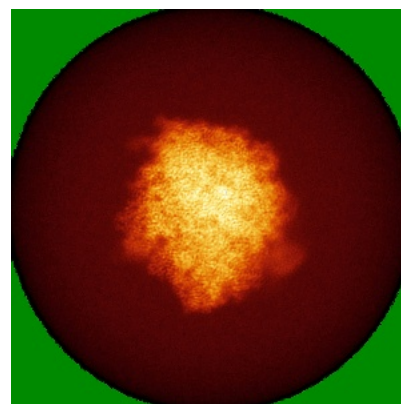
6.4.1 Primary map



X

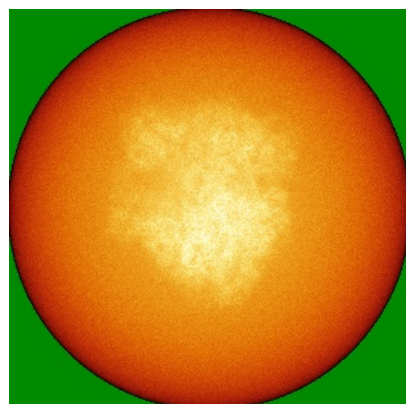


Y

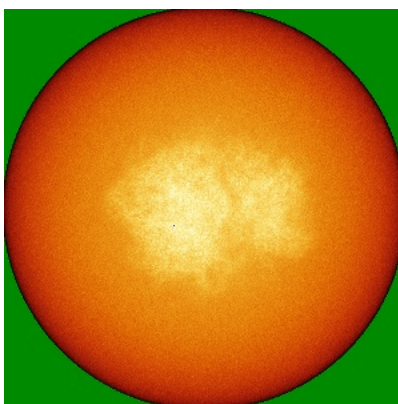


Z

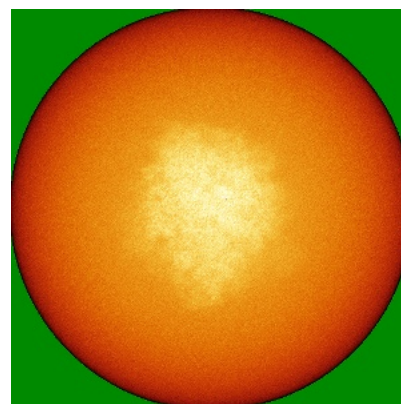
6.4.2 Raw map



X



Y



Z

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

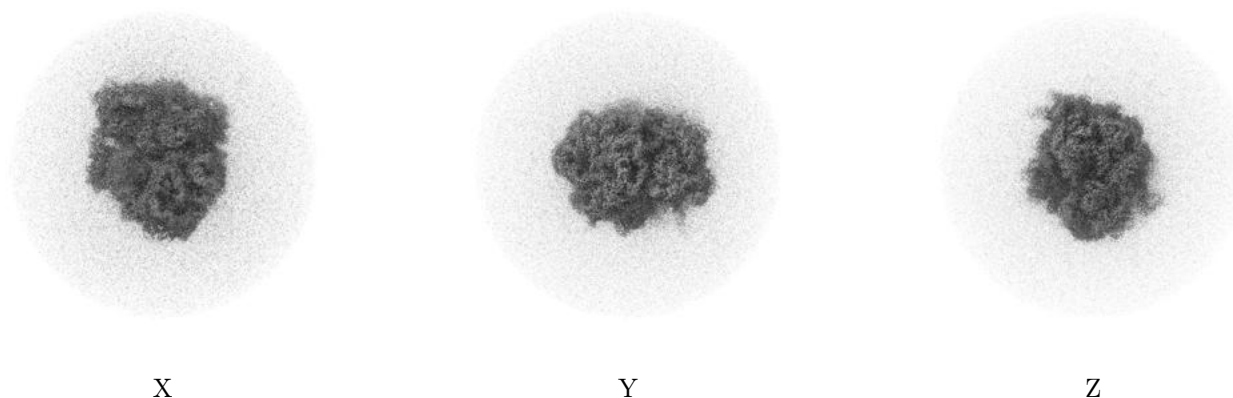
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

