



Full wwPDB EM Validation Report ⓘ

Feb 23, 2022 – 01:02 pm GMT

PDB ID : 7OIG
EMDB ID : EMD-12929
Title : CspA-27 cotranslational folding intermediate 3
Authors : Agirrezabala, X.; Samatova, E.; Macher, M.; Liutkute, M.; Gil-Carton, D.;
Novacek, J.; Valle, M.; Rodnina, M.V.
Deposited on : 2021-05-11
Resolution : 3.20 Å(reported)
Based on initial model : 6ORE

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

EMDB validation analysis : 0.0.0.dev97
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

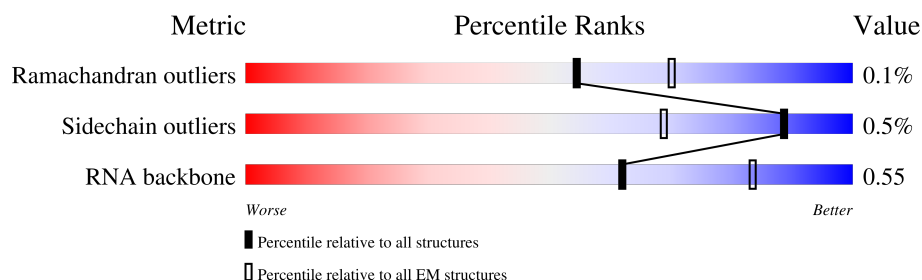
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	2903	
2	2	1534	
3	3	120	
4	4	6	
5	C	271	
6	D	209	
7	E	201	
8	F	177	

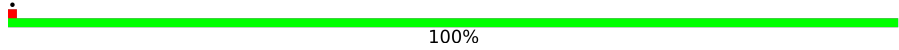
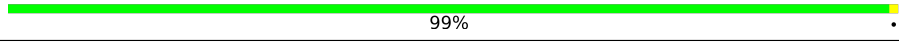
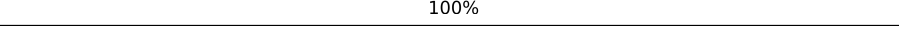
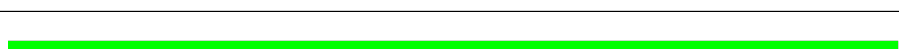

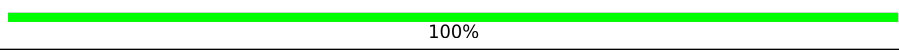
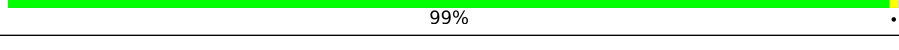
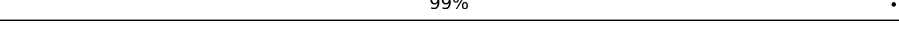
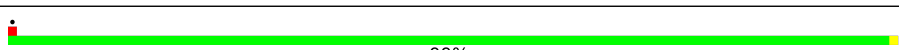

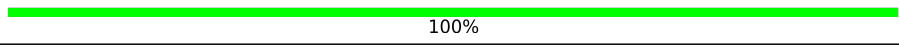
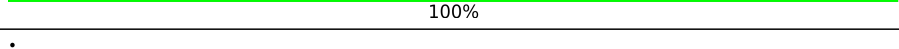
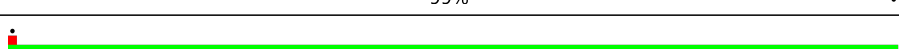
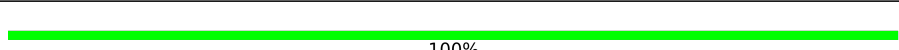
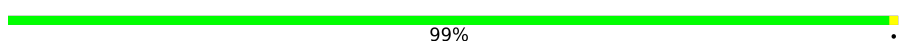
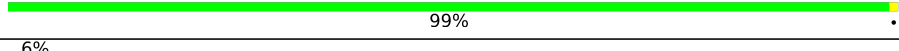
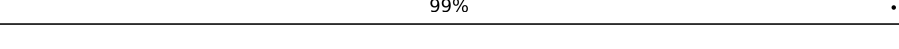





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Mol	Chain	Length	Quality of chain
9	G	175	100%
10	H	149	52% 97%
11	I	142	100%
12	J	123	99%
13	K	144	99%
14	L	136	99%
15	M	119	100%
16	N	116	99%
17	O	114	100%
18	P	117	99%
19	Q	103	98%
20	R	110	100%
21	S	94	100%
22	T	103	100%
23	U	94	100%
24	V	80	99%
25	W	77	100%
26	X	62	100%
27	Y	58	100%
28	Z	66	100%
29	a	56	100%
30	b	52	100%
31	c	46	100%
32	d	64	98%
33	e	38	100%

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Mol	Chain	Length	Quality of chain
34	f	225	 100%
35	g	208	 99%
36	h	205	 100%
37	i	156	 99%
38	j	104	 100%
39	k	151	 100%
40	l	129	 100%
41	m	127	 99%
42	n	99	 99%
43	o	117	 99%
44	p	123	 99%
45	q	116	 100%
46	r	100	 100%
47	s	88	 100%
48	t	82	 99%
49	u	80	 100%
50	v	66	 100%
51	w	83	 99%
52	x	86	 99%
53	y	70	 6%
54	z	88	 51%42%7%
55	B	27	 7%93%

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 145136 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	6	Total	C	N	O	P	0	0
			126	56	20	44	6		

- Molecule 5 is a protein called 50S ribosomal protein L2.

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

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

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

- Molecule 8 is a protein called 50S ribosomal protein L5.

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

- Molecule 9 is a protein called 50S ribosomal protein L6.

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

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

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

- Molecule 13 is a protein called 50S ribosomal protein L15.

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

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

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

- Molecule 16 is a protein called 50S ribosomal protein L18.

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

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

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

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	103	Total	C	N	O		0	0
			788	498	148	142			

- Molecule 23 is a protein called 50S ribosomal protein L25.

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

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	80	Total	C	N	O	S	0	0
			601	370	121	109	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

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

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L31.

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

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	52	Total	C	N	O	S	0	0
			426	275	78	73			

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a protein called 30S ribosomal protein S2.

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

- Molecule 35 is a protein called 30S ribosomal protein S3.

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

- Molecule 36 is a protein called 30S ribosomal protein S4.

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

- Molecule 37 is a protein called 30S ribosomal protein S5.

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

- Molecule 38 is a protein called 30S ribosomal protein S6.

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

- Molecule 39 is a protein called 30S ribosomal protein S7.

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

- Molecule 40 is a protein called 30S ribosomal protein S8.

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

- Molecule 41 is a protein called 30S ribosomal protein S9.

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

- Molecule 42 is a protein called 30S ribosomal protein S10.

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

- Molecule 43 is a protein called 30S ribosomal protein S11.

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

- Molecule 44 is a protein called 30S ribosomal protein S12.

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

- Molecule 45 is a protein called 30S ribosomal protein S13.

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

- Molecule 46 is a protein called 30S ribosomal protein S14.

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

- Molecule 47 is a protein called 30S ribosomal protein S15.

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

- Molecule 48 is a protein called 30S ribosomal protein S16.

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

- Molecule 49 is a protein called 30S ribosomal protein S17.

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

- Molecule 50 is a protein called 30S ribosomal protein S18.

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

- Molecule 51 is a protein called 30S ribosomal protein S19.

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

- Molecule 52 is a protein called 30S ribosomal protein S20.

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

- Molecule 53 is a protein called 30S ribosomal protein S21.

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

- Molecule 54 is a RNA chain called tRNA-Ser.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	88	Total	C	N	O	P	0	0
			1891	841	341	621	88		

- Molecule 55 is a protein called CspA transcriptional activator.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B	27	Total	C	N	O	S	0	0
			205	132	32	39	2		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	1	270	Total 270	Mg 270	0
56	2	113	Total 113	Mg 113	0
56	3	8	Total 8	Mg 8	0
56	4	1	Total 1	Mg 1	0
56	C	1	Total 1	Mg 1	0
56	D	2	Total 2	Mg 2	0
56	M	1	Total 1	Mg 1	0
56	a	1	Total 1	Mg 1	0
56	h	1	Total 1	Mg 1	0
56	q	1	Total 1	Mg 1	0
56	z	1	Total 1	Mg 1	0

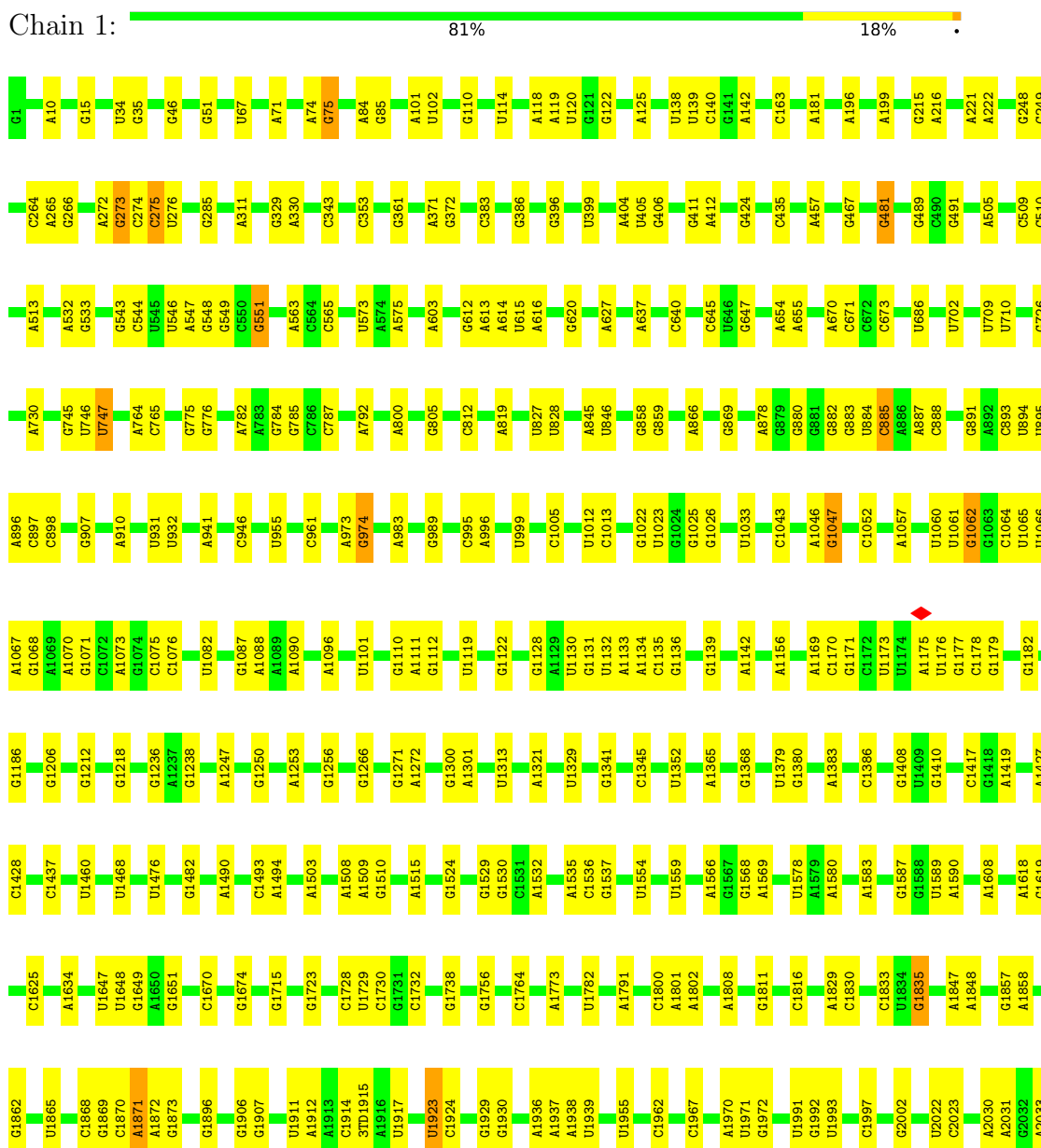
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

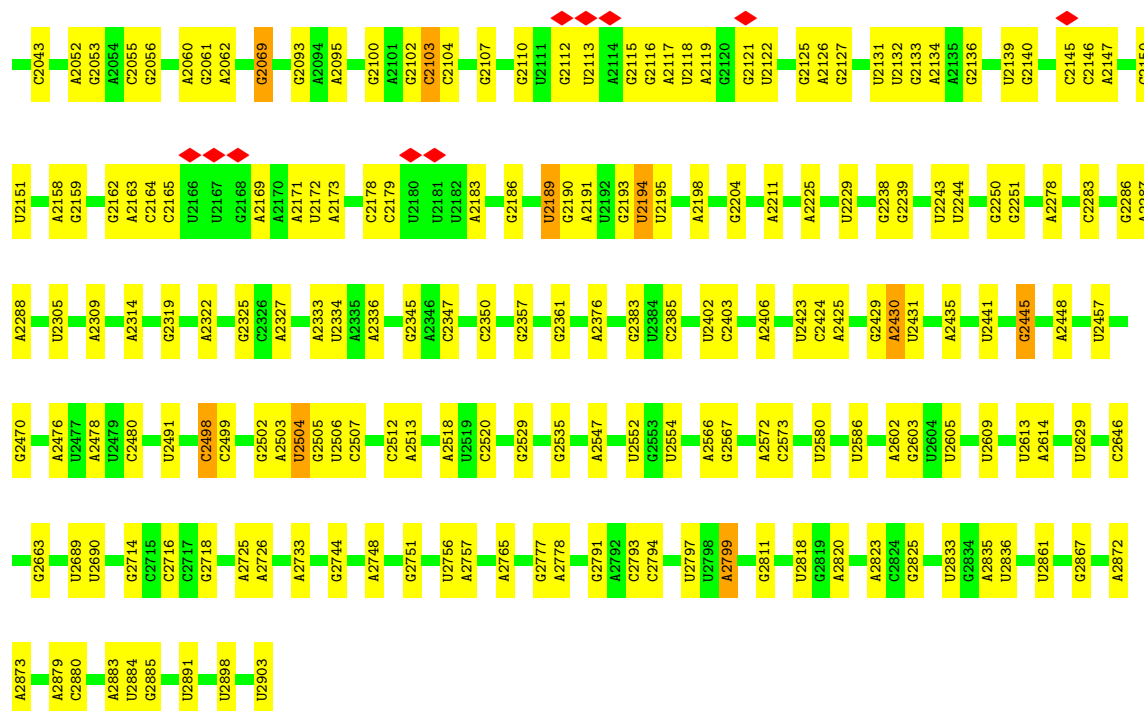
Mol	Chain	Residues	Atoms		AltConf
57	Z	1	Total 1	Zn 1	0
57	e	1	Total 1	Zn 1	0

3 Residue-property plots

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

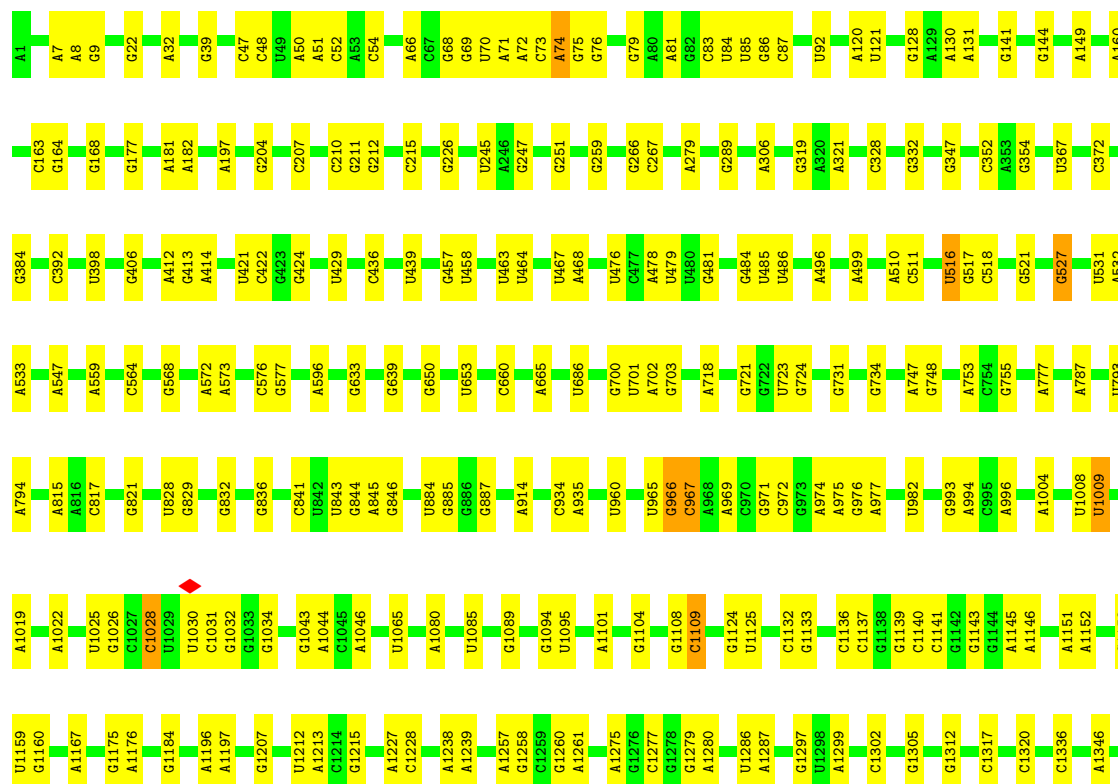
• Molecule 1: 23S rRNA





• Molecule 2: 16S rRNA

Chain 2: 82% 17% .





