



Full wwPDB EM Validation Report ⓘ

Mar 9, 2024 – 12:32 PM EST

PDB ID : 6O8W
EMDB ID : EMD-0656
Title : Cryo-EM image reconstruction of the 70S Ribosome *Enterococcus faecalis* Class01
Authors : Jogl, G.; Khayat, R.
Deposited on : 2019-03-12
Resolution : 3.53 Å (reported)
Based on initial models : 4YBB, 5LI0

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:

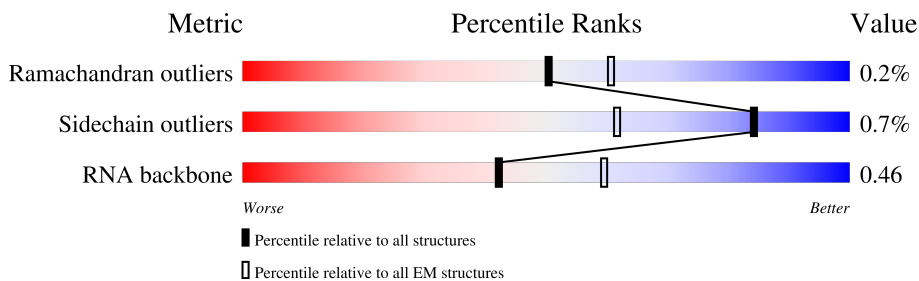
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.53 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.



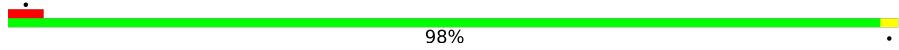
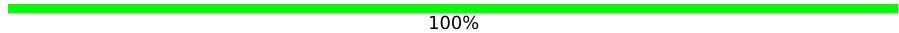
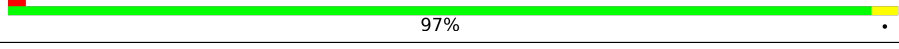
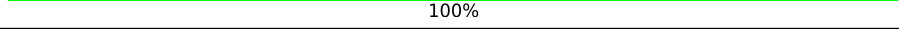
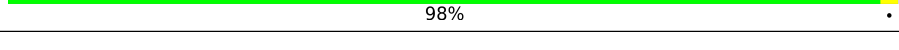
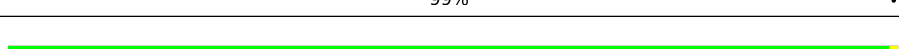
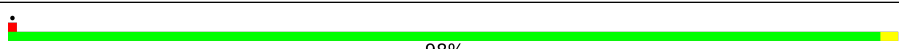
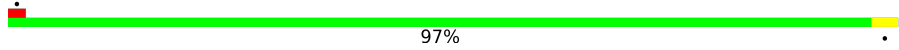
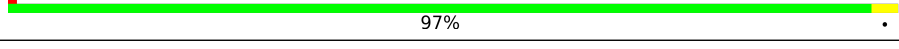
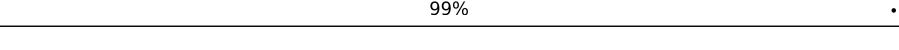



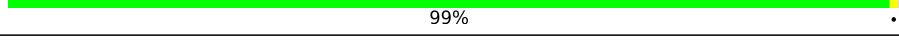
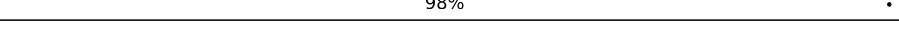

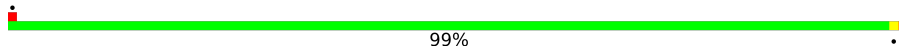
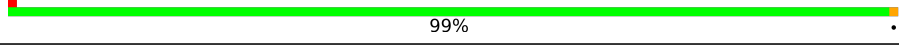
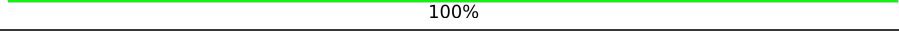
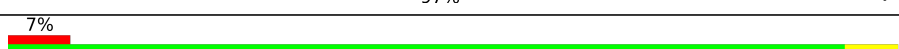
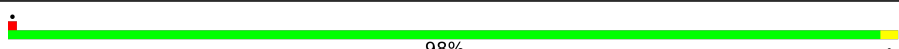



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	a	1523	
2	c	204	
3	d	201	
4	e	163	
5	f	97	
6	g	154	
7	h	131	
8	i	128	

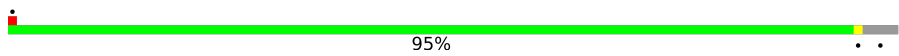
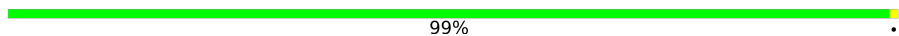
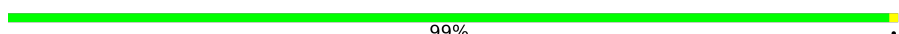
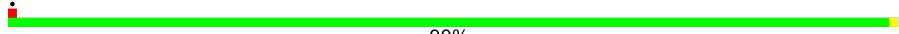




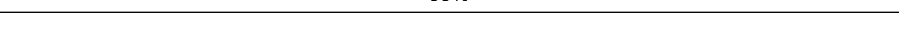
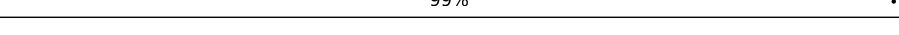
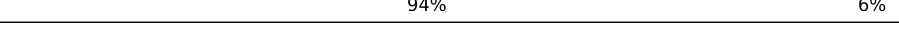
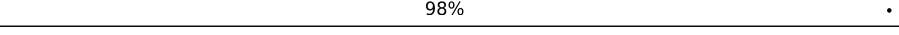
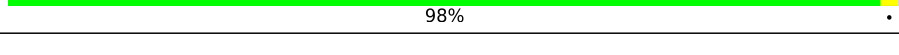
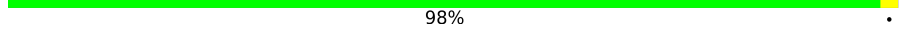
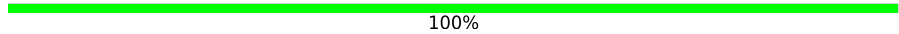
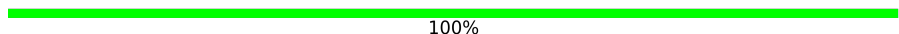
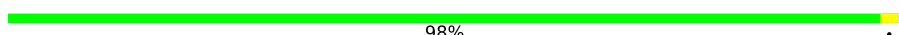
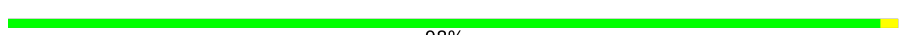
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Mol	Chain	Length	Quality of chain
9	j	99	 98%
10	k	117	 100%
11	l	136	 97%
12	m	112	 100%
13	n	60	 98%
14	o	88	 99%
15	p	89	 99%
16	q	83	 98%
17	r	66	 97%
18	s	78	 97%
19	t	81	 99%
20	u	76	 57% 36% 8%
21	v	5	 60% 40%
22	A	2903	 70% 27%
23	B	116	 59% 36%
24	C	275	 99%
25	D	207	 98%
26	E	206	 99%
27	F	177	 99%
28	G	176	 99%
29	K	145	 99%
30	L	122	 100%
31	M	146	 97%
32	N	141	 7% 94% 6%
33	O	123	98%

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Mol	Chain	Length	Quality of chain
34	P	117	 95%
35	Q	114	 99%
36	R	118	 99%
37	S	102	 99%
38	T	112	 100%
39	U	89	 96%
40	V	101	 94% 5%
41	W	94	 63% 99%
42	X	76	 99%
43	Y	54	 94% 6%
44	Z	61	 98%
45	0	58	 100%
46	1	59	 98%
47	2	56	 100%
48	3	49	 100%
49	4	44	 98%
50	5	64	 98%
51	6	38	 100%