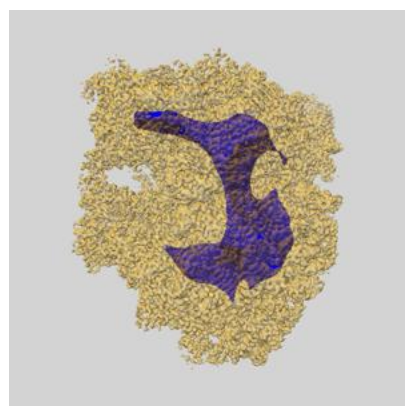
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

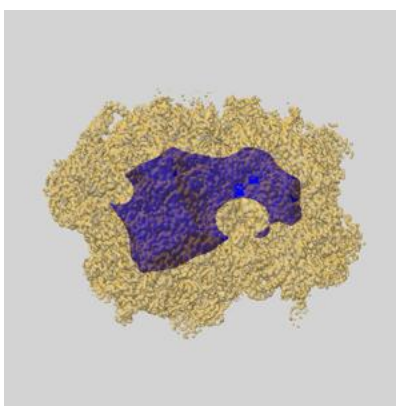
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

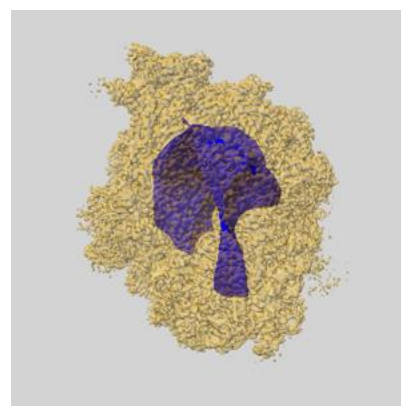
6.6.1 emd_12261_msk_1.map [i](#)