- Molecule 3: 5S rRNA

Chain 3: 88% 12%



- Molecule 4: mRNA

Chain 4: 83% 17%



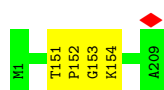
- Molecule 5: 50S ribosomal protein L2

Chain C: 100%



- Molecule 6: 50S ribosomal protein L3

Chain D: 98%



- Molecule 7: 50S ribosomal protein L4

Chain E: 100%

There are no outlier residues recorded for this chain.

- Molecule 8: 50S ribosomal protein L5

Chain F: 99%

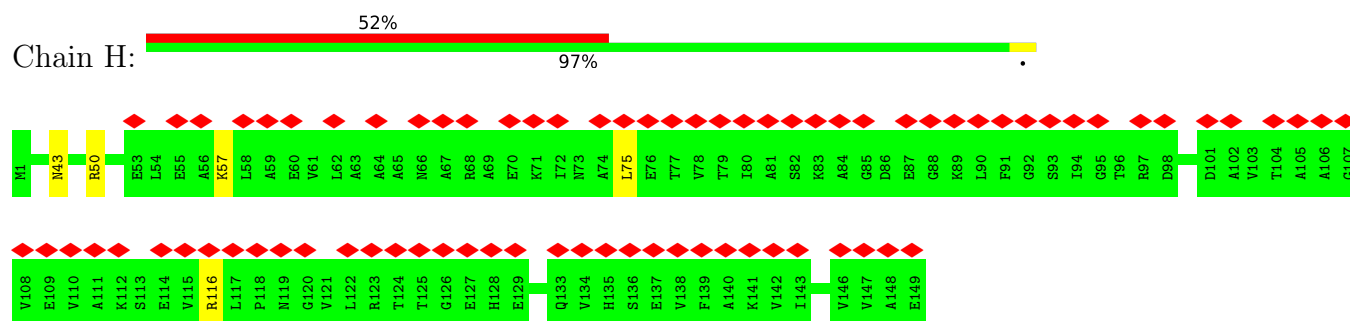


- Molecule 9: 50S ribosomal protein L6

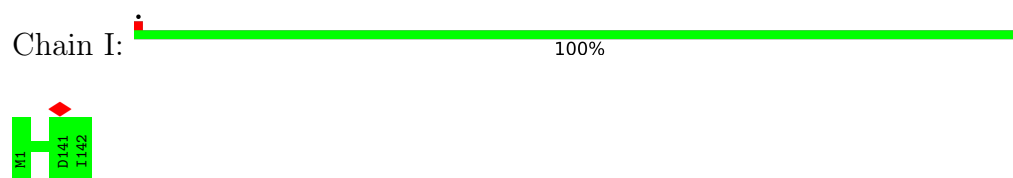
Chain G: 100%

There are no outlier residues recorded for this chain.

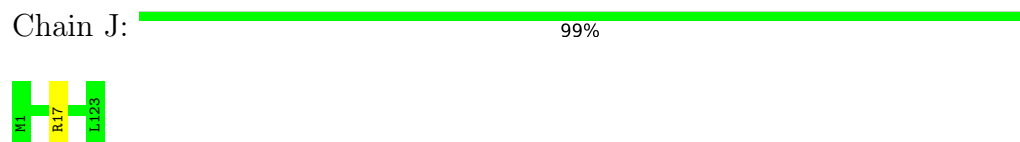
- Molecule 10: 50S ribosomal protein L9



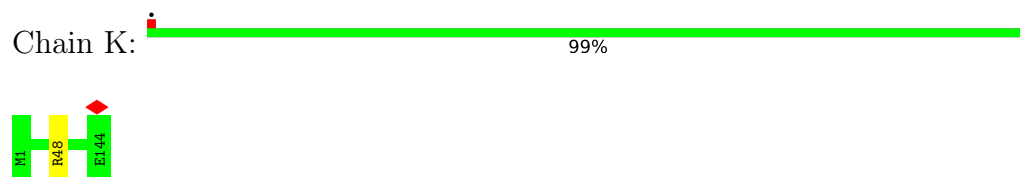
- Molecule 11: 50S ribosomal protein L13



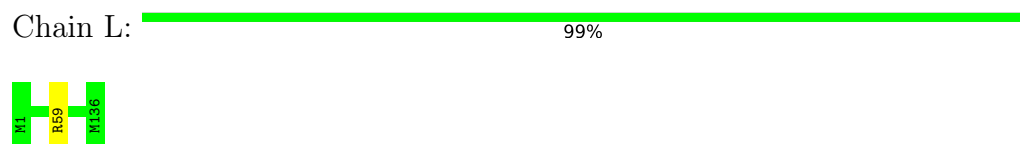
- Molecule 12: 50S ribosomal protein L14



- Molecule 13: 50S ribosomal protein L15



- Molecule 14: 50S ribosomal protein L16



- Molecule 15: 50S ribosomal protein L17



There are no outlier residues recorded for this chain.

- Molecule 16: 50S ribosomal protein L18





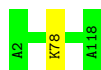
- Molecule 17: 50S ribosomal protein L19

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: 50S ribosomal protein L20

Chain P:  99%



- Molecule 19: 50S ribosomal protein L21

Chain Q:  98%



- Molecule 20: 50S ribosomal protein L22

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 21: 50S ribosomal protein L23

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 22: 50S ribosomal protein L24

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 23: 50S ribosomal protein L25

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 24: 50S ribosomal protein L27

Chain V:  99%



- Molecule 25: 50S ribosomal protein L28

Chain W:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: 50S ribosomal protein L29

Chain X:  100%



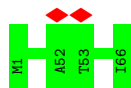
- Molecule 27: 50S ribosomal protein L30

Chain Y:  100%



- Molecule 28: 50S ribosomal protein L31

Chain Z:  100%



- Molecule 29: 50S ribosomal protein L32

Chain a:  100%



- Molecule 30: 50S ribosomal protein L33

Chain b:  100%



- Molecule 31: 50S ribosomal protein L34

Chain c:  100%



- Molecule 32: 50S ribosomal protein L35

Chain d:  98%



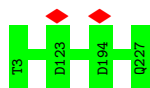
- Molecule 33: 50S ribosomal protein L36

Chain e:  100%



- Molecule 34: 30S ribosomal protein S2

Chain f:  100%



- Molecule 35: 30S ribosomal protein S3

Chain g:  99%



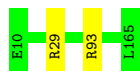
- Molecule 36: 30S ribosomal protein S4

Chain h:  100%



- Molecule 37: 30S ribosomal protein S5

Chain i:  99%



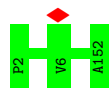
- Molecule 38: 30S ribosomal protein S6

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 39: 30S ribosomal protein S7

Chain k:  100%



- Molecule 40: 30S ribosomal protein S8

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 41: 30S ribosomal protein S9

Chain m:  99%



- Molecule 42: 30S ribosomal protein S10

Chain n:  99%



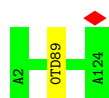
- Molecule 43: 30S ribosomal protein S11

Chain o:  99%



- Molecule 44: 30S ribosomal protein S12

Chain p:  99%



- Molecule 45: 30S ribosomal protein S13

Chain q:  100%



- Molecule 46: 30S ribosomal protein S14

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 47: 30S ribosomal protein S15

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 30S ribosomal protein S16

Chain t:  99%



- Molecule 49: 30S ribosomal protein S17

Chain u:  100%



- Molecule 50: 30S ribosomal protein S18

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 51: 30S ribosomal protein S19

Chain w:  99%

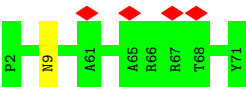


- Molecule 52: 30S ribosomal protein S20

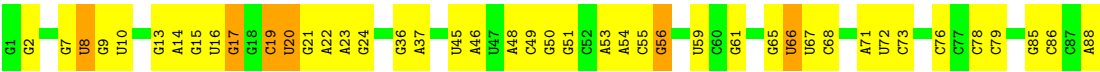
Chain x:  99%



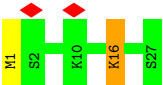
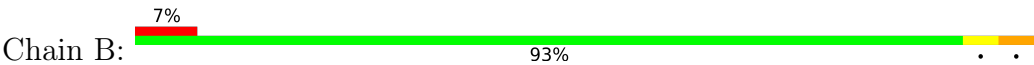
- Molecule 53: 30S ribosomal protein S21



• Molecule 54: tRNA-Ser



• Molecule 55: CspA transcriptional activator



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15459	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.132	Depositor
Minimum map value	-0.058	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	1.08	4/69286 (0.0%)	1.08	74/108087 (0.1%)
2	2	0.98	0/36590	1.04	11/57074 (0.0%)
3	3	0.96	0/2872	1.03	0/4478
4	4	0.62	0/139	1.02	0/214
5	C	0.77	0/2121	0.63	0/2852
6	D	0.77	0/1586	0.62	0/2134
7	E	0.68	0/1571	0.62	0/2113
8	F	0.56	0/1434	0.61	0/1926
9	G	0.54	0/1333	0.62	0/1805
10	H	0.43	0/1122	0.70	1/1515 (0.1%)
11	I	0.74	0/1152	0.59	0/1551
12	J	0.73	0/955	0.63	0/1279
13	K	0.69	0/1062	0.66	0/1413
14	L	0.70	0/1093	0.62	0/1460
15	M	0.69	0/964	0.64	0/1289
16	N	0.61	0/902	0.62	0/1209
17	O	0.74	0/929	0.58	0/1242
18	P	0.80	0/960	0.62	0/1278
19	Q	0.70	0/829	0.62	0/1107
20	R	0.75	0/864	0.64	0/1156
21	S	0.71	0/752	0.59	0/1005
22	T	0.62	0/796	0.61	0/1062
23	U	0.62	0/766	0.60	0/1025
24	V	0.71	0/608	0.62	0/804
25	W	0.69	0/635	0.61	0/848
26	X	0.57	0/502	0.65	0/667
27	Y	0.64	0/452	0.60	0/605
28	Z	0.47	0/531	0.59	0/709
29	a	0.68	0/450	0.63	0/599
30	b	0.62	0/433	0.59	0/576
31	c	0.73	0/380	0.64	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	d	0.73	0/513	0.65	0/676
33	e	0.74	0/303	0.61	0/397
34	f	0.51	0/1791	0.62	0/2413
35	g	0.61	0/1663	0.60	0/2241
36	h	0.59	0/1665	0.60	0/2227
37	i	0.70	0/1165	0.66	0/1568
38	j	0.58	0/867	0.57	0/1171
39	k	0.53	0/1195	0.61	0/1602
40	l	0.65	0/989	0.60	0/1326
41	m	0.58	0/1034	0.64	0/1375
42	n	0.55	0/800	0.67	0/1082
43	o	0.59	0/893	0.60	0/1205
44	p	0.69	0/960	0.62	0/1286
45	q	0.54	0/909	0.64	0/1215
46	r	0.58	0/817	0.60	0/1088
47	s	0.58	0/722	0.58	0/964
48	t	0.64	0/659	0.62	0/884
49	u	0.61	0/657	0.59	0/881
50	v	0.58	0/553	0.66	0/743
51	w	0.53	0/680	0.58	0/915
52	x	0.56	0/675	0.65	0/895
53	y	0.48	0/597	0.61	0/792
54	z	1.05	11/2062 (0.5%)	1.30	13/3208 (0.4%)
55	B	0.41	0/200	0.57	0/267
All	All	0.95	15/156438 (0.0%)	0.97	99/234001 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	20	U	C2-N3	16.02	1.49	1.37
54	z	20	U	C5-C6	14.97	1.47	1.34
54	z	9	G	OP3-P	-10.99	1.48	1.61
54	z	20	U	N1-C2	10.89	1.48	1.38
54	z	20	U	N3-C4	8.00	1.45	1.38
54	z	20	U	OP3-P	-7.93	1.51	1.61
54	z	20	U	N1-C6	7.83	1.45	1.38
54	z	67	U	OP3-P	-7.53	1.52	1.61
54	z	8	U	OP3-P	-7.29	1.52	1.61
54	z	20	U	C4-C5	5.82	1.48	1.43
1	1	2499	C	N1-C6	-5.71	1.33	1.37
54	z	20	U	C4-O4	-5.48	1.19	1.23
1	1	671	C	N1-C6	-5.37	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	673	C	N1-C6	-5.25	1.33	1.37
1	1	787	C	N1-C6	-5.04	1.34	1.37