2 Entry composition [i](#)

There are 52 unique types of molecules in this entry. The entry contains 139953 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1523	32646	14564	5967	10592	1523	0	0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	c	204	1610	1012	303	292	3	0	0

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	d	201	1620	1016	303	297	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	e	163	1204	759	222	221	2	0	0

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	f	97	795	501	137	154	3	0	0

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	g	154	1229	765	236	222	6	0	0

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	h	131	1041	662	184	193	2	0	0

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	i	128	990	615	197	177	1	0	0

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	j	99	800	504	147	147	2	0	0

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	k	117	863	533	165	161	4	0	0

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	l	136	1065	661	214	188	2	0	0

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	m	112	884	540	180	163	1	0	0

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	n	60	492	310	100	77	5	0	0

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	88	Total	C	N	O	S	0	0
			741	455	152	133	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	p	89	Total	C	N	O	S	0	0
			708	448	131	127	2		

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	q	83	Total	C	N	O	S	0	0
			681	427	127	124	3		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	r	66	Total	C	N	O	S	0	0
			537	343	99	94	1		

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	s	78	Total	C	N	O	S	0	0
			634	410	113	109	2		

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	t	81	Total	C	N	O	S	0	0
			610	372	119	117	2		

- Molecule 20 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	u	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 21 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	v	5	Total	C	N	O	P	0	0
			100	45	11	39	5		

- Molecule 22 is a RNA chain called 50S subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A	2903	Total	C	N	O	P	0	0
			62301	27808	11456	20134	2903		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	116	Total	C	N	O	P	0	0
			2478	1106	442	814	116		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C	275	Total	C	N	O	S	0	0
			2113	1310	415	381	7		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	D	207	Total	C	N	O	S	0	0
			1578	993	292	289	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	E	206	Total	C	N	O	S	0	0
			1573	983	290	298	2		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	177	Total	C	N	O	S	0	0
			1391	886	239	260	6		

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	176	Total	C	N	O	S	0	0
			1344	841	244	255	4		

- Molecule 29 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	K	145	Total	C	N	O	S	0	0
			1129	713	205	207	4		

- Molecule 30 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	L	122	Total	C	N	O	S	0	0
			921	573	176	170	2		

- Molecule 31 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	M	146	Total	C	N	O	S	0	0
			1094	676	212	205	1		

- Molecule 32 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	N	141	Total	C	N	O	S	0	0
			1118	710	216	185	7		

- Molecule 33 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	O	123	Total	C	N	O	S	0	0
			978	602	190	183	3		

- Molecule 34 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	P	112	Total	C	N	O	S	0	0
			862	533	169	159	1		

- Molecule 35 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Q	114	Total	C	N	O	0	0
			923	581	185	157		

- Molecule 36 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	R	118	Total	C	N	O	S	0	0
			950	602	184	160	4		

- Molecule 37 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	S	102	Total	C	N	O	S	0	0
			783	499	139	143	2		

- Molecule 38 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	T	112	Total	C	N	O	S	0	0
			848	531	156	159	2		

- Molecule 39 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	U	89	Total	C	N	O	S	0	0
			720	458	127	132	3		

- Molecule 40 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	V	101	Total	C	N	O	S	0	0
			762	485	135	140	2		

- Molecule 41 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	W	94	Total	C	N	O	S	0	0
			758	479	135	140	4		

- Molecule 42 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	X	76	Total	C	N	O	0	0
			571	350	109	112		

- Molecule 43 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Y	54	Total	C	N	O	S	0	0
			425	265	86	72	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	51	ALA	THR	conflict	UNP A0A1B4XRZ8

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Z	61	Total	C	N	O	S	0	0
			504	314	94	95	1		

- Molecule 45 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	0	58	Total	C	N	O	S	0	0
			434	270	81	82	1		

- Molecule 46 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1	59	Total	C	N	O	S	0	0
			472	300	74	96	2		

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2	56	Total	C	N	O	S	0	0
			428	261	88	73	6		

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	3	49	Total	C	N	O	S	0	0
			419	253	86	76	4		

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	4	44	Total	C	N	O	S	0	0
			374	227	91	54	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	5	64	Total	C	N	O	S	0	0
			521	320	122	77	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	6	38	Total	C	N	O	S	0	0
			304	188	66	44	6		

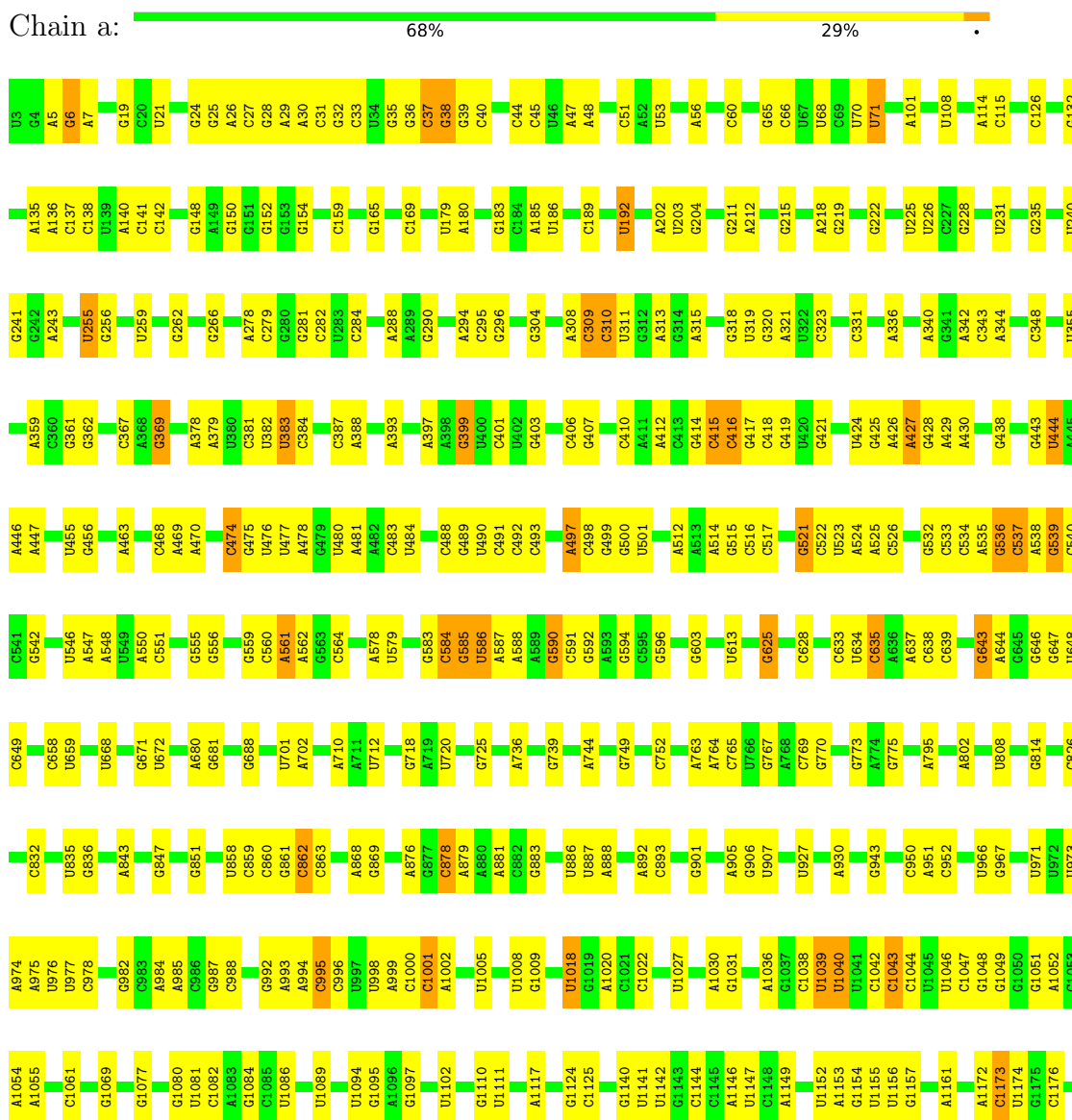
- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