X



Y

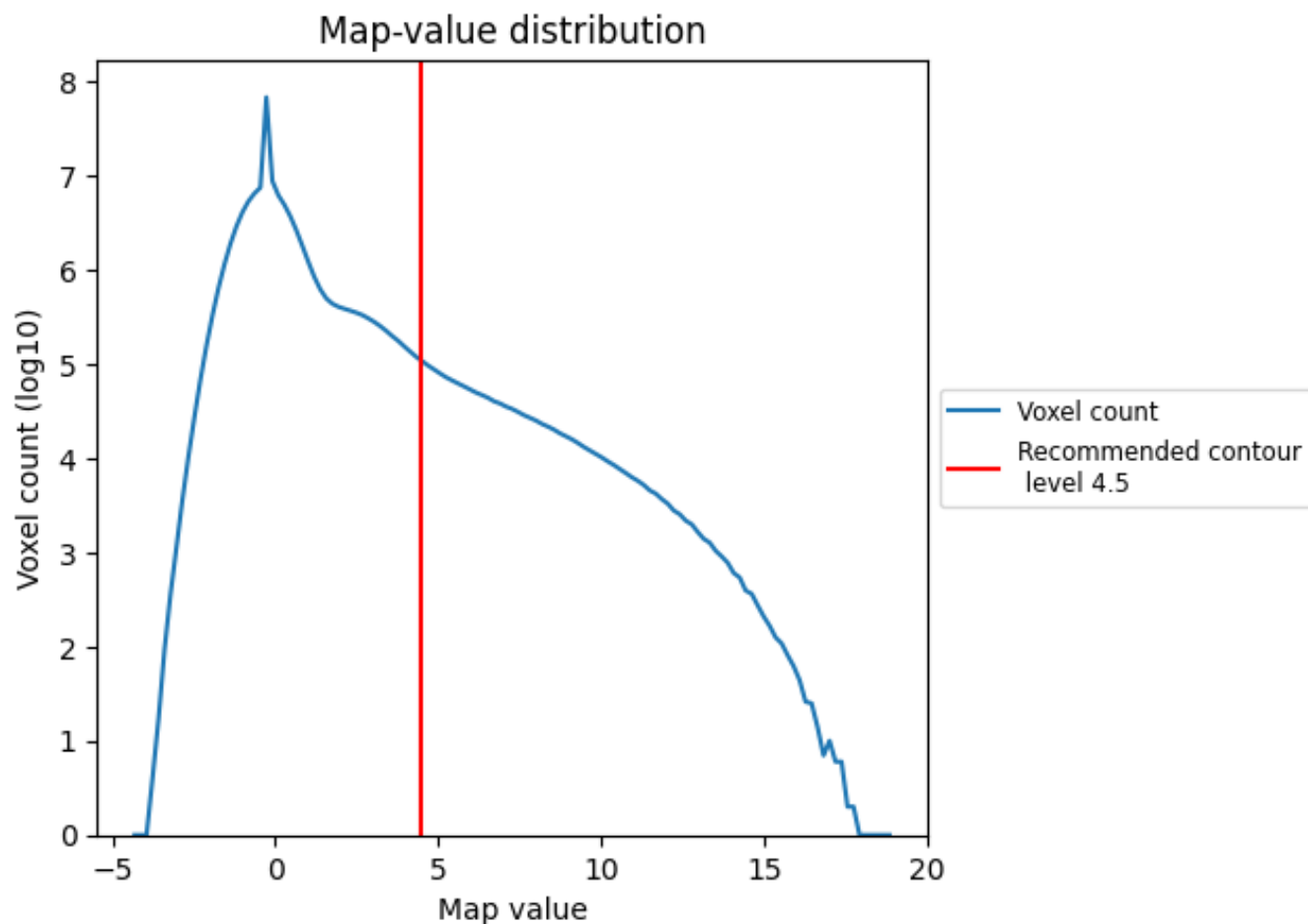


Z

7 Map analysis [i](#)

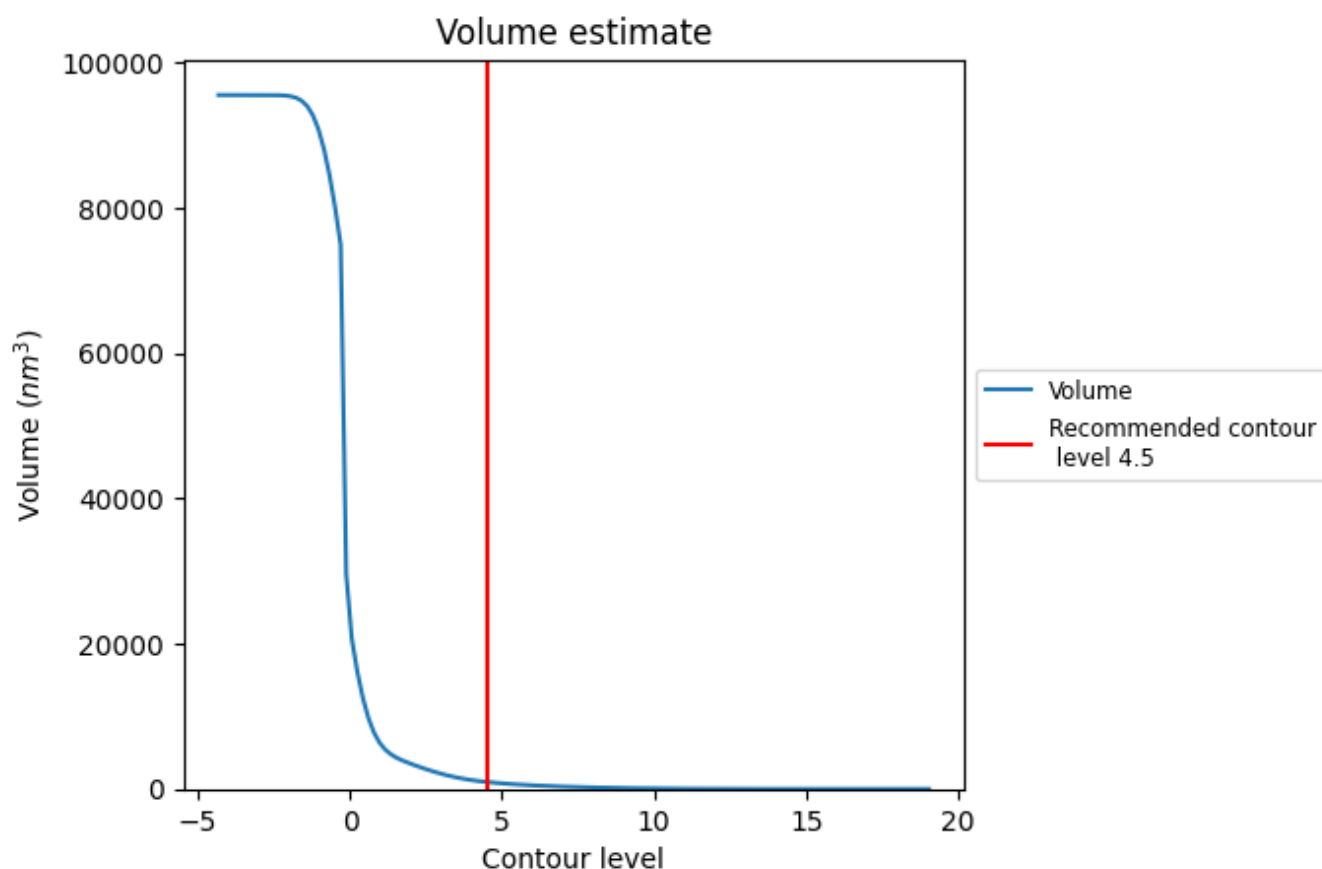
This section contains the results of statistical analysis of the map.