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	z	67	U	O5'-P-OP1	-21.44	84.97	110.70
54	z	8	U	O5'-P-OP1	-19.48	87.33	110.70
54	z	20	U	C2-N3-C4	-12.49	119.50	127.00
54	z	20	U	C5-C4-O4	-10.73	119.46	125.90
54	z	20	U	N3-C4-C5	9.52	120.31	114.60
1	1	2193	G	C4-N9-C1'	8.71	137.82	126.50
54	z	20	U	N1-C2-N3	8.64	120.08	114.90
54	z	19	C	OP1-P-O3'	-8.56	86.36	105.20
1	1	2103	C	N1-C2-O2	8.45	123.97	118.90
1	1	1062	G	N3-C4-N9	8.38	131.03	126.00
1	1	2179	C	N3-C2-O2	-8.14	116.20	121.90
1	1	2193	G	C8-N9-C1'	-7.90	116.73	127.00
1	1	1313	U	C2-N1-C1'	7.86	127.13	117.70
54	z	19	C	OP2-P-O3'	-7.85	87.92	105.20
1	1	2193	G	C6-C5-N7	-7.82	125.71	130.40
1	1	2614	A	C6-N1-C2	-7.15	114.31	118.60
54	z	20	U	OP1-P-OP2	7.10	130.24	119.60
1	1	1076	C	N3-C2-O2	-7.09	116.94	121.90
1	1	1062	G	C4-N9-C1'	7.05	135.67	126.50
54	z	67	U	O5'-P-OP2	7.01	119.11	110.70
1	1	974	G	O4'-C1'-N9	6.80	113.64	108.20
1	1	2189	U	O4'-C1'-N1	6.78	113.62	108.20
1	1	221	A	O4'-C1'-N9	6.75	113.60	108.20
54	z	8	U	O5'-P-OP2	6.75	118.80	110.70
1	1	1047	G	O4'-C1'-N9	6.72	113.58	108.20
1	1	2193	G	N3-C4-N9	6.65	129.99	126.00
1	1	1313	U	C6-N1-C1'	-6.61	111.94	121.20
1	1	481	G	O4'-C1'-N9	6.60	113.48	108.20
1	1	2244	U	N3-C4-O4	6.58	124.01	119.40
1	1	67	U	C5-C4-O4	-6.56	121.97	125.90
1	1	1062	G	C8-N9-C1'	-6.53	118.51	127.00
1	1	640	C	C6-N1-C2	-6.49	117.71	120.30
1	1	1871	A	O4'-C1'-N9	6.43	113.34	108.20
1	1	2053	G	C5-N7-C8	-6.42	101.09	104.30
1	1	2244	U	C5-C4-O4	-6.41	122.05	125.90
1	1	67	U	N3-C4-O4	6.40	123.88	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1109	C	C3'-C2'-C1'	6.33	106.56	101.50
1	1	2512	C	C5'-C4'-C3'	6.25	125.99	116.00
1	1	2193	G	C4-C5-N7	6.21	113.29	110.80
1	1	2103	C	N3-C2-O2	-6.20	117.56	121.90
1	1	1923	U	O4'-C1'-N1	6.12	113.10	108.20
1	1	620	G	P-O3'-C3'	-6.09	112.39	119.70
2	2	74	A	O4'-C1'-N9	6.08	113.06	108.20
1	1	1857	G	O4'-C1'-N9	6.08	113.06	108.20
1	1	2186	G	N3-C4-C5	6.06	131.63	128.60
1	1	2195	U	O4'-C1'-N1	6.05	113.04	108.20
1	1	1062	G	N3-C4-C5	-5.99	125.61	128.60
1	1	2314	A	O4'-C1'-N9	5.98	112.99	108.20
1	1	274	C	N1-C2-O2	5.97	122.48	118.90
1	1	2053	G	C4-C5-N7	5.93	113.17	110.80
1	1	75	G	N3-C4-N9	-5.92	122.45	126.00
1	1	1728	C	C2-N1-C1'	-5.90	112.31	118.80
1	1	1062	G	C6-C5-N7	-5.88	126.87	130.40
2	2	1028	C	O4'-C1'-N1	-5.86	103.51	108.20
1	1	2194	U	O4'-C1'-N1	5.84	112.87	108.20
1	1	2179	C	C6-N1-C2	-5.83	117.97	120.30
2	2	259	G	N3-C4-N9	-5.80	122.52	126.00
2	2	215	C	C2-N1-C1'	5.80	125.18	118.80
1	1	1410	G	P-O3'-C3'	5.77	126.63	119.70
1	1	2136	G	P-O3'-C3'	5.76	126.61	119.70
1	1	1830	C	C2-N1-C1'	5.74	125.12	118.80
1	1	2104	C	C6-N1-C2	-5.66	118.04	120.30
2	2	1009	U	O4'-C1'-N1	5.59	112.67	108.20
1	1	1075	C	N1-C2-O2	5.58	122.25	118.90
1	1	2179	C	N1-C2-O2	5.57	122.24	118.90
1	1	565	C	C6-N1-C2	5.53	122.51	120.30
1	1	551	G	C8-N9-C1'	-5.52	119.82	127.00
2	2	207	C	C2-N1-C1'	-5.51	112.74	118.80
1	1	1052	C	N1-C2-O2	-5.49	115.61	118.90
10	H	116	ARG	NE-CZ-NH1	5.47	123.04	120.30
2	2	686	U	O4'-C1'-N1	5.43	112.55	108.20
1	1	2799	A	C6-C5-N7	-5.40	128.52	132.30
1	1	275	C	C2-N1-C1'	-5.36	112.90	118.80
1	1	1075	C	N3-C2-O2	-5.34	118.16	121.90
1	1	114	U	C2-N1-C1'	5.30	124.06	117.70
1	1	551	G	C4-N9-C1'	5.28	133.37	126.50
1	1	1625	C	N1-C2-O2	5.27	122.06	118.90
54	z	9	G	OP1-P-OP2	5.27	127.51	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1830	C	C6-N1-C1'	-5.27	114.48	120.80
1	1	1313	U	O4'-C1'-N1	5.27	112.42	108.20
1	1	2430	A	N1-C6-N6	5.26	121.76	118.60
1	1	2799	A	N9-C4-C5	-5.26	103.70	105.80
2	2	168	G	C8-N9-C1'	-5.25	120.17	127.00
1	1	2150	C	O4'-C1'-N1	-5.21	104.03	108.20
1	1	640	C	C5-C6-N1	5.19	123.59	121.00
1	1	1568	G	N3-C4-C5	5.18	131.19	128.60
2	2	207	C	N1-C2-O2	-5.17	115.80	118.90
1	1	2194	U	C2-N1-C1'	-5.15	111.52	117.70
1	1	640	C	C2-N1-C1'	5.15	124.47	118.80
54	z	56	G	N9-C4-C5	-5.15	103.34	105.40
1	1	1670	C	C5-C4-N4	-5.15	116.60	120.20
1	1	2193	G	N7-C8-N9	5.11	115.65	113.10
1	1	1082	U	O4'-C1'-N1	5.10	112.28	108.20
1	1	1062	G	N9-C4-C5	-5.08	103.37	105.40
1	1	885	C	N1-C2-O2	-5.08	115.85	118.90
1	1	1728	C	N1-C2-O2	-5.08	115.86	118.90
1	1	273	G	C8-N9-C1'	-5.07	120.41	127.00
2	2	168	G	C6-C5-N7	-5.06	127.37	130.40
1	1	883	G	N3-C4-N9	-5.01	122.99	126.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	269/271 (99%)	256 (95%)	13 (5%)	0	100	100
6	D	207/209 (99%)	201 (97%)	3 (1%)	3 (1%)	11	46
7	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
8	F	175/177 (99%)	165 (94%)	9 (5%)	1 (1%)	25	64
9	G	173/175 (99%)	161 (93%)	12 (7%)	0	100	100
10	H	147/149 (99%)	137 (93%)	10 (7%)	0	100	100
11	I	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
12	J	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
13	K	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	L	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
15	M	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
16	N	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
17	O	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
18	P	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
19	Q	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	7	38
20	R	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
21	S	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
22	T	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
23	U	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
24	V	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
25	W	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
26	X	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
27	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
28	Z	64/66 (97%)	59 (92%)	5 (8%)	0	100	100
29	a	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
30	b	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
31	c	44/46 (96%)	44 (100%)	0	0	100	100
32	d	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
33	e	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
34	f	223/225 (99%)	207 (93%)	16 (7%)	0	100	100
35	g	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
36	h	203/205 (99%)	201 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	i	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
38	j	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
39	k	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
40	l	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
41	m	125/127 (98%)	118 (94%)	7 (6%)	0	100	100
42	n	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
43	o	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
44	p	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
45	q	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
46	r	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
47	s	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
48	t	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
49	u	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
50	v	64/66 (97%)	64 (100%)	0	0	100	100
51	w	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
52	x	84/86 (98%)	84 (100%)	0	0	100	100
53	y	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
55	B	25/27 (93%)	13 (52%)	11 (44%)	1 (4%)	3	21
All	All	5637/5738 (98%)	5424 (96%)	206 (4%)	7 (0%)	54	83

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	152	PRO
6	D	153	GLY
6	D	154	LYS
19	Q	52	PRO
19	Q	53	PHE
55	B	16	LYS
8	F	124	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	
5	C	216/216 (100%)	216 (100%)	0	100	100
6	D	164/164 (100%)	163 (99%)	1 (1%)	86	94
7	E	165/165 (100%)	165 (100%)	0	100	100
8	F	148/148 (100%)	148 (100%)	0	100	100
9	G	136/136 (100%)	136 (100%)	0	100	100
10	H	114/114 (100%)	110 (96%)	4 (4%)	36	69
11	I	116/116 (100%)	116 (100%)	0	100	100
12	J	104/104 (100%)	103 (99%)	1 (1%)	76	90
13	K	103/103 (100%)	102 (99%)	1 (1%)	76	90
14	L	109/109 (100%)	108 (99%)	1 (1%)	78	91
15	M	99/99 (100%)	99 (100%)	0	100	100
16	N	86/86 (100%)	85 (99%)	1 (1%)	71	88
17	O	99/99 (100%)	99 (100%)	0	100	100
18	P	89/89 (100%)	88 (99%)	1 (1%)	73	88
19	Q	84/84 (100%)	84 (100%)	0	100	100
20	R	93/93 (100%)	93 (100%)	0	100	100
21	S	81/81 (100%)	81 (100%)	0	100	100
22	T	84/84 (100%)	84 (100%)	0	100	100
23	U	78/78 (100%)	78 (100%)	0	100	100
24	V	59/59 (100%)	58 (98%)	1 (2%)	60	83
25	W	67/67 (100%)	67 (100%)	0	100	100
26	X	54/54 (100%)	54 (100%)	0	100	100
27	Y	48/48 (100%)	48 (100%)	0	100	100
28	Z	59/59 (100%)	59 (100%)	0	100	100
29	a	47/47 (100%)	47 (100%)	0	100	100
30	b	47/47 (100%)	47 (100%)	0	100	100
31	c	38/38 (100%)	38 (100%)	0	100	100
32	d	51/51 (100%)	50 (98%)	1 (2%)	55	80
33	e	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	f	187/187 (100%)	187 (100%)	0	100	100
35	g	171/171 (100%)	169 (99%)	2 (1%)	71	88
36	h	172/172 (100%)	171 (99%)	1 (1%)	86	94
37	i	119/119 (100%)	117 (98%)	2 (2%)	60	83
38	j	91/91 (100%)	91 (100%)	0	100	100
39	k	124/124 (100%)	124 (100%)	0	100	100
40	l	104/104 (100%)	104 (100%)	0	100	100
41	m	105/105 (100%)	104 (99%)	1 (1%)	76	90
42	n	86/86 (100%)	85 (99%)	1 (1%)	71	88
43	o	90/90 (100%)	89 (99%)	1 (1%)	73	88
44	p	102/102 (100%)	102 (100%)	0	100	100
45	q	94/94 (100%)	94 (100%)	0	100	100
46	r	83/83 (100%)	83 (100%)	0	100	100
47	s	76/76 (100%)	76 (100%)	0	100	100
48	t	65/65 (100%)	64 (98%)	1 (2%)	65	85
49	u	74/74 (100%)	74 (100%)	0	100	100
50	v	57/57 (100%)	57 (100%)	0	100	100
51	w	72/72 (100%)	71 (99%)	1 (1%)	67	86
52	x	65/65 (100%)	64 (98%)	1 (2%)	65	85
53	y	60/60 (100%)	59 (98%)	1 (2%)	60	83
55	B	20/20 (100%)	19 (95%)	1 (5%)	24	60
All	All	4689/4689 (100%)	4664 (100%)	25 (0%)	89	95

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	D	151	THR
10	H	43	ASN
10	H	50	ARG
10	H	57	LYS
10	H	75	LEU
12	J	17	ARG
13	K	48	ARG
14	L	59	ARG
16	N	53	THR

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Mol	Chain	Res	Type
18	P	78	LYS
24	V	14	ARG
32	d	31	HIS
35	g	164	ARG
35	g	172	ARG
36	h	138	SER
37	i	29	ARG
37	i	93	ARG
41	m	106	ARG
42	n	5	ARG
43	o	56	ARG
48	t	1	MET
51	w	78	ARG
52	x	85	LYS
53	y	9	ASN
55	B	16	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
32	d	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2898/2903 (99%)	494 (17%)	11 (0%)
2	2	1529/1534 (99%)	260 (17%)	4 (0%)
3	3	119/120 (99%)	15 (12%)	0
4	4	5/6 (83%)	1 (20%)	0
54	z	87/88 (98%)	41 (47%)	0
All	All	4638/4651 (99%)	811 (17%)	15 (0%)

All (811) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	34	U
1	1	35	G
1	1	46	G

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Mol	Chain	Res	Type
1	1	51	G
1	1	71	A
1	1	74	A
1	1	75	G
1	1	84	A
1	1	85	G
1	1	101	A
1	1	102	U
1	1	110	G
1	1	118	A
1	1	119	A
1	1	120	U
1	1	122	G
1	1	125	A
1	1	138	U
1	1	139	U
1	1	140	C
1	1	142	A
1	1	163	C
1	1	181	A
1	1	196	A
1	1	199	A
1	1	215	G
1	1	216	A
1	1	222	A
1	1	248	G
1	1	249	C
1	1	264	C
1	1	265	A
1	1	266	G
1	1	272	A
1	1	273	G
1	1	275	C
1	1	276	U
1	1	285	G
1	1	311	A
1	1	329	G
1	1	330	A
1	1	343	C
1	1	353	C
1	1	361	G
1	1	371	A

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Mol	Chain	Res	Type
1	1	372	G
1	1	383	C
1	1	386	G
1	1	396	G
1	1	399	U
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	424	G
1	1	435	C
1	1	457	A
1	1	467	G
1	1	481	G
1	1	489	G
1	1	491	G
1	1	505	A
1	1	509	C
1	1	510	C
1	1	513	A
1	1	532	A
1	1	533	G
1	1	543	G
1	1	544	C
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	551	G
1	1	563	A
1	1	573	U
1	1	575	A
1	1	603	A
1	1	612	G
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	627	A
1	1	637	A
1	1	645	C
1	1	647	G

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Mol	Chain	Res	Type
1	1	654	A
1	1	655	A
1	1	670	A
1	1	686	U
1	1	702	U
1	1	709	U
1	1	710	U
1	1	726	G
1	1	730	A
1	1	747	5MU
1	1	764	A
1	1	765	C
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	792	A
1	1	800	A
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	845	A
1	1	846	U
1	1	858	G
1	1	859	G
1	1	866	A
1	1	869	G
1	1	878	A
1	1	880	G
1	1	882	G
1	1	884	U
1	1	885	C
1	1	887	A
1	1	888	C
1	1	891	G
1	1	893	C
1	1	894	U
1	1	895	U
1	1	896	A

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Mol	Chain	Res	Type
1	1	897	C
1	1	898	C
1	1	907	G
1	1	910	A
1	1	931	U
1	1	932	U
1	1	941	A
1	1	946	C
1	1	961	C
1	1	973	A
1	1	974	G
1	1	983	A
1	1	989	G
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1012	U
1	1	1013	C
1	1	1022	G
1	1	1023	U
1	1	1025	G
1	1	1026	G
1	1	1033	U
1	1	1043	C
1	1	1046	A
1	1	1047	G
1	1	1057	A
1	1	1060	U
1	1	1061	U
1	1	1062	G
1	1	1064	C
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1070	A
1	1	1071	G
1	1	1073	A
1	1	1087	G
1	1	1088	A
1	1	1090	A