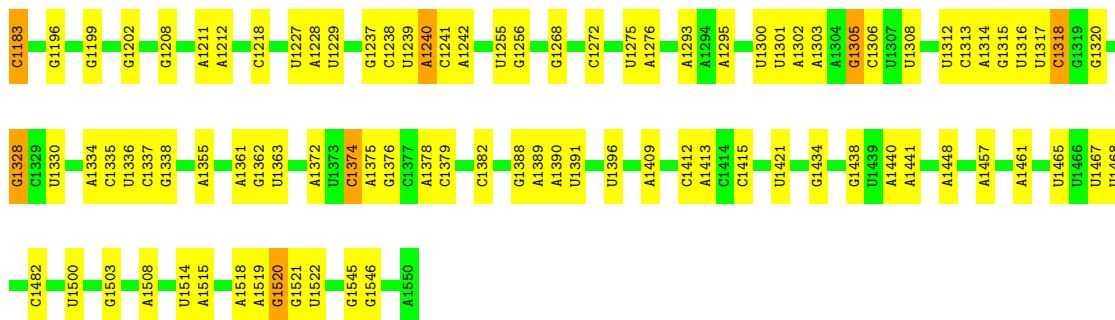
Mol	Chain	Residues	Atoms		AltConf
52	n	1	Total	Zn	0
			1	1	
52	2	1	Total	Zn	0
			1	1	
52	3	1	Total	Zn	0
			1	1	
52	6	1	Total	Zn	0
			1	1	

3 Residue-property plots

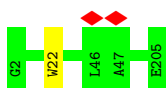
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

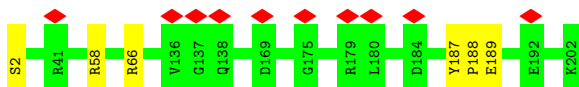




- Molecule 2: 30S ribosomal protein S3



- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5

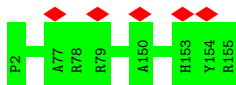


- Molecule 5: 30S ribosomal protein S6



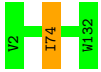
There are no outlier residues recorded for this chain.

- Molecule 6: 30S ribosomal protein S7



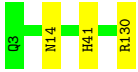
- Molecule 7: 30S ribosomal protein S8





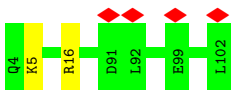
- Molecule 8: 30S ribosomal protein S9

Chain i: 98%



- Molecule 9: 30S ribosomal protein S10

Chain j: 98%



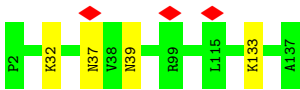
- Molecule 10: 30S ribosomal protein S11

Chain k: 100%

There are no outlier residues recorded for this chain.

- Molecule 11: 30S ribosomal protein S12

Chain l: 97%



- Molecule 12: 30S ribosomal protein S13

Chain m: 100%

There are no outlier residues recorded for this chain.

- Molecule 13: 30S ribosomal protein S14 type Z

Chain n: 98%



- Molecule 14: 30S ribosomal protein S15

Chain o: 99%



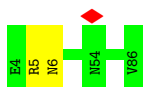
- Molecule 15: 30S ribosomal protein S16

Chain p:  99%



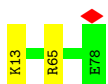
- Molecule 16: 30S ribosomal protein S17

Chain q:  98%



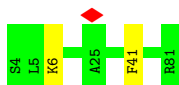
- Molecule 17: 30S ribosomal protein S18

Chain r:  97%



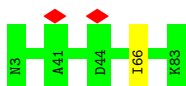
- Molecule 18: 30S ribosomal protein S19

Chain s:  97%



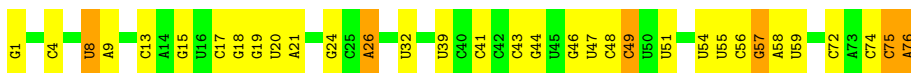
- Molecule 19: 30S ribosomal protein S20