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.

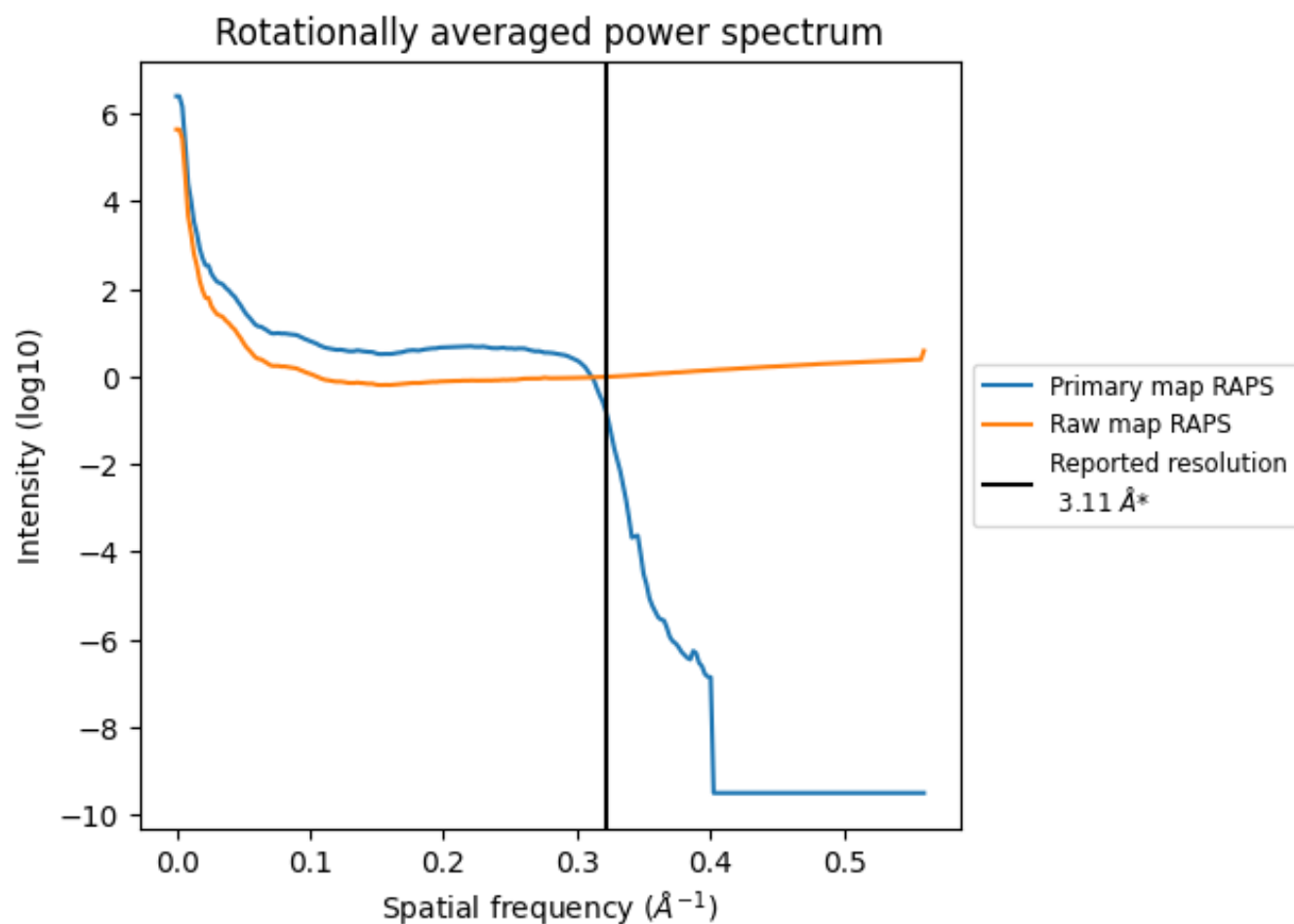
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 959 nm^3 ; this corresponds to an approximate mass of 867 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 ⓘ