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Mol	Chain	Res	Type
1	1	1096	A
1	1	1101	U
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1119	U
1	1	1122	G
1	1	1128	G
1	1	1130	U
1	1	1131	G
1	1	1132	U
1	1	1133	A
1	1	1134	A
1	1	1135	C
1	1	1136	G
1	1	1139	G
1	1	1142	A
1	1	1156	A
1	1	1169	A
1	1	1170	C
1	1	1171	G
1	1	1173	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1179	G
1	1	1182	G
1	1	1186	G
1	1	1206	G
1	1	1212	G
1	1	1218	G
1	1	1236	G
1	1	1238	G
1	1	1247	A
1	1	1250	G
1	1	1253	A
1	1	1256	G
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1300	G

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Mol	Chain	Res	Type
1	1	1301	A
1	1	1321	A
1	1	1329	U
1	1	1341	G
1	1	1345	C
1	1	1352	U
1	1	1365	A
1	1	1368	G
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1386	C
1	1	1408	G
1	1	1417	C
1	1	1419	A
1	1	1427	A
1	1	1428	C
1	1	1437	C
1	1	1460	U
1	1	1468	U
1	1	1476	U
1	1	1482	G
1	1	1490	A
1	1	1493	C
1	1	1494	A
1	1	1503	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1524	G
1	1	1529	G
1	1	1530	G
1	1	1532	A
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1554	U
1	1	1559	U
1	1	1566	A
1	1	1569	A
1	1	1578	U

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Mol	Chain	Res	Type
1	1	1580	A
1	1	1583	A
1	1	1587	G
1	1	1589	U
1	1	1590	A
1	1	1608	A
1	1	1619	G
1	1	1634	A
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G
1	1	1674	G
1	1	1715	G
1	1	1723	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1756	G
1	1	1764	C
1	1	1773	A
1	1	1782	U
1	1	1791	A
1	1	1800	C
1	1	1801	A
1	1	1802	A
1	1	1808	A
1	1	1811	G
1	1	1816	C
1	1	1829	A
1	1	1833	C
1	1	1835	2MG
1	1	1847	A
1	1	1848	A
1	1	1858	A
1	1	1862	G
1	1	1865	U
1	1	1868	C
1	1	1869	G
1	1	1870	C
1	1	1871	A

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Mol	Chain	Res	Type
1	1	1872	A
1	1	1873	G
1	1	1896	G
1	1	1906	G
1	1	1907	G
1	1	1912	A
1	1	1914	C
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1937	A
1	1	1938	A
1	1	1955	U
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2022	U
1	1	2023	C
1	1	2031	A
1	1	2033	A
1	1	2043	C
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2093	G
1	1	2095	A
1	1	2100	G
1	1	2102	G
1	1	2103	C
1	1	2107	G

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Mol	Chain	Res	Type
1	1	2110	G
1	1	2112	G
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2119	A
1	1	2121	G
1	1	2122	U
1	1	2125	G
1	1	2126	A
1	1	2127	G
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2139	U
1	1	2140	G
1	1	2145	C
1	1	2146	C
1	1	2147	A
1	1	2151	U
1	1	2158	A
1	1	2159	G
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2169	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2178	C
1	1	2183	A
1	1	2189	U
1	1	2190	G
1	1	2191	A
1	1	2194	U
1	1	2198	A
1	1	2204	G
1	1	2211	A

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Mol	Chain	Res	Type
1	1	2225	A
1	1	2229	U
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2250	G
1	1	2278	A
1	1	2283	C
1	1	2286	G
1	1	2287	A
1	1	2288	A
1	1	2305	U
1	1	2309	A
1	1	2319	G
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2334	U
1	1	2336	A
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2357	G
1	1	2361	G
1	1	2376	A
1	1	2383	G
1	1	2385	C
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2435	A
1	1	2441	U
1	1	2445	2MG
1	1	2448	A
1	1	2470	G

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Mol	Chain	Res	Type
1	1	2476	A
1	1	2478	A
1	1	2480	C
1	1	2491	U
1	1	2498	OMC
1	1	2502	G
1	1	2504	PSU
1	1	2505	G
1	1	2506	U
1	1	2507	C
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2529	G
1	1	2535	G
1	1	2547	A
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2586	U
1	1	2602	A
1	1	2603	G
1	1	2609	U
1	1	2613	U
1	1	2629	U
1	1	2646	C
1	1	2663	G
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2716	C
1	1	2718	G
1	1	2725	A
1	1	2726	A
1	1	2733	A
1	1	2744	G
1	1	2748	A
1	1	2751	G
1	1	2757	A
1	1	2765	A

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Mol	Chain	Res	Type
1	1	2777	G
1	1	2778	A
1	1	2791	G
1	1	2793	C
1	1	2794	C
1	1	2797	U
1	1	2799	A
1	1	2811	G
1	1	2818	U
1	1	2820	A
1	1	2823	A
1	1	2825	G
1	1	2833	U
1	1	2835	A
1	1	2836	U
1	1	2861	U
1	1	2867	G
1	1	2872	A
1	1	2873	A
1	1	2879	A
1	1	2880	C
1	1	2883	A
1	1	2884	U
1	1	2885	G
1	1	2891	U
1	1	2898	U
1	1	2903	U
2	2	7	A
2	2	8	A
2	2	9	G
2	2	22	G
2	2	32	A
2	2	39	G
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	54	C
2	2	66	A
2	2	68	G
2	2	69	G

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Mol	Chain	Res	Type
2	2	70	U
2	2	71	A
2	2	72	A
2	2	73	C
2	2	74	A
2	2	75	G
2	2	76	G
2	2	79	G
2	2	81	A
2	2	83	C
2	2	84	U
2	2	85	U
2	2	86	G
2	2	87	C
2	2	92	U
2	2	120	A
2	2	121	U
2	2	128	G
2	2	130	A
2	2	131	A
2	2	141	G
2	2	144	G
2	2	149	A
2	2	160	A
2	2	163	C
2	2	164	G
2	2	177	G
2	2	181	A
2	2	182	A
2	2	197	A
2	2	204	G
2	2	210	C
2	2	211	G
2	2	212	G
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	266	G
2	2	267	C
2	2	279	A
2	2	289	G

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Mol	Chain	Res	Type
2	2	306	A
2	2	319	G
2	2	321	A
2	2	328	C
2	2	332	G
2	2	347	G
2	2	352	C
2	2	354	G
2	2	367	U
2	2	372	C
2	2	384	G
2	2	392	C
2	2	398	U
2	2	406	G
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	429	U
2	2	436	C
2	2	439	U
2	2	457	G
2	2	458	U
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	476	U
2	2	478	A
2	2	479	U
2	2	481	G
2	2	484	G
2	2	485	U
2	2	486	U
2	2	496	A
2	2	499	A
2	2	510	A
2	2	511	C
2	2	517	G
2	2	518	C

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Mol	Chain	Res	Type
2	2	521	G
2	2	527	G7M
2	2	531	U
2	2	532	A
2	2	533	A
2	2	547	A
2	2	559	A
2	2	564	C
2	2	568	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	596	A
2	2	633	G
2	2	639	G
2	2	650	G
2	2	653	U
2	2	660	C
2	2	665	A
2	2	700	G
2	2	701	U
2	2	702	A
2	2	703	G
2	2	718	A
2	2	721	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	747	A
2	2	748	G
2	2	753	A
2	2	755	G
2	2	777	A
2	2	787	A
2	2	793	U
2	2	794	A
2	2	815	A
2	2	817	C
2	2	821	G
2	2	828	U

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Mol	Chain	Res	Type
2	2	829	G
2	2	832	G
2	2	836	G
2	2	841	C
2	2	843	U
2	2	844	G
2	2	845	A
2	2	846	G
2	2	884	U
2	2	885	G
2	2	887	G
2	2	914	A
2	2	934	C
2	2	935	A
2	2	960	U
2	2	965	U
2	2	966	2MG
2	2	967	5MC
2	2	969	A
2	2	971	G
2	2	972	C
2	2	974	A
2	2	975	A
2	2	976	G
2	2	977	A
2	2	982	U
2	2	993	G
2	2	994	A
2	2	996	A
2	2	1004	A
2	2	1008	U
2	2	1009	U
2	2	1019	A
2	2	1022	A
2	2	1025	U
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1032	G
2	2	1034	G
2	2	1043	G

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Mol	Chain	Res	Type
2	2	1044	A
2	2	1046	A
2	2	1065	U
2	2	1080	A
2	2	1085	U
2	2	1089	G
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1104	G
2	2	1108	G
2	2	1124	G
2	2	1125	U
2	2	1132	C
2	2	1133	G
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1143	G
2	2	1145	A
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1158	C
2	2	1159	U
2	2	1160	G
2	2	1167	A
2	2	1175	G
2	2	1176	A
2	2	1184	G
2	2	1196	A
2	2	1197	A
2	2	1212	U
2	2	1213	A
2	2	1215	G
2	2	1227	A
2	2	1228	C
2	2	1238	A
2	2	1239	A
2	2	1257	A

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Mol	Chain	Res	Type
2	2	1258	G
2	2	1260	G
2	2	1261	A
2	2	1275	A
2	2	1277	C
2	2	1279	G
2	2	1280	A
2	2	1286	U
2	2	1287	A
2	2	1297	G
2	2	1299	A
2	2	1302	C
2	2	1305	G
2	2	1312	G
2	2	1317	C
2	2	1320	C
2	2	1336	C
2	2	1346	A
2	2	1353	G
2	2	1363	A
2	2	1370	G
2	2	1379	G
2	2	1381	U
2	2	1419	G
2	2	1441	A
2	2	1446	A
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1529	G
2	2	1530	G
2	2	1534	A
3	3	2	G
3	3	9	G
3	3	13	G
3	3	24	G
3	3	35	C
3	3	36	C
3	3	45	A

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Mol	Chain	Res	Type
3	3	51	G
3	3	56	G
3	3	66	A
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	109	A
4	4	2	G
54	z	2	G
54	z	7	G
54	z	8	U
54	z	10	U
54	z	13	G
54	z	14	A
54	z	15	G
54	z	16	U
54	z	17	OMG
54	z	19	C
54	z	20	U
54	z	21	G
54	z	22	A
54	z	23	A
54	z	24	G
54	z	36	G
54	z	37	A
54	z	45	U
54	z	46	A
54	z	48	A
54	z	49	C
54	z	50	G
54	z	51	G
54	z	53	A
54	z	54	A
54	z	55	C
54	z	56	G
54	z	59	U
54	z	61	G
54	z	65	G
54	z	66	5MU
54	z	68	C
54	z	71	A