Chain t:  99%



- Molecule 20: tRNA

Chain u:  57% 36% 8%

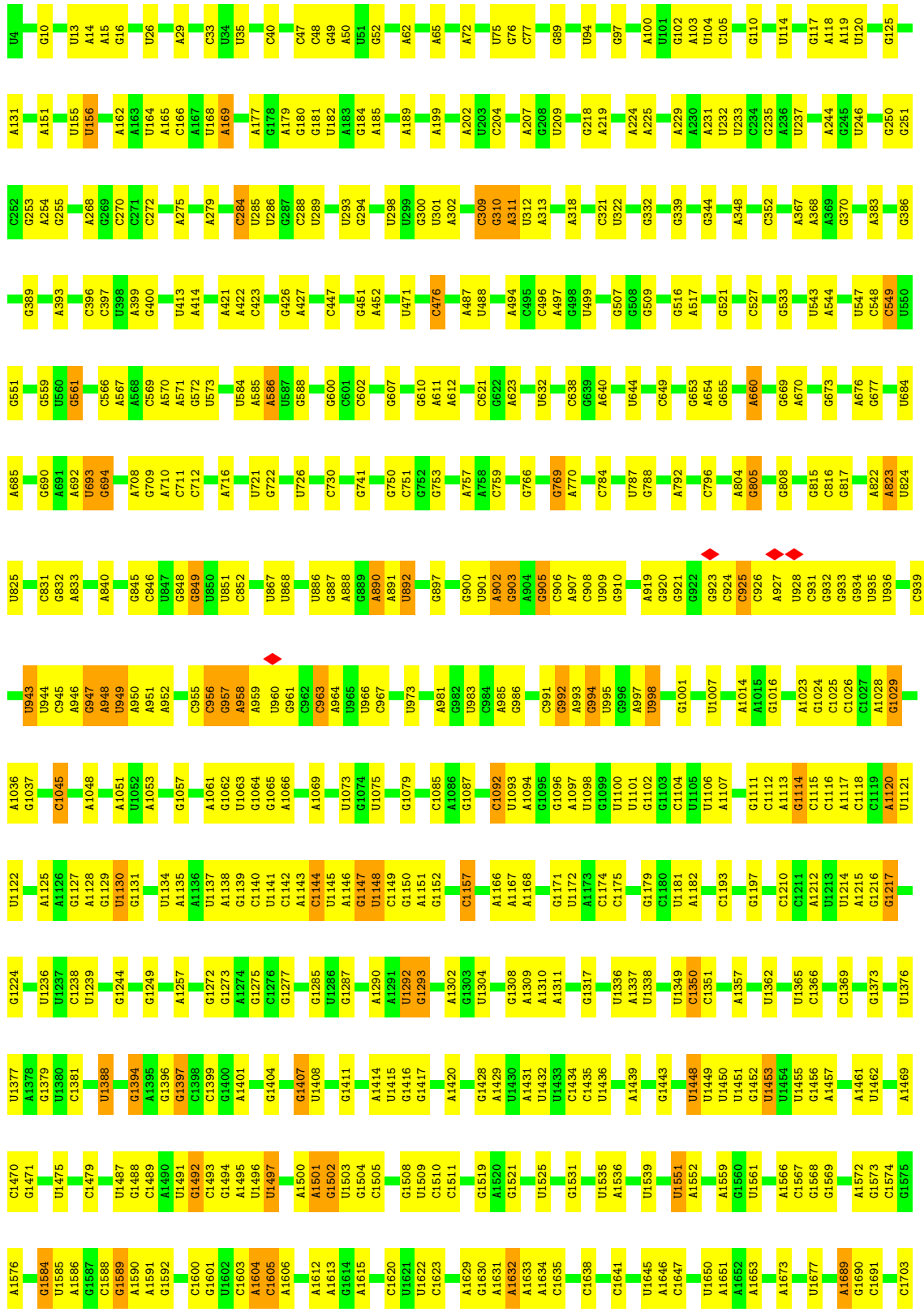


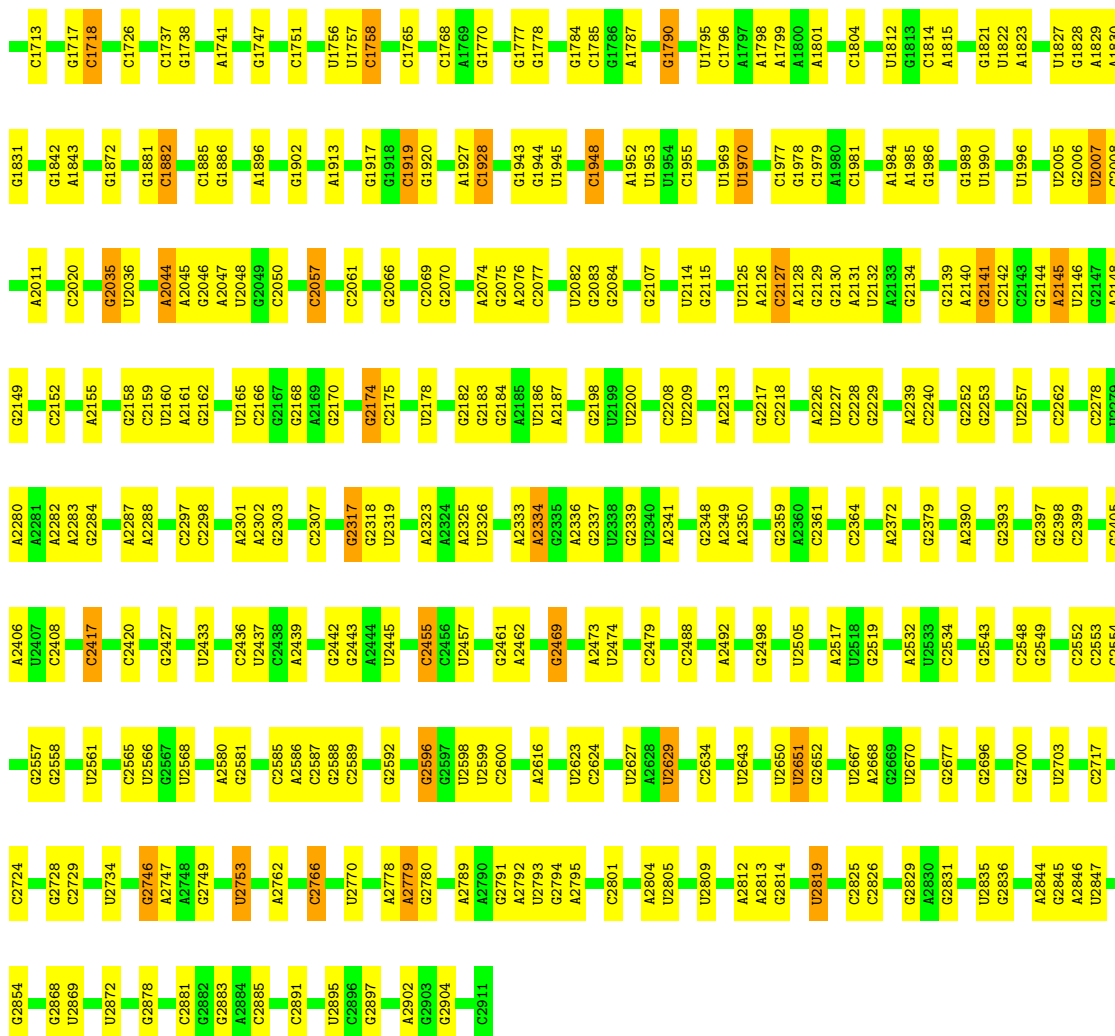
- Molecule 21: mRNA

Chain v:  60% 40%

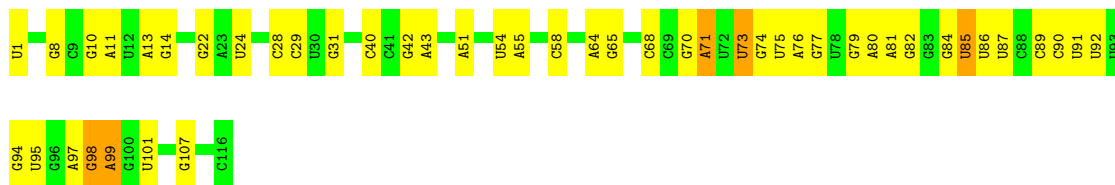


• Molecule 22: 50S subunit





• Molecule 23: 5S rRNA

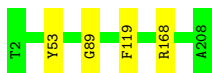


• Molecule 24: 50S ribosomal protein L2



• Molecule 25: 50S ribosomal protein L3

Chain D:  98%



- Molecule 26: 50S ribosomal protein L4

Chain E:  99%



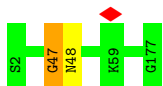
- Molecule 27: 50S ribosomal protein L5

Chain F:  99%



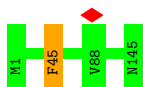
- Molecule 28: 50S ribosomal protein L6

Chain G:  99%



- Molecule 29: 50S ribosomal protein L13

Chain K:  99%



- Molecule 30: 50S ribosomal protein L14

Chain L:  100%

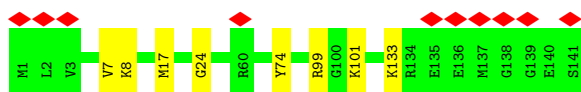
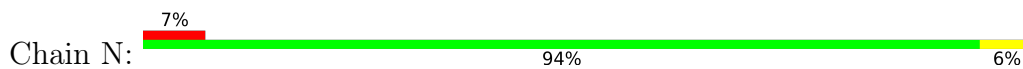
There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L15

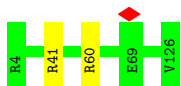
Chain M:  97%



- Molecule 32: 50S ribosomal protein L16



- Molecule 33: 50S ribosomal protein L17



- Molecule 34: 50S ribosomal protein L18



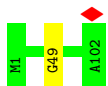
- Molecule 35: 50S ribosomal protein L19



- Molecule 36: 50S ribosomal protein L20



- Molecule 37: 50S ribosomal protein L21



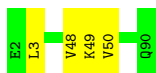
- Molecule 38: 50S ribosomal protein L22



There are no outlier residues recorded for this chain.