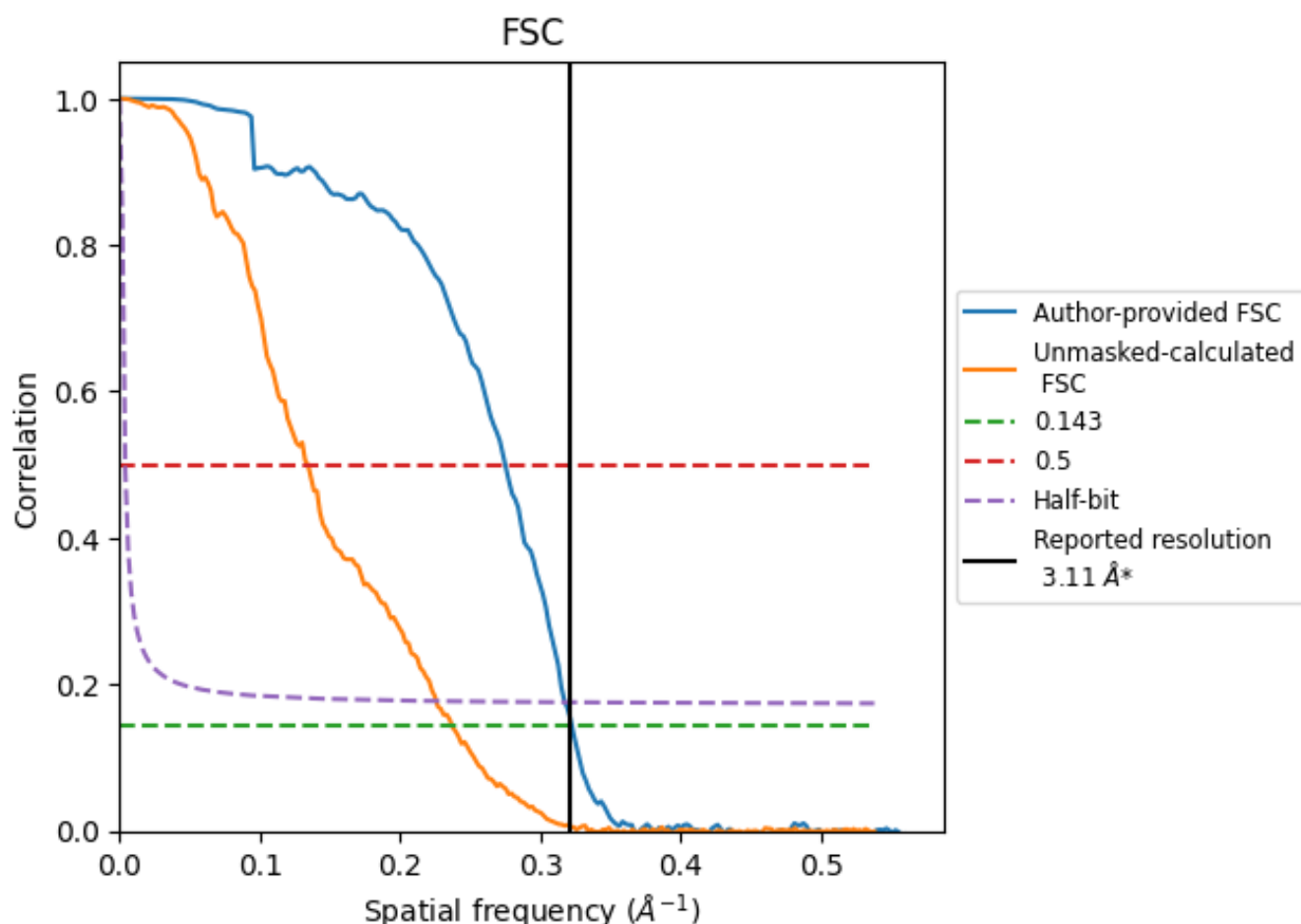


*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

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 0.322 Å⁻¹

8.2 Resolution estimates [i](#)

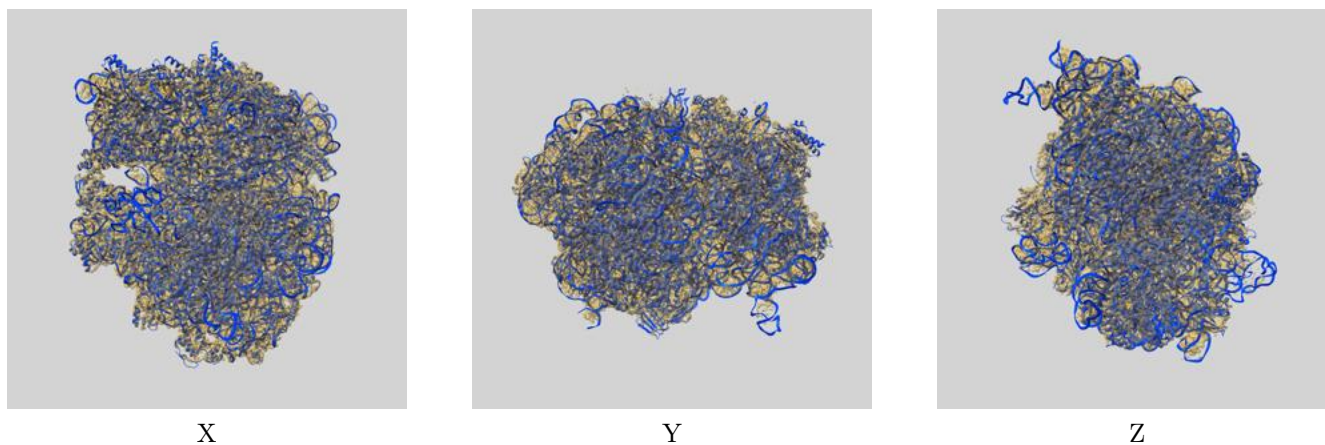
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.10	3.64	3.15