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Mol	Chain	Res	Type
54	z	72	U
54	z	73	C
54	z	76	C
54	z	78	C
54	z	79	C
54	z	85	G
54	z	86	C
54	z	88	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	404	A
1	1	613	A
1	1	784	G
1	1	894	U
1	1	896	A
1	1	1379	U
1	1	2102	G
1	1	2146	C
1	1	2189	U
1	1	2602	A
1	1	2756	U
2	2	516	PSU
2	2	966	2MG
2	2	1109	C
2	2	1145	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PSU	1	2504	1	17,21,22	1.27	3 (17%)	20,30,33	2.99	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1	746	1,56	17,21,22	1.13	2 (11%)	20,30,33	3.07	6 (30%)
1	PSU	1	2457	1	17,21,22	1.30	3 (17%)	20,30,33	2.99	7 (35%)
1	OMC	1	2498	1,56	15,22,23	2.92	6 (40%)	17,31,34	1.33	3 (17%)
1	PSU	1	2580	1	17,21,22	1.38	3 (17%)	20,30,33	3.05	8 (40%)
1	5MC	1	1962	1	15,22,23	2.89	5 (33%)	19,32,35	1.40	2 (10%)
2	5MC	2	1407	2	15,22,23	2.71	5 (33%)	19,32,35	1.28	2 (10%)
1	OMG	1	2251	1,54,56	18,26,27	3.12	7 (38%)	20,38,41	1.63	4 (20%)
2	2MG	2	1207	2	19,26,27	4.09	7 (36%)	21,38,41	2.01	8 (38%)
44	0TD	p	89	44	4,9,10	1.54	0	3,11,13	1.33	1 (33%)
1	6MZ	1	1618	1	18,25,26	1.78	2 (11%)	16,36,39	3.60	3 (18%)
1	G7M	1	2069	1	20,26,27	3.22	8 (40%)	20,39,42	2.19	6 (30%)
55	FME	B	1	55	8,9,10	0.90	0	7,9,11	1.39	1 (14%)
1	PSU	1	2605	1	17,21,22	1.33	2 (11%)	20,30,33	3.23	7 (35%)
2	UR3	2	1498	2	14,22,23	2.81	3 (21%)	15,32,35	0.93	1 (6%)
2	4OC	2	1402	2	16,23,24	2.99	6 (37%)	17,32,35	1.30	1 (5%)
1	3TD	1	1915	1	17,22,23	3.13	8 (47%)	19,32,35	1.68	4 (21%)
54	5MU	z	66	54	15,22,23	2.85	3 (20%)	16,32,35	2.63	2 (12%)
1	2MA	1	2503	1,56	17,25,26	3.49	6 (35%)	19,37,40	1.90	4 (21%)
1	PSU	1	955	1,56	17,21,22	1.29	3 (17%)	20,30,33	2.98	5 (25%)
2	2MG	2	1516	2	19,26,27	4.15	7 (36%)	21,38,41	2.05	7 (33%)
1	1MG	1	745	1	18,26,27	3.59	5 (27%)	19,39,42	2.45	3 (15%)
2	PSU	2	516	2,56	17,21,22	1.03	2 (11%)	20,30,33	3.01	5 (25%)
2	5MC	2	967	2	15,22,23	2.95	5 (33%)	19,32,35	1.25	1 (5%)
1	6MZ	1	2030	1	18,25,26	1.79	3 (16%)	16,36,39	3.30	3 (18%)
2	MA6	2	1518	2	19,26,27	1.23	2 (10%)	18,38,41	3.31	2 (11%)
2	2MG	2	966	2	19,26,27	4.24	7 (36%)	21,38,41	2.05	8 (38%)
2	MA6	2	1519	2	19,26,27	1.23	2 (10%)	18,38,41	3.70	2 (11%)
1	PSU	1	1917	1	17,21,22	1.31	3 (17%)	20,30,33	2.99	6 (30%)
2	G7M	2	527	2	20,26,27	3.26	8 (40%)	20,39,42	2.41	5 (25%)
1	OMU	1	2552	1	14,22,23	3.21	5 (35%)	14,31,34	0.88	1 (7%)
1	2MG	1	1835	1	19,26,27	4.06	7 (36%)	21,38,41	1.93	7 (33%)
1	5MU	1	747	1	15,22,23	2.71	3 (20%)	16,32,35	2.60	2 (12%)
1	PSU	1	1911	1	17,21,22	1.30	3 (17%)	20,30,33	3.10	6 (30%)
54	OMG	z	17	54	22,27,27	4.41	7 (31%)	27,41,41	2.67	9 (33%)
1	5MU	1	1939	1,56	15,22,23	2.75	3 (20%)	16,32,35	2.72	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	1	2445	1	19,26,27	3.84	9 (47%)	21,38,41	1.94	7 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	1	746	1,56	-	2/7/25/26	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2498	1,56	-	0/7/27/28	0/2/2/2
1	PSU	1	2580	1	-	1/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	0/5/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/5/25/26	0/2/2/2
1	OMG	1	2251	1,54,56	-	0/5/27/28	0/3/3/3
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
44	0TD	p	89	44	-	1/3/12/14	-
1	6MZ	1	1618	1	-	3/5/27/28	0/3/3/3
1	G7M	1	2069	1	-	1/3/25/26	0/3/3/3
55	FME	B	1	55	-	3/7/9/11	-
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
2	UR3	2	1498	2	-	0/5/25/26	0/2/2/2
2	4OC	2	1402	2	-	2/9/29/30	0/2/2/2
1	3TD	1	1915	1	-	2/7/25/26	0/2/2/2
54	5MU	z	66	54	-	2/5/25/26	0/2/2/2
1	2MA	1	2503	1,56	-	2/3/25/26	0/3/3/3
1	PSU	1	955	1,56	-	0/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
2	PSU	2	516	2,56	-	2/7/25/26	0/2/2/2
2	5MC	2	967	2	-	0/5/25/26	0/2/2/2
1	6MZ	1	2030	1	-	2/5/27/28	0/3/3/3
2	MA6	2	1518	2	-	1/7/29/30	0/3/3/3
2	2MG	2	966	2	-	2/5/27/28	0/3/3/3
2	MA6	2	1519	2	-	5/7/29/30	0/3/3/3
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
2	G7M	2	527	2	-	3/3/25/26	0/3/3/3
1	OMU	1	2552	1	-	0/7/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
1	5MU	1	747	1	-	0/5/25/26	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
54	OMG	z	17	54	-	5/8/28/28	0/3/3/3
1	5MU	1	1939	1,56	-	0/5/25/26	0/2/2/2
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	17	OMG	C4-N3	12.45	1.55	1.35
2	2	1516	2MG	C2-N2	12.39	1.44	1.34
2	2	966	2MG	C2-N2	12.32	1.44	1.34
2	2	1207	2MG	C2-N2	11.84	1.44	1.34
1	1	1835	2MG	C2-N2	11.84	1.44	1.34
1	1	2445	2MG	C2-N2	10.80	1.43	1.34
54	z	66	5MU	C5-C4	9.52	1.61	1.41
1	1	1939	5MU	C5-C4	8.77	1.60	1.41
1	1	747	5MU	C5-C4	8.67	1.60	1.41
2	2	966	2MG	C4-N3	8.42	1.48	1.35
1	1	1835	2MG	C4-N3	8.33	1.48	1.35
54	z	17	OMG	C2-N1	8.32	1.50	1.35
2	2	527	G7M	C4-N3	8.32	1.48	1.35
2	2	1207	2MG	C4-N3	8.28	1.48	1.35
1	1	2503	2MA	C4-N3	8.22	1.48	1.35
54	z	17	OMG	O6-C6	-8.08	1.04	1.24
2	2	1516	2MG	C4-N3	8.02	1.48	1.35
1	1	745	1MG	C4-N3	7.91	1.48	1.35
1	1	2445	2MG	C4-N3	7.75	1.47	1.35
1	1	745	1MG	C2-N2	7.65	1.49	1.33
1	1	2069	G7M	C4-N3	7.64	1.47	1.35
1	1	2251	OMG	C4-N3	7.58	1.47	1.35
54	z	17	OMG	C5-C6	7.39	1.54	1.41
1	1	2503	2MA	C5-C6	7.31	1.52	1.41
1	1	2552	OMU	C4-N3	7.14	1.45	1.33
2	2	966	2MG	C5-C6	7.09	1.53	1.41
1	1	1962	5MC	C4-N3	7.07	1.45	1.35
1	1	745	1MG	C5-C6	7.02	1.52	1.41
2	2	967	5MC	C4-N3	6.87	1.44	1.35
2	2	1498	UR3	C6-N1	6.86	1.44	1.35
1	1	1915	3TD	C6-C5	6.81	1.48	1.38
2	2	1207	2MG	C5-C6	6.80	1.53	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	17	OMG	C6-N1	6.70	1.44	1.33
2	2	1402	4OC	C6-N1	6.68	1.44	1.35
2	2	1516	2MG	C5-C6	6.63	1.52	1.41
1	1	1835	2MG	C5-C6	6.50	1.52	1.41
1	1	2445	2MG	C5-C6	6.41	1.52	1.41
1	1	745	1MG	C2-N3	6.34	1.44	1.34
1	1	2251	OMG	C5-C6	6.30	1.52	1.41
2	2	527	G7M	C5-C6	6.29	1.52	1.41
1	1	2503	2MA	C2-N3	6.27	1.45	1.34
1	1	2069	G7M	C5-C6	6.25	1.52	1.41
2	2	1407	5MC	C4-N3	6.23	1.43	1.35
1	1	2498	OMC	C6-N1	6.08	1.43	1.35
1	1	2552	OMU	C6-N1	5.93	1.43	1.35
2	2	966	2MG	C6-N1	5.69	1.42	1.33
1	1	1618	6MZ	C6-N6	5.64	1.44	1.35
1	1	2069	G7M	C6-N1	5.60	1.42	1.33
2	2	527	G7M	C2-N2	5.56	1.45	1.33
1	1	2030	6MZ	C6-N6	5.54	1.44	1.35
1	1	2552	OMU	C2-N3	5.50	1.49	1.38
2	2	1516	2MG	C6-N1	5.40	1.42	1.33
2	2	1207	2MG	C6-N1	5.39	1.42	1.33
1	1	2251	OMG	C6-N1	5.38	1.42	1.33
2	2	1498	UR3	C6-C5	5.30	1.49	1.38
2	2	527	G7M	C6-N1	5.23	1.42	1.33
1	1	1915	3TD	C2-N1	5.18	1.48	1.38
1	1	1835	2MG	C6-N1	5.18	1.42	1.33
1	1	1915	3TD	C6-N1	5.16	1.45	1.34
1	1	2498	OMC	C4-N3	5.12	1.43	1.35
1	1	1962	5MC	C2-N3	5.11	1.48	1.38
2	2	967	5MC	C2-N3	5.03	1.48	1.38
1	1	2069	G7M	C2-N2	5.01	1.43	1.33
1	1	2445	2MG	C6-N1	4.97	1.41	1.33
2	2	967	5MC	C5-C4	4.94	1.49	1.41
1	1	2498	OMC	C2-N3	4.93	1.47	1.38
2	2	1498	UR3	C4-N3	4.90	1.45	1.38
1	1	1915	3TD	C4-N3	4.86	1.45	1.38
1	1	2503	2MA	C2-N1	4.77	1.42	1.34
1	1	1939	5MU	C4-N3	-4.76	1.24	1.33
2	2	1402	4OC	C2-N3	4.74	1.47	1.38
2	2	1407	5MC	C2-N3	4.74	1.47	1.38
2	2	1402	4OC	C4-N3	4.72	1.43	1.34
1	1	2069	G7M	C2-N1	4.71	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1402	4OC	C6-C5	4.68	1.48	1.38
1	1	747	5MU	C4-N3	-4.68	1.24	1.33
2	2	527	G7M	C2-N1	4.68	1.43	1.35
54	z	17	OMG	C2-N2	4.56	1.43	1.33
1	1	1962	5MC	C4-N4	4.49	1.45	1.34
2	2	967	5MC	C4-N4	4.46	1.45	1.34
2	2	1407	5MC	C5-C4	4.36	1.48	1.41
1	1	2498	OMC	C6-C5	4.34	1.47	1.38
1	1	1962	5MC	C5-C4	4.30	1.48	1.41
1	1	2552	OMU	C6-C5	4.25	1.47	1.38
54	z	66	5MU	C4-N3	-4.18	1.25	1.33
1	1	1915	3TD	C5-C4	4.11	1.50	1.41
2	2	1402	4OC	C4-N4	4.01	1.44	1.36
1	1	2503	2MA	C6-N1	4.00	1.43	1.35
2	2	1407	5MC	C4-N4	3.96	1.44	1.34
1	1	2251	OMG	C2-N1	3.91	1.42	1.35
2	2	966	2MG	C2-N3	3.85	1.46	1.34
54	z	17	OMG	C2-N3	3.84	1.52	1.34
1	1	745	1MG	O6-C6	-3.81	1.15	1.24
1	1	2069	G7M	C5-C4	-3.77	1.34	1.39
1	1	1835	2MG	C2-N3	3.76	1.46	1.34
1	1	2251	OMG	C2-N2	3.75	1.41	1.33
2	2	1207	2MG	C2-N3	3.62	1.45	1.34
2	2	1516	2MG	C2-N3	3.53	1.45	1.34
2	2	1402	4OC	C5-C4	3.53	1.47	1.39
1	1	2445	2MG	C2-N3	3.45	1.45	1.34
1	1	2605	PSU	C5-C1'	-3.40	1.49	1.52
2	2	1519	MA6	C5-C4	-3.27	1.32	1.40
1	1	1915	3TD	C5-C1'	-3.23	1.49	1.52
1	1	1911	PSU	C5-C1'	-3.23	1.49	1.52
1	1	2580	PSU	C5-C1'	-3.23	1.49	1.52
1	1	2498	OMC	C4-N4	3.20	1.44	1.35
2	2	1518	MA6	C5-C4	-3.17	1.32	1.40
2	2	967	5MC	C6-C5	3.15	1.48	1.40
2	2	1407	5MC	C6-C5	3.14	1.48	1.40
1	1	1917	PSU	C5-C1'	-3.11	1.49	1.52
1	1	2457	PSU	C5-C1'	-3.10	1.49	1.52
1	1	2030	6MZ	C5-C4	-3.04	1.32	1.40
2	2	1516	2MG	C2-N1	3.03	1.43	1.34
1	1	1618	6MZ	C5-C4	-3.01	1.33	1.40
2	2	966	2MG	C2-N1	2.97	1.43	1.34
1	1	2504	PSU	C5-C1'	-2.96	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	955	PSU	C5-C1'	-2.95	1.49	1.52
2	2	527	G7M	C5-C4	-2.87	1.35	1.39
1	1	1962	5MC	C6-C5	2.86	1.48	1.40
2	2	1207	2MG	C2-N1	2.84	1.43	1.34
1	1	747	5MU	O4-C4	-2.78	1.17	1.24
1	1	1835	2MG	C2-N1	2.75	1.43	1.34
1	1	1911	PSU	C4-N3	2.71	1.37	1.33
1	1	746	PSU	C4-N3	2.68	1.37	1.33
1	1	1939	5MU	O4-C4	-2.68	1.17	1.24
1	1	2445	2MG	C2-N1	2.67	1.42	1.34
1	1	1917	PSU	C4-N3	2.66	1.37	1.33
1	1	1915	3TD	O4-C4	-2.66	1.17	1.24
1	1	2251	OMG	O6-C6	-2.62	1.18	1.24
54	z	66	5MU	O4-C4	-2.55	1.18	1.24
1	1	2457	PSU	C4-N3	2.53	1.37	1.33
2	2	516	PSU	C4-N3	2.51	1.37	1.33
1	1	2498	OMC	C5-C4	2.49	1.47	1.41
1	1	2580	PSU	C4-N3	2.46	1.37	1.33
2	2	527	G7M	O6-C6	-2.46	1.18	1.24
1	1	2445	2MG	O6-C6	-2.46	1.18	1.24
1	1	2504	PSU	C4-N3	2.45	1.37	1.33
1	1	2069	G7M	O6-C6	-2.42	1.18	1.24
1	1	955	PSU	C4-N3	2.42	1.37	1.33
1	1	1835	2MG	O6-C6	-2.41	1.18	1.24
2	2	527	G7M	C2-N3	2.38	1.45	1.34
2	2	1518	MA6	C2-N3	2.37	1.35	1.32
2	2	1207	2MG	O6-C6	-2.37	1.18	1.24
1	1	2605	PSU	C4-N3	2.34	1.37	1.33
2	2	1516	2MG	O6-C6	-2.33	1.18	1.24
1	1	2552	OMU	O4-C4	-2.33	1.18	1.24
2	2	1519	MA6	C2-N3	2.31	1.35	1.32
1	1	2251	OMG	C2-N3	2.24	1.45	1.34
2	2	966	2MG	O6-C6	-2.23	1.18	1.24
1	1	1915	3TD	O4'-C1'	-2.22	1.41	1.44
1	1	2503	2MA	C5-C4	-2.21	1.35	1.40
1	1	1911	PSU	O4'-C1'	-2.18	1.41	1.44
1	1	2504	PSU	O4'-C1'	-2.18	1.41	1.44
1	1	746	PSU	O4'-C1'	-2.18	1.41	1.44
1	1	2580	PSU	O4'-C1'	-2.17	1.41	1.44
2	2	516	PSU	C5-C1'	-2.16	1.50	1.52
1	1	1917	PSU	O4'-C1'	-2.11	1.41	1.44
1	1	955	PSU	O4'-C1'	-2.11	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2457	PSU	O4'-C1'	-2.09	1.41	1.44
1	1	2069	G7M	C2-N3	2.08	1.44	1.34
1	1	2445	2MG	C2'-C1'	-2.06	1.50	1.53
1	1	2445	2MG	C5-C4	-2.04	1.35	1.40
1	1	2030	6MZ	C6-N1	-2.03	1.31	1.34