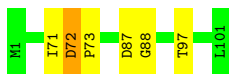
- Molecule 39: 50S ribosomal protein L23

Chain U:  96%



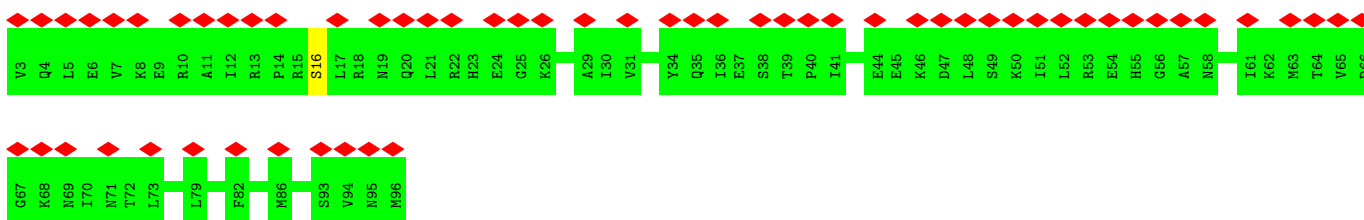
- Molecule 40: 50S ribosomal protein L24

Chain V:  94%



- Molecule 41: 50S ribosomal protein L25

Chain W:  63%



- Molecule 42: 50S ribosomal protein L27

Chain X:  99%



- Molecule 43: 50S ribosomal protein L28

Chain Y:  94%



- Molecule 44: 50S ribosomal protein L29

Chain Z:  98%



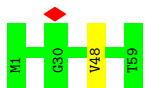
- Molecule 45: 50S ribosomal protein L30

Chain 0:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: 50S ribosomal protein L31 type B

Chain 1:  98%



- Molecule 47: 50S ribosomal protein L32

Chain 2:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 50S ribosomal protein L33

Chain 3:  100%

There are no outlier residues recorded for this chain.

- Molecule 49: 50S ribosomal protein L34

Chain 4:  98%



- Molecule 50: 50S ribosomal protein L35

Chain 5:  98%



- Molecule 51: 50S ribosomal protein L36

Chain 6:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35466	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.098	Depositor
Minimum map value	-0.790	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.238	Depositor
Map size (Å)	482.68, 482.68, 482.68	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.097, 1.097, 1.097	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	1.50	8/36545 (0.0%)	1.21	231/56995 (0.4%)
2	c	0.34	0/1635	0.57	0/2197
3	d	3.34	1/1650 (0.1%)	0.66	2/2217 (0.1%)
4	e	0.37	0/1217	0.62	0/1641
5	f	0.37	0/807	0.55	0/1087
6	g	0.31	0/1249	0.54	0/1682
7	h	0.37	0/1054	0.61	1/1417 (0.1%)
8	i	0.32	0/1003	0.59	0/1343
9	j	0.33	0/812	0.68	0/1093
10	k	0.34	0/878	0.60	0/1185
11	l	0.34	0/1082	0.66	0/1453
12	m	0.30	0/890	0.61	0/1195
13	n	0.33	0/504	0.55	0/669
14	o	0.35	0/751	0.59	0/1001
15	p	0.36	0/720	0.65	0/966
16	q	0.36	0/689	0.59	0/920
17	r	0.34	0/544	0.64	0/728
18	s	0.33	0/650	0.60	0/872
19	t	0.31	0/612	0.58	0/818
20	u	0.70	2/1813 (0.1%)	1.30	24/2823 (0.9%)
21	v	0.44	0/109	1.66	3/166 (1.8%)
22	A	0.99	9/69780 (0.0%)	1.23	504/108830 (0.5%)
23	B	0.82	3/2769 (0.1%)	1.31	25/4311 (0.6%)
24	C	0.57	0/2145	0.74	1/2881 (0.0%)
25	D	0.58	0/1599	0.76	0/2145
26	E	0.50	0/1594	0.63	0/2156
27	F	0.36	0/1409	0.65	0/1894
28	G	0.42	0/1362	0.66	0/1833
29	K	0.54	0/1148	0.71	0/1548
30	L	0.53	0/928	0.69	0/1245
31	M	0.47	0/1102	0.74	0/1470
32	N	0.49	0/1141	0.74	0/1519

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	O	0.54	0/985	0.82	2/1320 (0.2%)
34	P	0.45	0/870	0.62	0/1163
35	Q	0.54	0/935	0.68	0/1256
36	R	0.56	0/963	0.71	0/1280
37	S	0.53	0/793	0.68	0/1063
38	T	0.50	0/857	0.70	0/1156
39	U	0.52	0/727	0.76	2/972 (0.2%)
40	V	0.45	0/769	0.71	1/1027 (0.1%)
41	W	0.31	0/769	0.62	0/1034
42	X	0.59	0/576	0.68	0/770
43	Y	0.46	0/431	0.59	0/574
44	Z	0.40	0/505	0.60	0/672
45	0	0.46	0/434	0.67	0/583
46	1	0.35	0/486	0.67	0/661
47	2	0.56	0/434	0.66	0/575
48	3	0.43	0/423	0.56	0/563
49	4	0.50	0/377	0.63	0/491
50	5	0.46	0/527	0.67	0/687
51	6	0.52	0/309	0.63	0/409
All	All	1.09	23/152361 (0.0%)	1.12	796/228556 (0.3%)

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
2	c	0	1
3	d	0	3
11	l	0	2
18	s	0	1
19	t	0	1
24	C	0	3
25	D	0	2
26	E	0	1
27	F	0	1
28	G	0	1
29	K	0	1
31	M	0	2
32	N	0	5
33	O	0	1
35	Q	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
37	S	0	1
40	V	0	3
42	X	0	1
43	Y	0	1
46	1	0	1
49	4	0	1
All	All	0	34

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	d	2	SER	CA-CB	135.02	3.55	1.52
1	a	561	A	N3-C4	134.90	2.15	1.34
1	a	561	A	C6-N1	119.25	2.19	1.35
1	a	561	A	C5-C4	98.00	2.07	1.38
1	a	561	A	C2-N3	89.48	2.14	1.33
1	a	561	A	N1-C2	89.18	2.14	1.34
1	a	561	A	C5-C6	86.65	2.19	1.41
20	u	1	G	OP3-P	-10.70	1.48	1.61
23	B	1	U	OP3-P	-10.61	1.48	1.61
22	A	958	A	N9-C4	8.30	1.42	1.37
22	A	2287	A	N7-C5	-8.29	1.34	1.39
20	u	76	A	N9-C4	-7.22	1.33	1.37
22	A	1689	A	N9-C4	6.72	1.41	1.37
22	A	2288	A	N7-C5	-6.51	1.35	1.39
1	a	561	A	C8-N7	6.42	1.36	1.31
22	A	1414	A	N9-C4	-5.85	1.34	1.37
22	A	1572	A	N9-C4	-5.41	1.34	1.37
22	A	769	G	N9-C4	-5.34	1.33	1.38
1	a	1390	A	N9-C4	-5.31	1.34	1.37
23	B	71	A	N9-C4	-5.26	1.34	1.37
22	A	1492	G	N9-C4	-5.17	1.33	1.38
23	B	99	A	N7-C5	-5.17	1.36	1.39
22	A	897	G	N9-C4	-5.03	1.33	1.38