Unmasked-calculated*	4.22	7.45	4.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 3.11 by more than 10 %

9 Map-model fit [i](#)

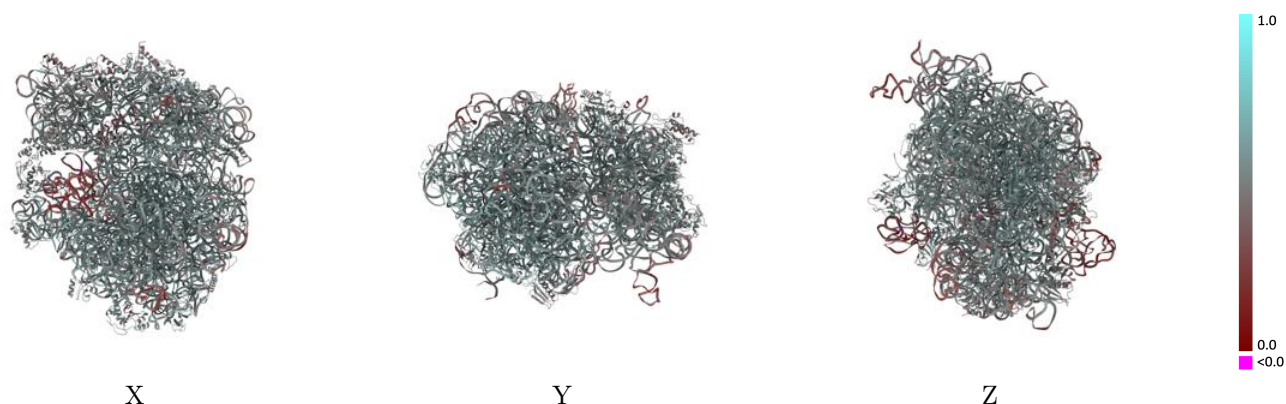
This section contains information regarding the fit between EMDB map EMD-12261 and PDB model 7NBU. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