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1519	MA6	N1-C6-N6	-14.51	101.79	117.06
2	2	1518	MA6	N1-C6-N6	-12.76	103.63	117.06
1	1	1618	6MZ	C1'-N9-C4	-11.97	105.60	126.64
1	1	2030	6MZ	C1'-N9-C4	-11.50	106.44	126.64
1	1	746	PSU	N3-C2-N1	-10.66	119.95	128.43
2	2	516	PSU	N3-C2-N1	-10.66	119.96	128.43
1	1	1917	PSU	N3-C2-N1	-10.04	120.45	128.43
1	1	1911	PSU	N3-C2-N1	-10.03	120.46	128.43
1	1	2605	PSU	N3-C2-N1	-9.87	120.58	128.43
1	1	955	PSU	N3-C2-N1	-9.86	120.59	128.43
1	1	2504	PSU	N3-C2-N1	-9.83	120.62	128.43
1	1	745	1MG	C1'-N9-C4	-9.62	109.74	126.64
1	1	2457	PSU	N3-C2-N1	-9.41	120.95	128.43
1	1	2580	PSU	N3-C2-N1	-9.19	121.12	128.43
1	1	1939	5MU	C5-C6-N1	-8.39	113.15	122.19
1	1	747	5MU	C5-C6-N1	-8.07	113.50	122.19
54	z	66	5MU	C5-C6-N1	-7.42	114.19	122.19
2	2	527	G7M	C1'-N9-C4	7.16	139.23	126.64
54	z	66	5MU	C2-N3-C4	6.77	120.86	115.14
1	1	1939	5MU	C2-N3-C4	6.16	120.34	115.14
1	1	747	5MU	C2-N3-C4	6.03	120.23	115.14
54	z	17	OMG	OP3-P-OP1	-5.87	87.70	110.68
1	1	2503	2MA	C1'-N9-C4	5.64	136.56	126.64
54	z	17	OMG	C4-C5-C6	-5.60	115.45	120.80
1	1	2605	PSU	C5-C1'-C2'	-5.49	105.53	115.32
2	2	1519	MA6	N3-C2-N1	-5.46	120.14	128.68
54	z	17	OMG	OP3-P-O5'	-5.35	92.51	106.73
1	1	1618	6MZ	C9-N6-C6	-5.32	118.29	122.87
2	2	1518	MA6	N3-C2-N1	-5.28	120.42	128.68
1	1	1618	6MZ	N3-C2-N1	-5.28	120.42	128.68
1	1	2069	G7M	C1'-N9-C4	5.27	135.90	126.64
1	1	2504	PSU	C2-N3-C4	5.18	119.52	115.14
2	2	527	G7M	N3-C2-N1	-5.13	120.38	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	746	PSU	C2-N3-C4	5.13	119.47	115.14
54	z	17	OMG	OP3-P-OP2	-5.12	88.07	107.64
54	z	17	OMG	OP2-P-OP1	5.03	130.36	110.68
1	1	2030	6MZ	N3-C2-N1	-4.97	120.90	128.68
1	1	2580	PSU	O4'-C1'-C5	4.95	117.60	109.93
2	2	516	PSU	C2-N3-C4	4.90	119.28	115.14
1	1	2069	G7M	N3-C2-N1	-4.89	120.70	127.22
1	1	955	PSU	C2-N3-C4	4.78	119.17	115.14
1	1	1917	PSU	C2-N3-C4	4.74	119.14	115.14
1	1	2580	PSU	C5-C4-N3	-4.67	119.35	125.36
1	1	1835	2MG	N2-C2-N3	4.66	121.44	116.96
2	2	1207	2MG	CM2-N2-C2	-4.56	118.08	123.59
1	1	1911	PSU	C5-C1'-C2'	-4.54	107.22	115.32
1	1	2580	PSU	C2-N3-C4	4.52	118.96	115.14
1	1	1911	PSU	C2-N3-C4	4.51	118.95	115.14
1	1	2457	PSU	C2-N3-C4	4.49	118.94	115.14
1	1	2457	PSU	C5-C4-N3	-4.46	119.61	125.36
1	1	2605	PSU	C2-N3-C4	4.39	118.85	115.14
1	1	955	PSU	C5-C4-N3	-4.38	119.72	125.36
1	1	2445	2MG	CM2-N2-C2	-4.37	118.31	123.59
1	1	1917	PSU	C5-C4-N3	-4.37	119.73	125.36
1	1	2504	PSU	C5-C4-N3	-4.36	119.74	125.36
1	1	1915	3TD	C5-C1'-C2'	-4.34	107.58	115.32
2	2	1402	4OC	CM4-N4-C4	-4.33	119.25	122.97
2	2	966	2MG	CM2-N2-C2	-4.29	118.41	123.59
1	1	2251	OMG	N3-C2-N1	-4.22	121.60	127.22
1	1	2605	PSU	C5-C4-N3	-4.19	119.97	125.36
1	1	1911	PSU	C5-C4-N3	-4.11	120.06	125.36
2	2	1516	2MG	C1'-N9-C4	-4.00	119.61	126.64
1	1	2605	PSU	C5-C6-N1	-3.96	119.57	124.44
1	1	746	PSU	C5-C4-N3	-3.96	120.26	125.36
1	1	1917	PSU	C5-C6-N1	-3.93	119.60	124.44
1	1	955	PSU	C5-C6-N1	-3.89	119.66	124.44
1	1	1911	PSU	C5-C6-N1	-3.88	119.67	124.44
1	1	2457	PSU	O4'-C1'-C5	3.87	115.92	109.93
1	1	1962	5MC	C4-N3-C2	3.80	120.60	116.02
1	1	2457	PSU	C5-C6-N1	-3.68	119.91	124.44
2	2	516	PSU	C5-C4-N3	-3.68	120.63	125.36
1	1	2503	2MA	C2-N3-C4	3.67	118.50	115.52
2	2	966	2MG	C2-N3-C4	3.63	119.40	115.28
1	1	2498	OMC	C4-N3-C2	3.59	119.98	116.34
2	2	1516	2MG	N2-C2-N1	3.56	120.38	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2445	2MG	C1'-N9-C4	-3.54	120.42	126.64
2	2	967	5MC	C4-N3-C2	3.53	120.28	116.02
1	1	2504	PSU	C5-C6-N1	-3.51	120.12	124.44
2	2	1407	5MC	C4-N3-C2	3.50	120.25	116.02
2	2	1516	2MG	C2-N3-C4	3.48	119.23	115.28
1	1	2580	PSU	C5-C6-N1	-3.46	120.19	124.44
2	2	1516	2MG	N3-C2-N1	-3.45	120.77	126.23
2	2	527	G7M	C2-N3-C4	3.43	119.27	115.36
54	z	17	OMG	N3-C2-N1	-3.42	122.67	127.22
1	1	2069	G7M	C2-N3-C4	3.39	119.23	115.36
2	2	1207	2MG	C1'-N9-C4	-3.38	120.71	126.64
2	2	516	PSU	C5-C6-N1	-3.35	120.33	124.44
2	2	1207	2MG	C2-N3-C4	3.32	119.05	115.28
1	1	1835	2MG	N3-C2-N1	-3.28	121.04	126.23
1	1	1835	2MG	C2-N3-C4	3.28	119.00	115.28
1	1	1911	PSU	C6-N1-C2	3.27	120.76	115.36
2	2	1516	2MG	CM2-N2-C2	-3.26	119.66	123.59
1	1	1915	3TD	C5-C6-N1	-3.23	120.46	124.44
1	1	746	PSU	C6-N1-C2	3.22	120.67	115.36
2	2	966	2MG	N3-C2-N1	-3.22	121.14	126.23
1	1	1835	2MG	CM2-N2-C2	-3.21	119.72	123.59
1	1	2605	PSU	C6-N1-C2	3.20	120.64	115.36
2	2	1207	2MG	N3-C2-N1	-3.19	121.19	126.23
2	2	966	2MG	C1'-N9-C4	-3.18	121.05	126.64
1	1	955	PSU	C6-N1-C2	3.15	120.56	115.36
1	1	1917	PSU	C6-N1-C2	3.15	120.55	115.36
2	2	516	PSU	C6-N1-C2	3.14	120.54	115.36
1	1	1962	5MC	N4-C4-N3	3.11	121.44	117.03
55	B	1	FME	C-CA-N	3.11	115.34	109.73
2	2	966	2MG	N2-C2-N3	3.10	119.94	116.96
1	1	2069	G7M	C5-C6-N1	-3.09	119.20	123.43
1	1	746	PSU	C5-C6-N1	-3.08	120.66	124.44
2	2	527	G7M	C5-C6-N1	-3.07	119.24	123.43
1	1	2030	6MZ	C9-N6-C6	-3.06	120.23	122.87
54	z	17	OMG	O5'-P-OP1	3.03	114.97	106.47
1	1	745	1MG	C2-N3-C4	3.00	118.78	115.36
1	1	2445	2MG	C5-C6-N1	-2.99	119.34	123.43
1	1	1835	2MG	C5-C6-N1	-2.96	119.38	123.43
54	z	17	OMG	OP2-P-O5'	2.96	114.61	106.73
2	2	1207	2MG	C5-C6-N1	-2.95	119.40	123.43
1	1	2445	2MG	N3-C2-N1	-2.95	121.57	126.23
1	1	2069	G7M	N2-C2-N1	2.94	121.82	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2445	2MG	C2-N3-C4	2.93	118.60	115.28
1	1	1915	3TD	C6-N1-C2	2.89	120.13	115.36
1	1	2504	PSU	C6-N1-C2	2.88	120.12	115.36
1	1	2251	OMG	C5-C6-N1	-2.88	119.49	123.43
2	2	966	2MG	C5-C6-N1	-2.86	119.52	123.43
1	1	2605	PSU	O4'-C1'-C5	2.84	114.32	109.93
1	1	2457	PSU	C6-N1-C2	2.82	120.02	115.36
2	2	1516	2MG	C5-C6-N1	-2.82	119.58	123.43
1	1	2251	OMG	C2-N3-C4	2.80	118.55	115.36
2	2	1498	UR3	C3U-N3-C4	2.77	121.78	118.12
1	1	2445	2MG	N2-C2-N3	2.73	119.58	116.96
1	1	2503	2MA	C5-C6-N1	-2.68	120.25	123.06
1	1	2580	PSU	C6-N1-C2	2.66	119.75	115.36
1	1	745	1MG	N2-C2-N3	2.65	121.70	117.40
1	1	2503	2MA	N3-C2-N1	-2.65	120.85	125.72
1	1	1835	2MG	C1'-N9-C4	-2.63	122.03	126.64
2	2	1207	2MG	N2-C2-N1	2.59	119.44	116.96
2	2	527	G7M	C2-N1-C6	2.58	120.03	115.93
1	1	746	PSU	O4'-C1'-C5	2.54	113.86	109.93
1	1	1835	2MG	C2-N1-C6	2.53	119.70	115.18
2	2	1207	2MG	N2-C2-N3	2.50	119.36	116.96
1	1	2504	PSU	C5-C1'-C2'	-2.50	110.87	115.32
2	2	1207	2MG	C2-N1-C6	2.45	119.56	115.18
1	1	2498	OMC	CM2-O2'-C2'	-2.44	108.12	114.52
2	2	1516	2MG	C2-N1-C6	2.40	119.47	115.18
2	2	1407	5MC	C5-C6-N1	-2.40	119.61	122.19
1	1	2580	PSU	O4'-C1'-C2'	2.36	108.49	104.66
1	1	2552	OMU	CM2-O2'-C2'	-2.33	108.41	114.52
1	1	2445	2MG	C2-N1-C6	2.32	119.33	115.18
2	2	966	2MG	C2-N1-C6	2.31	119.31	115.18
1	1	2457	PSU	O4'-C1'-C2'	2.27	108.34	104.66
1	1	1915	3TD	O4'-C1'-C5	2.25	113.42	109.93
1	1	2069	G7M	C2-N1-C6	2.19	119.40	115.93
44	p	89	0TD	CSB-SB-CB	2.18	106.15	101.85
1	1	2251	OMG	C2-N1-C6	2.10	119.26	115.93
1	1	1917	PSU	O4'-C1'-C2'	2.07	108.01	104.66
1	1	2498	OMC	N4-C4-N3	2.05	119.73	116.49
1	1	2580	PSU	C5-C1'-C2'	2.05	118.97	115.32
2	2	966	2MG	N2-C2-N1	2.04	118.92	116.96
54	z	17	OMG	C5-C6-N1	2.00	126.17	123.43

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	516	PSU	O4'-C1'-C5-C4
2	2	527	G7M	C3'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C10
44	p	89	0TD	CG-CB-SB-CSB
55	B	1	FME	O-C-CA-CB
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2504	PSU	O4'-C4'-C5'-O5'
54	z	17	OMG	C5'-O5'-P-OP2
54	z	17	OMG	C5'-O5'-P-OP3
54	z	17	OMG	C1'-C2'-O2'-CM2
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
2	2	527	G7M	O4'-C4'-C5'-O5'
2	2	966	2MG	O4'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C4'-C5'-O5'
2	2	1519	MA6	N1-C6-N6-C10
54	z	17	OMG	C3'-C2'-O2'-CM2
55	B	1	FME	N-CA-CB-CG
2	2	966	2MG	C3'-C4'-C5'-O5'
1	1	1835	2MG	C3'-C4'-C5'-O5'
1	1	1835	2MG	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
54	z	66	5MU	O4'-C4'-C5'-O5'
2	2	1518	MA6	C5-C6-N6-C10
2	2	1519	MA6	C5-C6-N6-C9
2	2	516	PSU	O4'-C1'-C5-C6
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	2503	2MA	C3'-C4'-C5'-O5'
54	z	66	5MU	C3'-C4'-C5'-O5'
2	2	527	G7M	C4'-C5'-O5'-P
1	1	746	PSU	O4'-C1'-C5-C6
1	1	746	PSU	O4'-C1'-C5-C4
1	1	1618	6MZ	N1-C6-N6-C9
2	2	1402	4OC	C3'-C4'-C5'-O5'
1	1	2580	PSU	C2'-C1'-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	B	1	FME	C-CA-CB-CG
1	1	2069	G7M	O4'-C4'-C5'-O5'
54	z	17	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 402 ligands modelled in this entry, 402 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

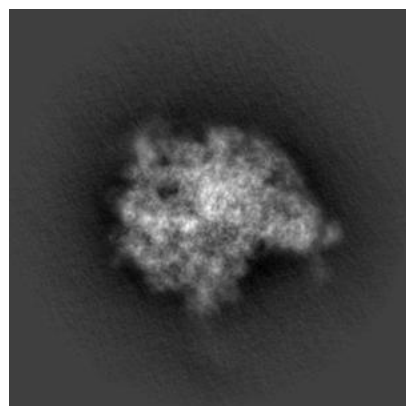
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12929. These allow visual inspection of the internal detail of the map and identification of artifacts.

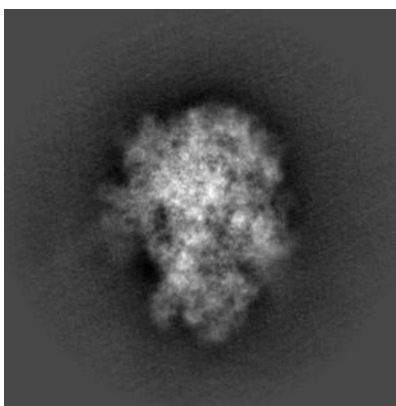
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

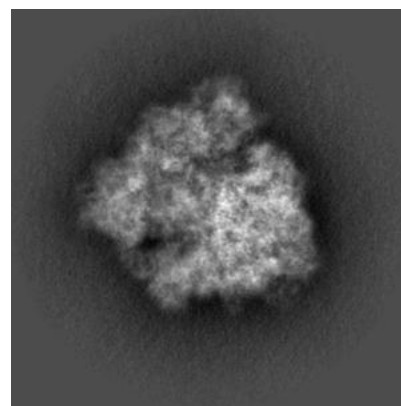
6.1.1 Primary map



X

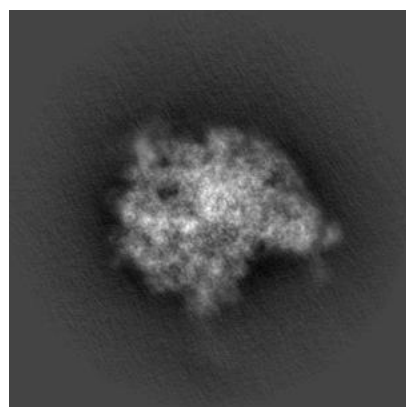


Y

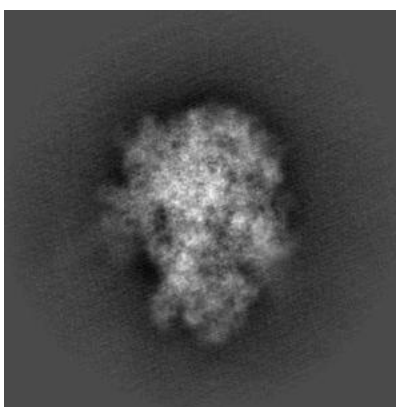


Z

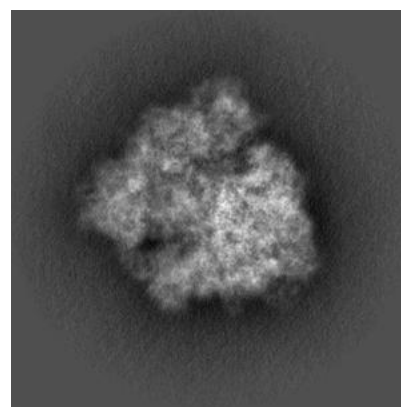
6.1.2 Raw map



X



Y

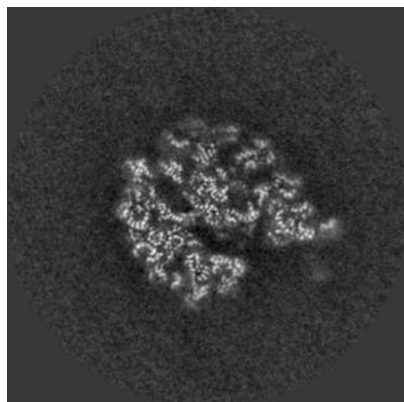


Z

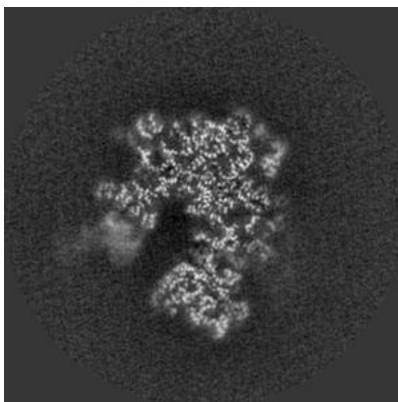
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