All (796) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	561	A	N1-C2-N3	-35.11	111.74	129.30
1	a	561	A	C2-N3-C4	30.76	125.98	110.60
1	a	561	A	N7-C8-N9	26.12	126.86	113.80
1	a	561	A	C4-C5-N7	-25.89	97.75	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	561	A	N3-C4-N9	16.81	140.84	127.40
1	a	561	A	N9-C4-C5	-16.18	99.33	105.80
1	a	561	A	C6-C5-N7	14.70	142.59	132.30
22	A	998	U	C2-N1-C1'	12.20	132.34	117.70
21	v	18	U	O3'-P-O5'	-12.17	80.87	104.00
1	a	561	A	C6-N1-C2	12.17	125.90	118.60
22	A	1130	U	C2-N1-C1'	11.77	131.83	117.70
23	B	99	A	N7-C8-N9	11.42	119.51	113.80
22	A	1551	U	C2-N1-C1'	11.04	130.95	117.70
22	A	1551	U	N1-C2-O2	10.96	130.47	122.80
22	A	1349	U	N3-C2-O2	-10.70	114.71	122.20
22	A	1130	U	N3-C2-O2	-10.54	114.82	122.20
22	A	644	U	N3-C2-O2	-10.33	114.97	122.20
3	d	2	SER	CB-CA-C	10.32	129.71	110.10
23	B	99	A	C8-N9-C4	-10.29	101.69	105.80
22	A	1130	U	N1-C2-O2	10.12	129.89	122.80
22	A	1115	C	N1-C2-O2	10.05	124.93	118.90
1	a	561	A	N3-C4-C5	-10.02	119.79	126.80
22	A	905	G	N3-C4-C5	-9.94	123.63	128.60
1	a	586	U	N3-C2-O2	-9.88	115.28	122.20
22	A	958	A	C2-N3-C4	9.80	115.50	110.60
23	B	29	C	N1-C2-O2	9.72	124.73	118.90
20	u	39	U	N3-C2-O2	-9.70	115.41	122.20
22	A	1758	C	N1-C2-O2	9.60	124.66	118.90
1	a	1082	C	N1-C2-O2	9.53	124.62	118.90
1	a	995	C	N1-C2-O2	9.52	124.61	118.90
22	A	1551	U	N3-C2-O2	-9.29	115.69	122.20
22	A	1148	U	C2-N1-C1'	9.28	128.83	117.70
1	a	579	U	N3-C2-O2	-9.20	115.76	122.20
22	A	2007	U	N3-C2-O2	-9.09	115.83	122.20
22	A	164	U	N1-C2-N3	9.08	120.35	114.90
22	A	998	U	N1-C2-O2	9.05	129.14	122.80
23	B	68	C	C2-N1-C1'	9.02	128.72	118.80
22	A	164	U	C2-N3-C4	-8.88	121.67	127.00
22	A	956	C	C6-N1-C2	-8.87	116.75	120.30
22	A	998	U	N3-C2-O2	-8.84	116.01	122.20
1	a	561	A	C5-N7-C8	8.79	108.30	103.90
22	A	2766	C	N1-C2-O2	8.79	124.17	118.90
22	A	897	G	N3-C4-N9	-8.79	120.73	126.00
23	B	68	C	N1-C2-O2	8.74	124.14	118.90
21	v	18	U	OP2-P-O3'	8.73	124.41	105.20
22	A	1349	U	C2-N1-C1'	8.73	128.18	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1349	U	N1-C2-O2	8.69	128.88	122.80
22	A	2825	C	N1-C2-O2	8.69	124.11	118.90
22	A	849	G	N1-C6-O6	-8.64	114.71	119.90
22	A	1591	A	N7-C8-N9	8.64	118.12	113.80
1	a	1082	C	C2-N1-C1'	8.63	128.29	118.80
22	A	2825	C	N3-C2-O2	-8.52	115.94	121.90
1	a	579	U	N1-C2-O2	8.51	128.76	122.80
22	A	769	G	N3-C4-N9	-8.49	120.91	126.00
22	A	2007	U	N1-C2-O2	8.48	128.74	122.80
22	A	1115	C	N3-C2-O2	-8.46	115.98	121.90
22	A	905	G	C8-N9-C4	-8.36	103.06	106.40
22	A	1448	U	N1-C2-O2	8.34	128.64	122.80
22	A	1970	U	N1-C2-O2	8.32	128.62	122.80
1	a	192	U	N1-C2-O2	8.24	128.57	122.80
22	A	1948	C	C2-N1-C1'	8.24	127.86	118.80
22	A	905	G	C4-N9-C1'	8.20	137.17	126.50
22	A	1758	C	C2-N1-C1'	8.20	127.82	118.80
20	u	39	U	N1-C2-O2	8.14	128.50	122.80
23	B	89	C	N3-C2-O2	-8.13	116.21	121.90
22	A	730	C	C6-N1-C2	-8.12	117.05	120.30
22	A	1092	C	C2-N1-C1'	8.10	127.71	118.80
1	a	863	C	N3-C2-O2	-8.04	116.27	121.90
22	A	1689	A	C2-N3-C4	8.03	114.61	110.60
22	A	1758	C	N3-C2-O2	-8.00	116.30	121.90
22	A	958	A	N3-C4-C5	-7.97	121.22	126.80
1	a	635	C	N1-C2-O2	7.87	123.62	118.90
22	A	549	C	N1-C2-O2	7.87	123.62	118.90
22	A	1970	U	N3-C2-O2	-7.86	116.70	122.20
22	A	1591	A	C8-N9-C4	-7.85	102.66	105.80
22	A	998	U	C5-C6-N1	7.84	126.62	122.70
1	a	952	C	N1-C2-O2	7.82	123.59	118.90
22	A	2651	U	C2-N1-C1'	7.80	127.06	117.70
23	B	29	C	C2-N1-C1'	7.76	127.34	118.80
1	a	878	C	C2-N1-C1'	7.73	127.31	118.80
20	u	49	C	C2-N1-C1'	7.70	127.27	118.80
1	a	192	U	N3-C2-O2	-7.69	116.82	122.20
22	A	1641	C	N1-C2-O2	7.67	123.50	118.90
22	A	2142	C	C6-N1-C2	-7.67	117.23	120.30
22	A	849	G	C5-C6-O6	7.66	133.20	128.60
22	A	1092	C	C5-C6-N1	7.64	124.82	121.00
23	B	98	G	P-O3'-C3'	7.64	128.87	119.70
1	a	988	C	N1-C2-O2	7.63	123.48	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	644	U	N1-C2-O2	7.62	128.13	122.80
22	A	1551	U	C6-N1-C1'	-7.61	110.54	121.20
22	A	2408	C	N1-C2-O2	7.61	123.47	118.90
1	a	996	C	N1-C2-O2	7.60	123.46	118.90
1	a	491	C	C5-C6-N1	7.59	124.80	121.00
22	A	823	A	C2-N3-C4	7.55	114.38	110.60
23	B	29	C	N3-C2-O2	-7.55	116.61	121.90
22	A	769	G	N3-C4-C5	7.51	132.36	128.60
22	A	1130	U	C5-C6-N1	7.49	126.44	122.70
22	A	905	G	C2-N3-C4	7.48	115.64	111.90
22	A	958	A	C8-N9-C4	-7.48	102.81	105.80
20	u	39	U	C2-N1-C1'	7.47	126.66	117.70
1	a	1125	C	N1-C2-O2	7.46	123.37	118.90
22	A	998	U	C6-N1-C2	-7.43	116.54	121.00
22	A	2753	U	N1-C2-O2	7.43	128.00	122.80
22	A	1092	C	N1-C2-O2	7.42	123.35	118.90
22	A	1955	C	N1-C2-O2	7.40	123.34	118.90
1	a	1082	C	N3-C2-O2	-7.39	116.73	121.90
1	a	115	C	N3-C2-O2	-7.38	116.73	121.90
22	A	1024	G	N3-C4-C5	-7.35	124.92	128.60
22	A	1502	G	N3-C4-C5	-7.33	124.93	128.60