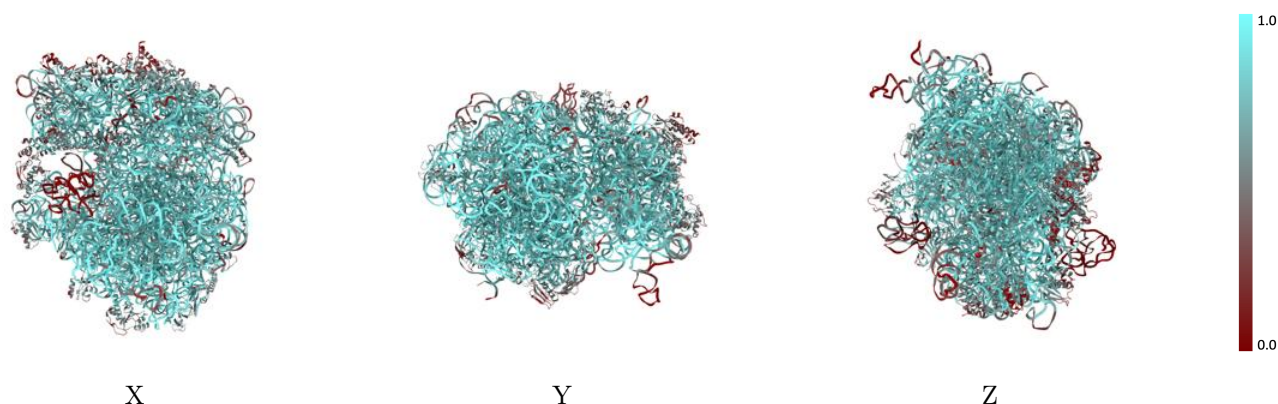
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