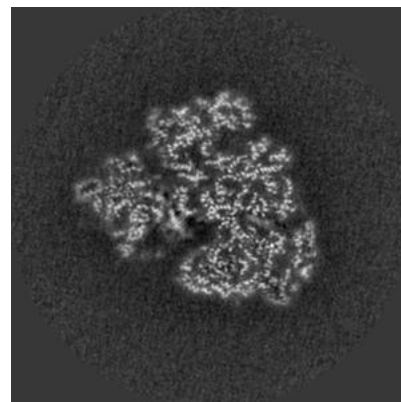
6.2.1 Primary map



X Index: 200

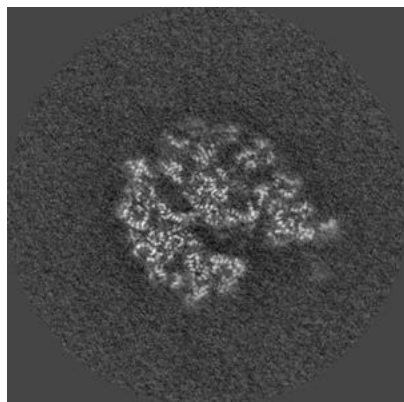


Y Index: 200

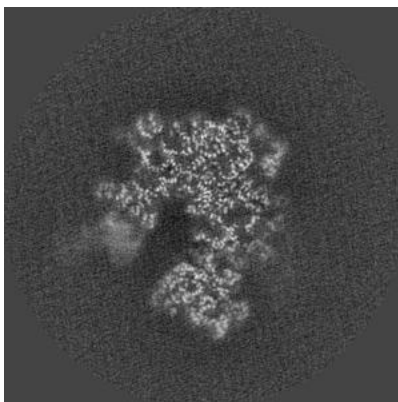


Z Index: 200

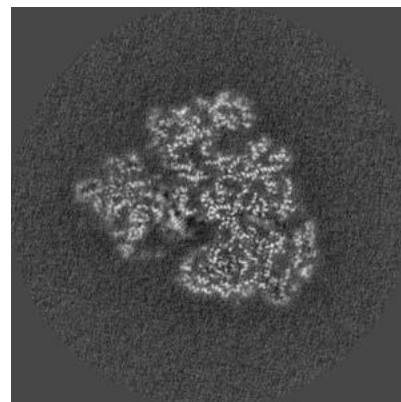
6.2.2 Raw map



X Index: 200



Y Index: 200

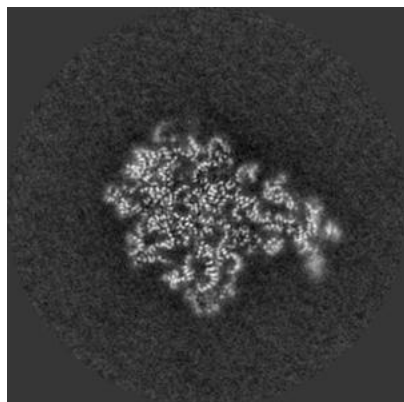


Z Index: 200

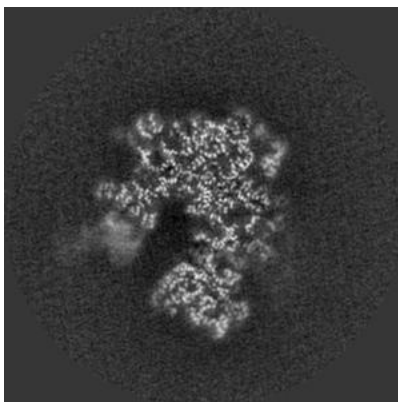
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

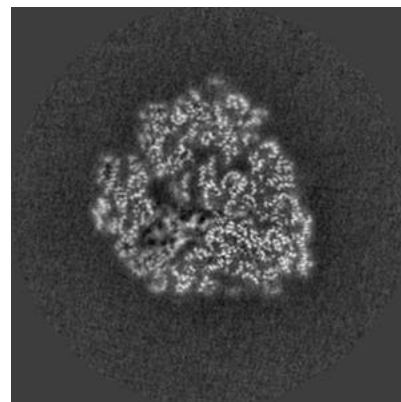
6.3.1 Primary map



X Index: 217

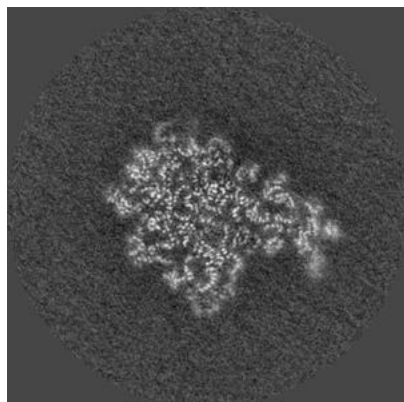


Y Index: 200

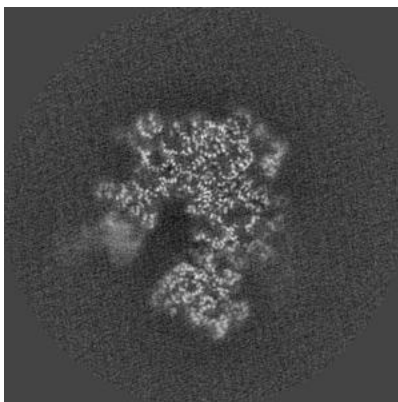


Z Index: 188

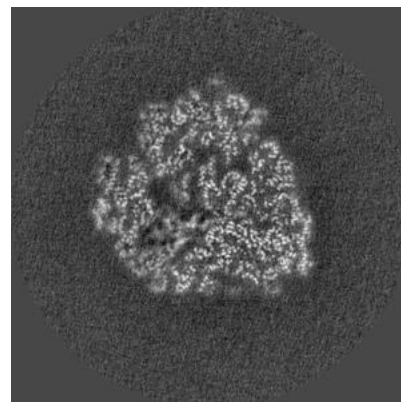
6.3.2 Raw map



X Index: 216



Y Index: 200



Z Index: 188

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



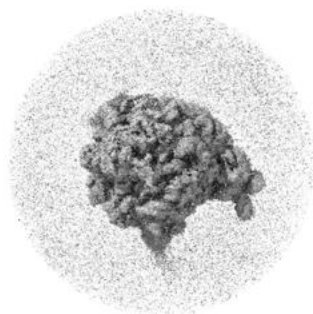
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

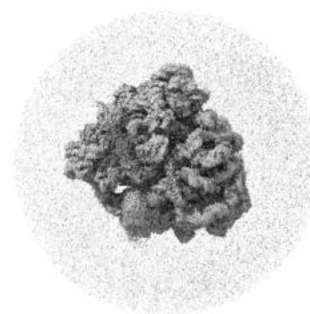
6.4.2 Raw map



X



Y



Z

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

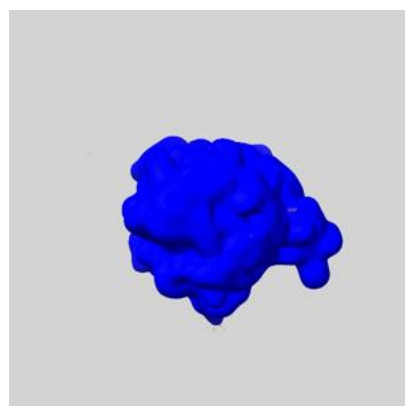
6.5 Mask visualisation [i](#)

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

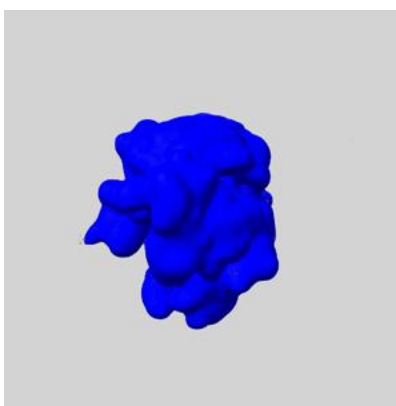
A mask typically either:

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

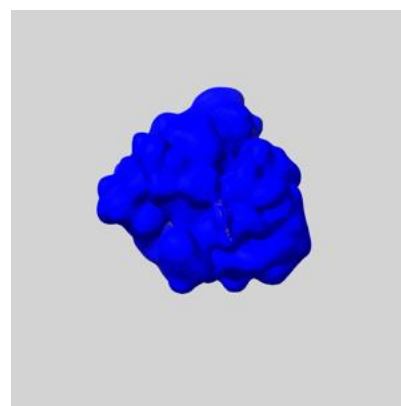
6.5.1 emd_12929_msk_1.map [i](#)



X



Y

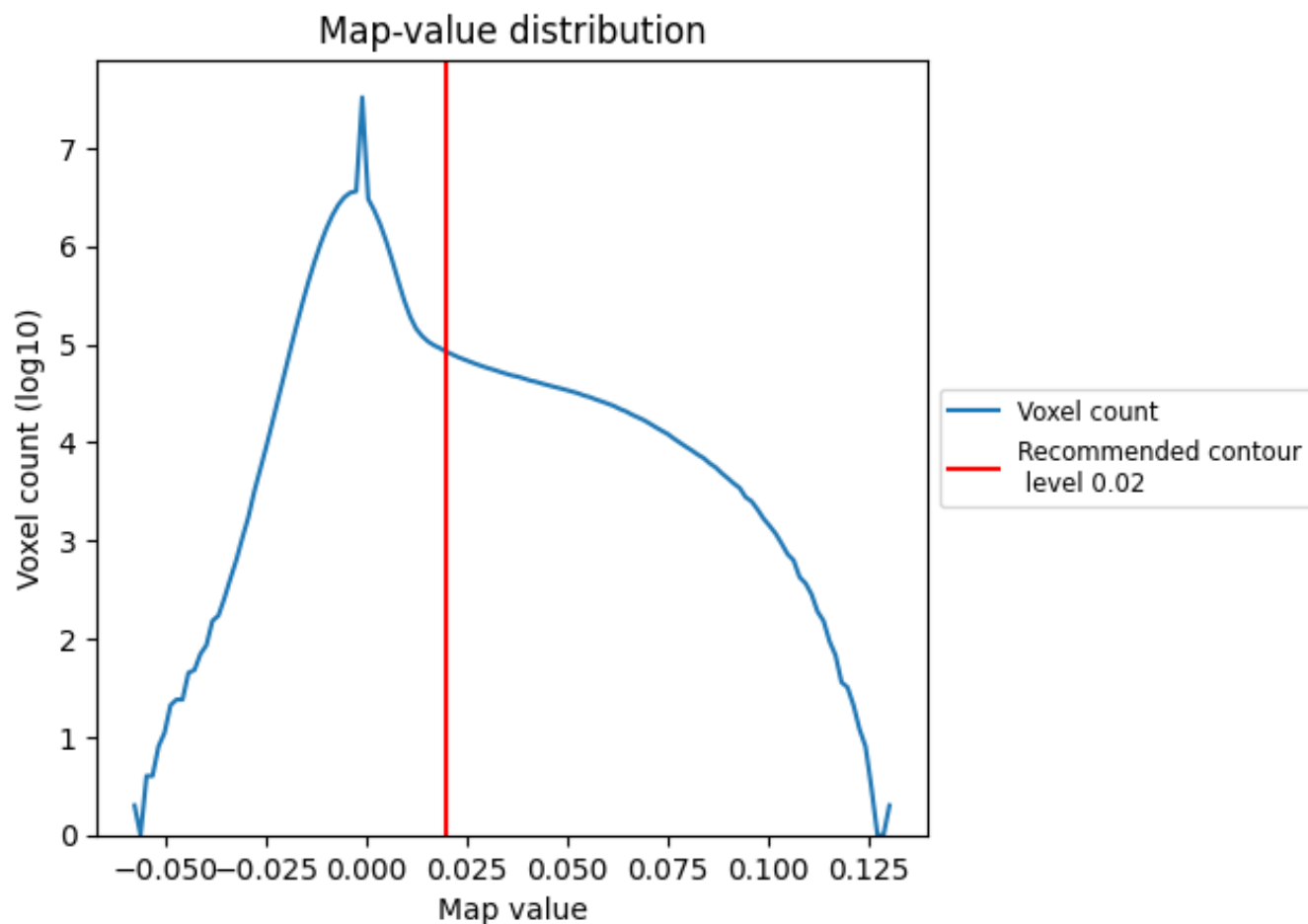


Z

7 Map analysis [i](#)

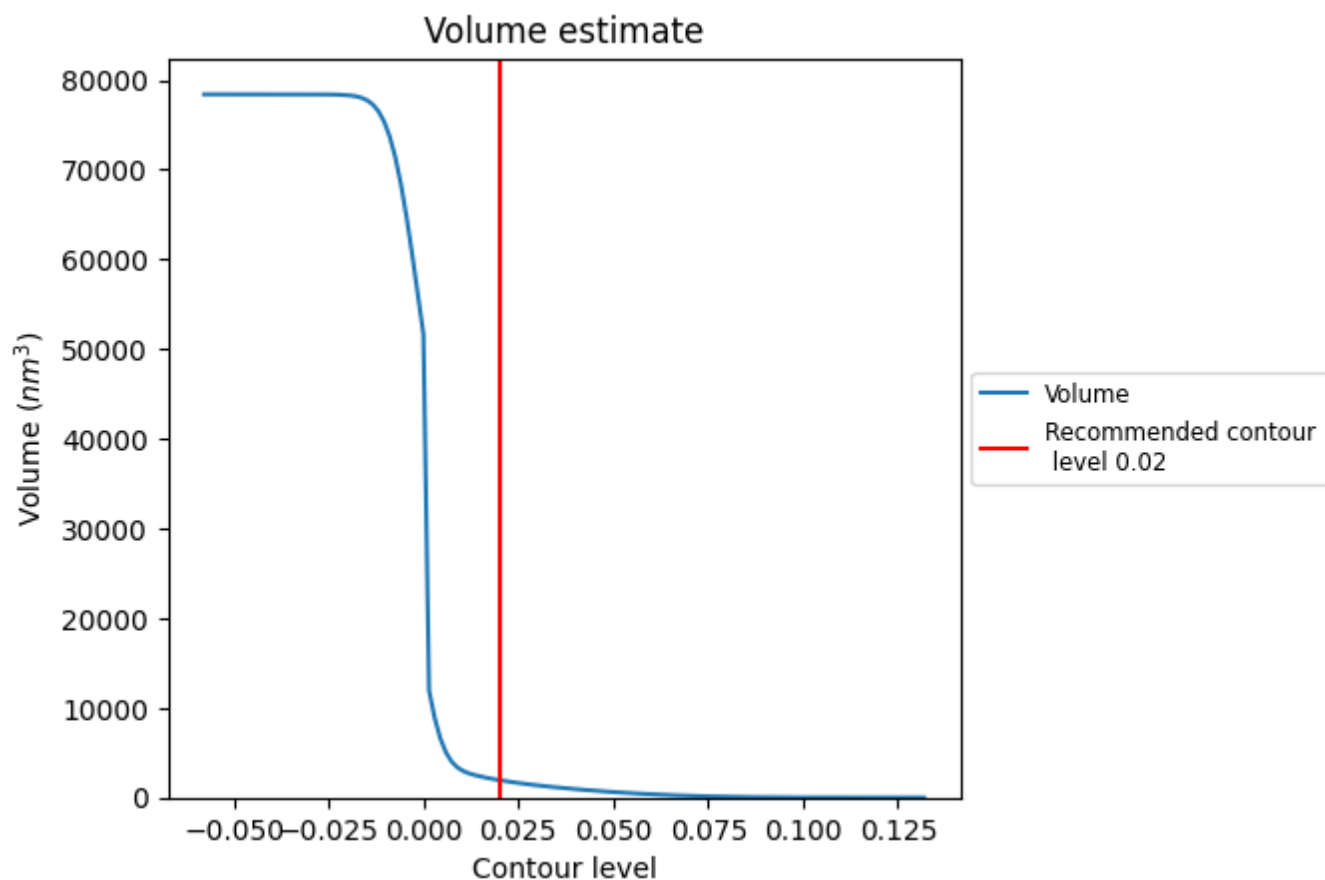
This section contains the results of statistical analysis of the map.