1	a	579	U	C2-N1-C1'	7.31	126.47	117.70
1	a	1318	C	C2-N1-C1'	7.30	126.83	118.80
1	a	585	G	C4-N9-C1'	7.29	135.98	126.50
22	A	1882	C	N1-C2-O2	7.29	123.28	118.90
1	a	115	C	N1-C2-O2	7.29	123.27	118.90
22	A	925	C	C2-N1-C1'	7.29	126.81	118.80
22	A	638	C	C6-N1-C2	-7.28	117.39	120.30
22	A	948	A	O5'-P-OP2	-7.28	99.15	105.70
22	A	2257	U	N3-C2-O2	-7.27	117.11	122.20
22	A	963	C	C6-N1-C2	-7.26	117.39	120.30
1	a	1082	C	C6-N1-C2	-7.26	117.40	120.30
22	A	602	C	C6-N1-C2	-7.25	117.40	120.30
1	a	551	C	C6-N1-C2	-7.23	117.41	120.30
22	A	998	U	C6-N1-C1'	-7.20	111.12	121.20
22	A	1502	G	N3-C4-N9	7.20	130.32	126.00
23	B	68	C	N3-C2-O2	-7.18	116.88	121.90
22	A	956	C	C5-C6-N1	7.18	124.59	121.00
22	A	1502	G	C4-N9-C1'	7.17	135.82	126.50
1	a	517	C	N3-C2-O2	-7.16	116.89	121.90
22	A	1130	U	C6-N1-C1'	-7.16	111.17	121.20
22	A	1148	U	N1-C2-O2	7.16	127.81	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1082	C	C5-C6-N1	7.16	124.58	121.00
22	A	1569	G	N3-C4-N9	-7.15	121.71	126.00
22	A	396	C	C2-N1-C1'	7.13	126.64	118.80
22	A	2753	U	N3-C2-O2	-7.13	117.21	122.20
22	A	2127	C	N1-C2-O2	7.12	123.17	118.90
1	a	1039	U	N3-C2-O2	-7.11	117.22	122.20
1	a	255	U	O4'-C1'-N1	7.10	113.88	108.20
1	a	995	C	N3-C2-O2	-7.10	116.93	121.90
22	A	1399	C	C6-N1-C2	-7.10	117.46	120.30
22	A	906	C	O5'-P-OP1	-7.08	99.33	105.70
1	a	309	C	N1-C2-O2	7.08	123.15	118.90
1	a	643	G	N3-C4-N9	-7.07	121.76	126.00
22	A	1350	C	C2-N1-C1'	7.05	126.55	118.80
22	A	2794	G	C4-N9-C1'	7.04	135.66	126.50
1	a	1482	C	N3-C2-O2	-7.03	116.98	121.90
22	A	1304	U	C2-N1-C1'	7.02	126.13	117.70
22	A	1130	U	C6-N1-C2	-7.01	116.79	121.00
20	u	43	C	C2-N1-C1'	7.01	126.51	118.80
22	A	925	C	N1-C2-O2	7.00	123.10	118.90
22	A	1604	A	P-O3'-C3'	7.00	128.10	119.70
20	u	75	C	N1-C2-O2	7.00	123.10	118.90
22	A	1641	C	N3-C2-O2	-7.00	117.00	121.90
1	a	625	G	C4-N9-C1'	6.98	135.57	126.50
22	A	1561	U	C2-N1-C1'	6.98	126.07	117.70
22	A	905	G	N3-C4-N9	6.96	130.18	126.00
22	A	2035	G	N3-C4-C5	-6.95	125.12	128.60
22	A	903	G	N3-C4-C5	6.94	132.07	128.60
22	A	1508	G	C5-C6-O6	6.93	132.76	128.60
22	A	1197	G	C6-C5-N7	-6.91	126.25	130.40
20	u	57	G	N3-C4-N9	-6.91	121.86	126.00
22	A	1197	G	N3-C4-N9	6.90	130.14	126.00
22	A	903	G	C8-N9-C4	6.89	109.16	106.40
22	A	1102	G	N3-C4-N9	6.88	130.13	126.00
22	A	973	U	N3-C2-O2	-6.87	117.39	122.20
22	A	1885	C	N1-C2-O2	6.87	123.02	118.90
1	a	988	C	N3-C2-O2	-6.85	117.11	121.90
22	A	693	U	P-O3'-C3'	6.84	127.91	119.70
22	A	1197	G	C4-N9-C1'	6.83	135.38	126.50
23	B	99	A	C5-N7-C8	-6.83	100.49	103.90
22	A	284	C	N1-C2-O2	6.82	122.99	118.90
1	a	1054	A	N7-C8-N9	6.81	117.21	113.80
22	A	621	C	C5-C6-N1	6.81	124.41	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1399	C	C2-N1-C1'	6.80	126.28	118.80
1	a	468	C	C6-N1-C2	-6.79	117.58	120.30
22	A	164	U	N3-C2-O2	-6.79	117.45	122.20
22	A	2585	C	C6-N1-C2	-6.79	117.59	120.30
1	a	613	U	N3-C2-O2	-6.78	117.45	122.20
22	A	1584	G	P-O3'-C3'	6.78	127.84	119.70
23	B	95	U	C5-C6-N1	6.78	126.09	122.70
1	a	424	U	N3-C2-O2	-6.77	117.46	122.20
22	A	769	G	C2-N3-C4	-6.74	108.53	111.90
22	A	892	U	N3-C2-O2	-6.74	117.48	122.20
1	a	38	G	N3-C4-N9	6.74	130.04	126.00
20	u	72	C	N3-C2-O2	-6.73	117.19	121.90
22	A	992	G	O4'-C1'-N9	6.73	113.58	108.20
1	a	1363	U	N3-C2-O2	-6.72	117.50	122.20
1	a	192	U	C2-N1-C1'	6.70	125.74	117.70
1	a	399	G	C4-N9-C1'	6.69	135.20	126.50
22	A	1703	C	C6-N1-C2	-6.68	117.63	120.30
22	A	1591	A	C4-N9-C1'	6.68	138.32	126.30
22	A	2408	C	N3-C2-O2	-6.67	117.23	121.90
22	A	509	G	O4'-C1'-N9	6.66	113.52	108.20
1	a	399	G	N3-C4-N9	6.65	129.99	126.00
1	a	1039	U	N1-C2-O2	6.64	127.45	122.80
22	A	973	U	N1-C2-O2	6.64	127.45	122.80
22	A	2554	C	N3-C2-O2	-6.63	117.26	121.90
1	a	38	G	C4-N9-C1'	6.63	135.12	126.50
1	a	108	U	N3-C2-O2	-6.63	117.56	122.20
22	A	1024	G	N3-C4-N9	6.61	129.97	126.00
22	A	2651	U	N1-C2-O2	6.61	127.43	122.80
22	A	2152	C	N3-C2-O2	-6.60	117.28	121.90
1	a	988	C	C2-N1-C1'	6.60	126.06	118.80
40	V	71	ILE	C-N-CA	6.60	138.19	121.70
20	u	75	C	C2-N1-C1'	6.59	126.06	118.80
22	A	1448	U	N3-C2-O2	-6.58	117.59	122.20
22	A	1831	G	C4-N9-C1'	6.58	135.05	126.50
22	A	1397	G	C8-N9-C4	-6.57	103.77	106.40
1	a	586	U	C2-N1-C1'	6.57	125.58	117.70
22	A	272	C	C2-N1-C1'	6.56	126.02	118.80
1	a	419	G	N3-C4-N9	6.55	129.93	126.00
33	O	41	ARG	CA-CB-CG	6.55	127.81	113.40
1	a	688	G	N3-C4-N9	6.54	129.92	126.00
1	a	38	G	N3-C4-C5	-6.53	125.33	128.60
22	A	422	A	C8-N9-C4	-6.53	103.19	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1492	G	N3-C4-N9	-6.53	122.08	126.00
22	A	1588	C	N3-C2-O2	-6.53	117.33	121.90
22	A	1102	G	N9-C4-C5	-6.53	102.79	105.40
22	A	2307	C	C5-C6-N1	6.52	124.26	121.00
22	A	1638	C	C2-N1-C1'	6.52	125.97	118.80