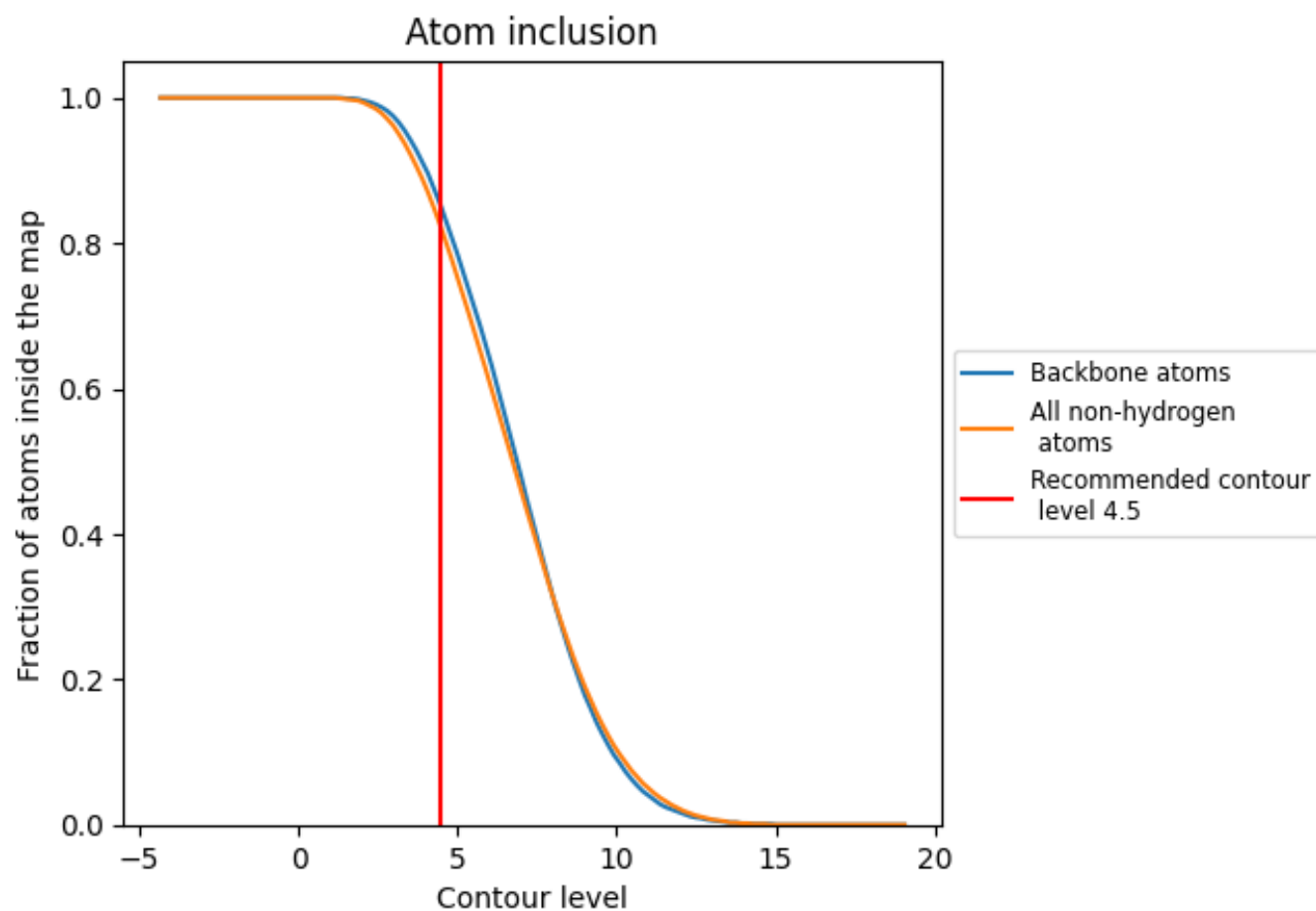
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 82% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.5210
0	 0.7430	 0.5470
1	 0.9490	 0.5690
2	 0.9230	 0.5710
3	 0.8770	 0.5800
A	 0.8640	 0.5130
B	 0.4110	 0.4710
C	 0.6620	 0.5210
D	 0.5910	 0.5040
E	 0.7560	 0.5430
F	 0.5990	 0.5010
G	 0.5350	 0.4760
H	 0.6710	 0.5300
I	 0.6120	 0.5060
J	 0.4970	 0.4690
K	 0.7420	 0.5280
L	 0.7770	 0.5360
M	 0.6000	 0.5090
N	 0.7120	 0.5230
O	 0.6970	 0.5200
P	 0.7100	 0.5320
Q	 0.6910	 0.5180
R	 0.6270	 0.4990
S	 0.5840	 0.4960
T	 0.6790	 0.5120
U	 0.4360	 0.4590
V	 0.9110	 0.4830
W	 0.5480	 0.4440
X	 0.5880	 0.4280
Y	 0.5760	 0.3740
Z	 0.7990	 0.5380
a	 0.8850	 0.5260
b	 0.8270	 0.5210
c	 0.9030	 0.5710
d	 0.7950	 0.5660



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Chain	Atom inclusion	Q-score
e	 0.6910	 0.5320
f	 0.5720	 0.4840
g	 0.4830	 0.4830
h	 0.5030	 0.4950
i	 0.8230	 0.5620
j	 0.8270	 0.5550
k	 0.7550	 0.5500
l	 0.6410	 0.5180
m	 0.8710	 0.5620
n	 0.6310	 0.5180
o	 0.7590	 0.5580
p	 0.8570	 0.5660
q	 0.6750	 0.5430
r	 0.8190	 0.5490
s	 0.7360	 0.5300
t	 0.6190	 0.5250
u	 0.6500	 0.5320
v	 0.8380	 0.5610
w	 0.8420	 0.5530
x	 0.6120	 0.5010
y	 0.7670	 0.5470
z	 0.8110	 0.5590