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.

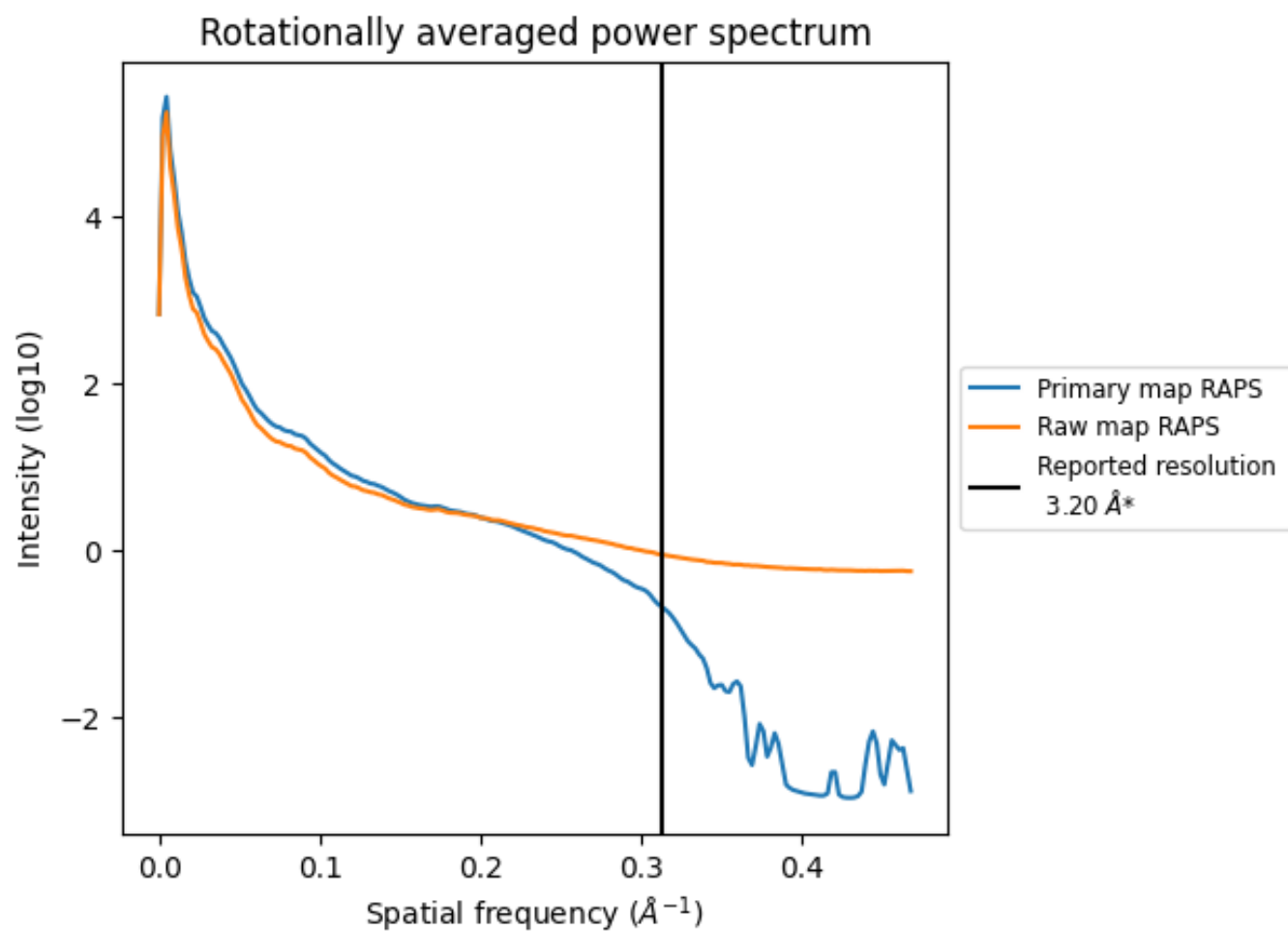
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1943 nm^3 ; this corresponds to an approximate mass of 1755 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 ⓘ

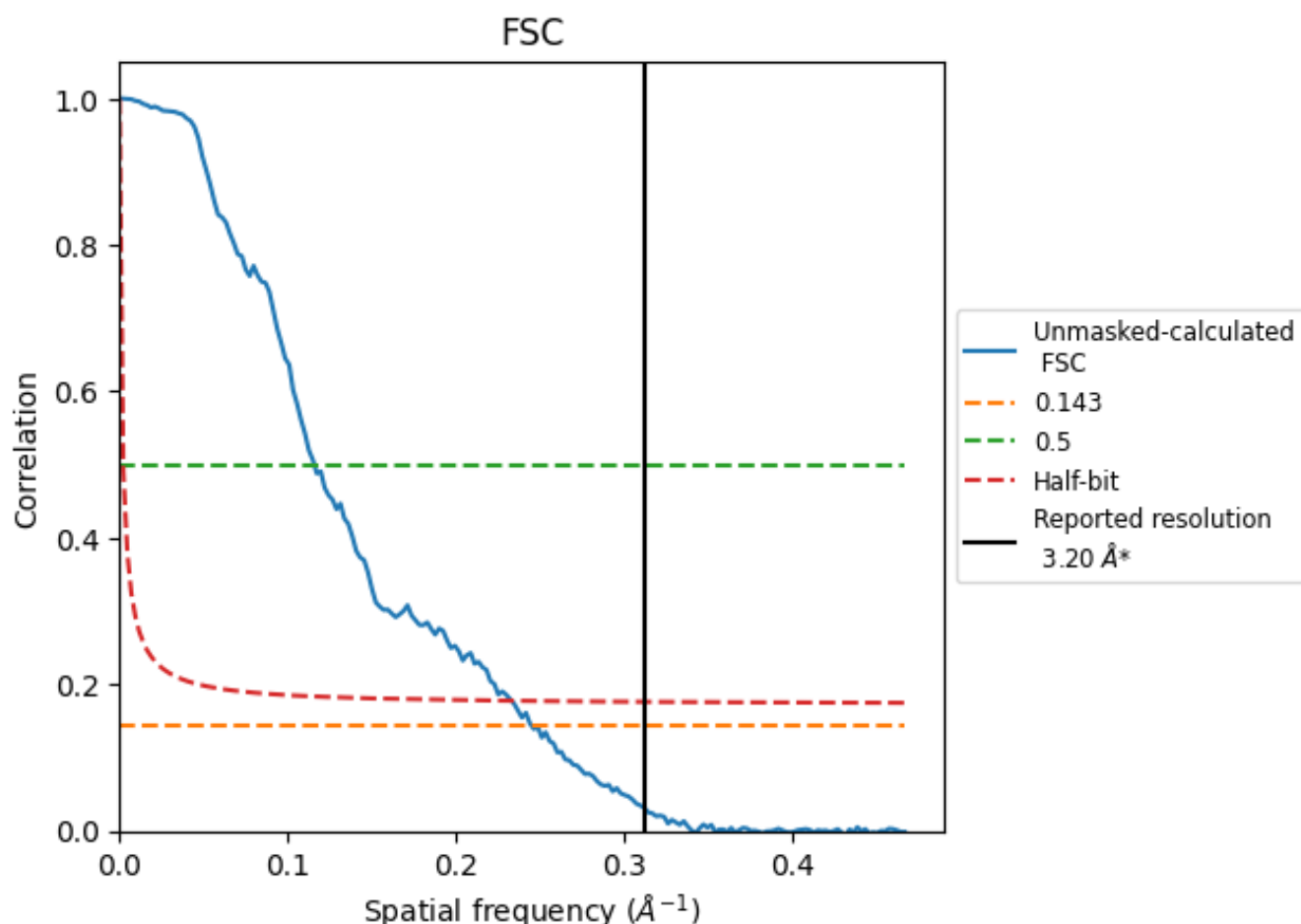


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

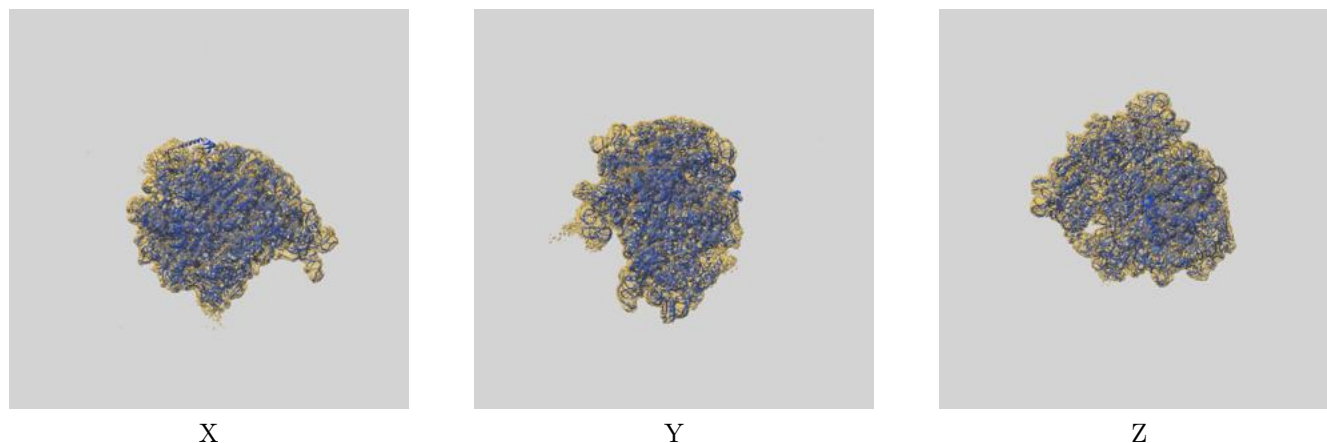
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.08	8.64	4.29

*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 4.08 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

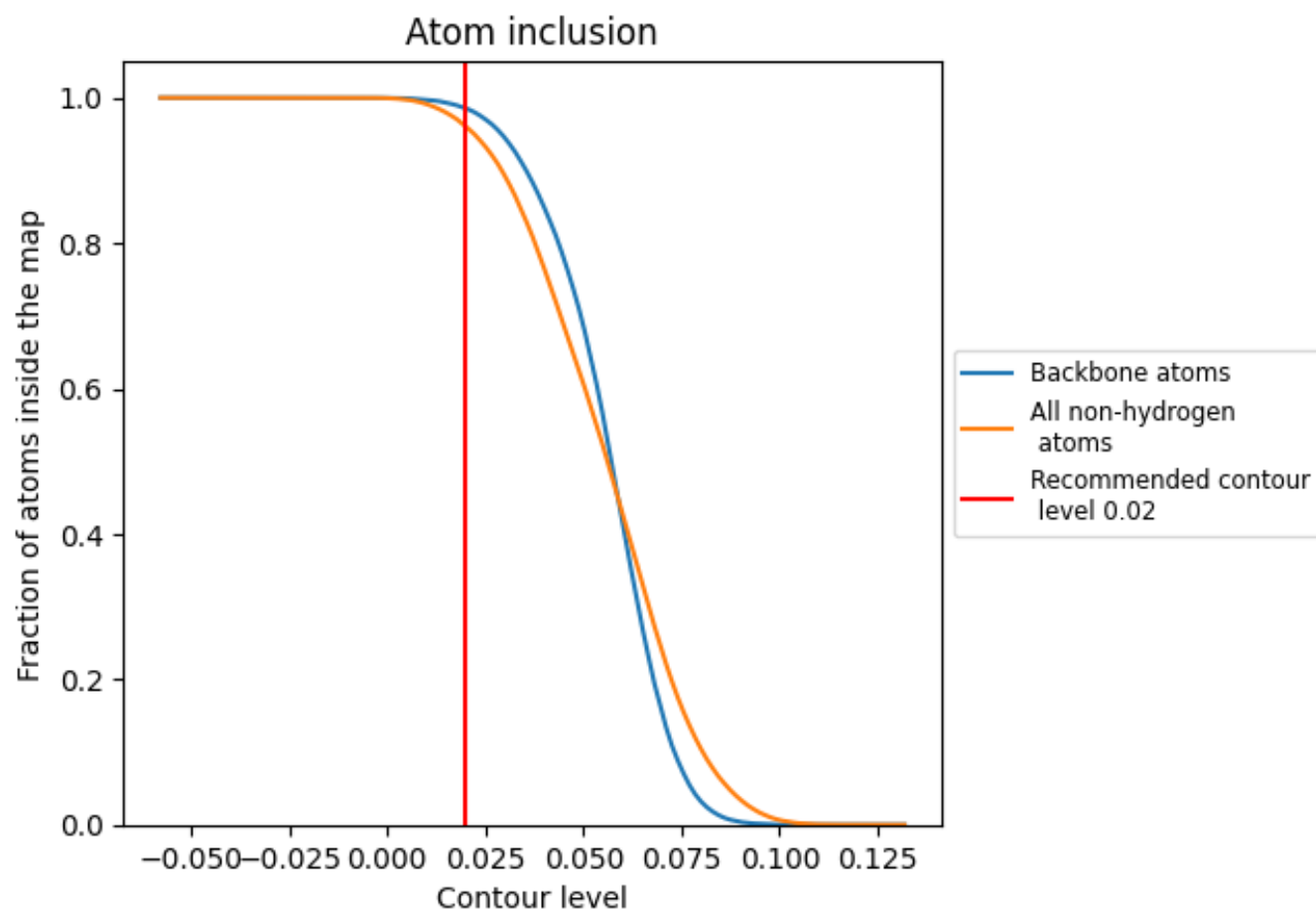
This section contains information regarding the fit between EMDB map EMD-12929 and PDB model 7OIG. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.02 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 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.