1	a	551	C	C5-C6-N1	6.52	124.26	121.00
22	A	561	G	C6-C5-N7	-6.51	126.49	130.40
22	A	931	C	C2-N1-C1'	6.51	125.96	118.80
22	A	607	G	N3-C4-C5	-6.50	125.35	128.60
22	A	2020	C	C6-N1-C2	-6.49	117.70	120.30
22	A	694	G	O5'-P-OP1	-6.49	99.86	105.70
22	A	2766	C	N3-C2-O2	-6.48	117.36	121.90
1	a	517	C	C6-N1-C2	-6.48	117.71	120.30
22	A	1882	C	C2-N1-C1'	6.48	125.92	118.80
22	A	275	A	N1-C2-N3	6.47	132.53	129.30
22	A	1561	U	N1-C2-O2	6.47	127.33	122.80
22	A	2670	U	C2-N1-C1'	6.47	125.46	117.70
21	v	18	U	P-O3'-C3'	-6.45	111.96	119.70
22	A	1561	U	N3-C2-O2	-6.45	117.68	122.20
1	a	1018	U	N1-C2-O2	6.44	127.31	122.80
22	A	2729	C	C5-C6-N1	6.43	124.22	121.00
23	B	68	C	C6-N1-C1'	-6.43	113.08	120.80
1	a	1363	U	N1-C2-O2	6.43	127.30	122.80
1	a	1421	U	N1-C2-O2	6.42	127.30	122.80
22	A	1379	G	C4-N9-C1'	6.42	134.84	126.50
22	A	1148	U	C6-N1-C1'	-6.41	112.22	121.20
22	A	209	U	N1-C2-O2	6.41	127.29	122.80
1	a	340	A	N1-C6-N6	6.41	122.44	118.60
1	a	585	G	C8-N9-C1'	-6.41	118.67	127.00
1	a	1363	U	C2-N1-C1'	6.39	125.37	117.70
22	A	958	A	N1-C6-N6	-6.38	114.77	118.60
1	a	426	A	C5-C6-N6	-6.38	118.60	123.70
22	A	1238	C	C6-N1-C2	-6.38	117.75	120.30
22	A	1497	U	N3-C2-O2	-6.38	117.74	122.20
1	a	559	G	N3-C4-N9	-6.37	122.18	126.00
22	A	2734	U	N3-C2-O2	-6.37	117.74	122.20
22	A	2729	C	C6-N1-C2	-6.37	117.75	120.30
1	a	331	C	C2-N1-C1'	6.36	125.80	118.80
1	a	628	C	N3-C2-O2	-6.36	117.45	121.90
1	a	1328	G	C4-N9-C1'	6.36	134.76	126.50
22	A	2035	G	N3-C4-N9	6.36	129.81	126.00
22	A	1197	G	C8-N9-C1'	-6.35	118.74	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1948	C	C6-N1-C2	-6.35	117.76	120.30
1	a	586	U	N1-C2-O2	6.33	127.23	122.80
22	A	1647	C	C6-N1-C2	-6.33	117.77	120.30
22	A	422	A	N7-C8-N9	6.32	116.96	113.80
22	A	897	G	C8-N9-C1'	6.32	135.22	127.00
22	A	1362	U	N3-C2-O2	-6.31	117.78	122.20
1	a	399	G	C8-N9-C1'	-6.30	118.81	127.00
1	a	907	U	N1-C2-O2	6.30	127.21	122.80
22	A	209	U	N3-C2-O2	-6.30	117.79	122.20
1	a	444	U	N3-C4-O4	6.30	123.81	119.40
22	A	1641	C	C6-N1-C2	-6.30	117.78	120.30
22	A	1024	G	C4-N9-C1'	6.29	134.67	126.50
22	A	1147	G	C4-C5-N7	6.28	113.31	110.80
1	a	1173	C	C2-N1-C1'	6.26	125.68	118.80
1	a	419	G	N3-C4-C5	-6.26	125.47	128.60
22	A	1641	C	C2-N1-C1'	6.25	125.67	118.80
22	A	2766	C	C2-N1-C1'	6.25	125.67	118.80
22	A	784	C	C5-C6-N1	6.25	124.12	121.00
22	A	413	U	N3-C2-O2	-6.23	117.84	122.20
22	A	1197	G	C4-C5-N7	6.22	113.29	110.80
1	a	1173	C	N3-C2-O2	-6.22	117.54	121.90
22	A	1505	C	C6-N1-C2	-6.22	117.81	120.30
22	A	963	C	C6-N1-C1'	6.21	128.26	120.80
22	A	1147	G	C6-C5-N7	-6.21	126.67	130.40
1	a	355	U	N3-C2-O2	-6.20	117.86	122.20
22	A	1508	G	N1-C6-O6	-6.19	116.19	119.90
22	A	2307	C	C6-N1-C2	-6.19	117.82	120.30
1	a	426	A	N1-C6-N6	6.19	122.31	118.60
1	a	1089	U	N3-C2-O2	-6.19	117.87	122.20
22	A	2895	U	N3-C2-O2	-6.18	117.87	122.20
22	A	527	C	N1-C2-O2	6.18	122.61	118.90
22	A	77	C	C5-C6-N1	6.17	124.08	121.00
1	a	995	C	C2-N1-C1'	6.16	125.58	118.80
1	a	279	C	C6-N1-C2	-6.16	117.84	120.30
1	a	1001	C	C2-N1-C1'	6.16	125.57	118.80
22	A	2035	G	C4-N9-C1'	6.15	134.50	126.50
23	B	73	U	P-O3'-C3'	6.15	127.08	119.70
22	A	237	U	N3-C2-O2	-6.14	117.90	122.20
22	A	905	G	N7-C8-N9	6.14	116.17	113.10
1	a	492	C	N1-C2-O2	6.13	122.58	118.90
22	A	2141	G	N3-C4-N9	-6.13	122.32	126.00
22	A	1102	G	C6-C5-N7	-6.12	126.73	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	2152	C	C6-N1-C2	-6.12	117.85	120.30
1	a	521	G	C6-C5-N7	-6.12	126.73	130.40
22	A	730	C	C2-N1-C1'	6.12	125.53	118.80
22	A	638	C	C2-N1-C1'	6.12	125.53	118.80
1	a	586	U	C6-N1-C2	-6.12	117.33	121.00
1	a	1125	C	N3-C2-O2	-6.11	117.62	121.90
22	A	1588	C	N1-C2-O2	6.11	122.56	118.90
1	a	952	C	C6-N1-C2	-6.11	117.86	120.30
1	a	1005	U	N3-C2-O2	-6.10	117.93	122.20
22	A	1605	C	P-O3'-C3'	6.10	127.02	119.70
1	a	584	C	C5-C6-N1	6.10	124.05	121.00
1	a	1421	U	N3-C2-O2	-6.09	117.94	122.20
1	a	1173	C	N1-C2-O2	6.09	122.55	118.90
22	A	1453	U	C5-C6-N1	6.09	125.74	122.70
22	A	1751	C	C6-N1-C2	-6.08	117.87	120.30
1	a	537	C	N1-C2-O2	6.08	122.55	118.90
22	A	2881	C	C6-N1-C2	-6.08	117.87	120.30
22	A	2554	C	N1-C2-O2	6.07	122.54	118.90
1	a	1520	G	P-O3'-C3'	6.07	126.98	119.70
1	a	1482	C	N1-C2-O2	6.06	122.54	118.90
1	a	795	A	C8-N9-C4	-6.06	103.38	105.80
22	A	897	G	N9-C4-C5	6.06	107.82	105.40
22	A	1885	C	C6-N1-C2	-6.06	117.88	120.30
1	a	551	C	N1-C2-O2	6.05	122.53	118.90
22	A	2050	C	N1-C2-O2	6.05	122.53	118.90
22	A	527	C	N3-C2-O2	-6.04	117.67	121.90
22	A	1115	C	C2-N1-C1'	6.04	125.45	118.80
22	A	2596	G	C4-N9-C1'	6.04	134.36	126.50
22	A	1434	C	C2-N1-C1'	6.04	125.45	118.80
22	A	1448	U	C2-N1-C1'	6.04	124.95	117.70
22	A	561	G	N3-C4-N9	6.03	129.62	126.00
22	A	1689	A	N3-C4-C5	-6.03	122.58	126.80
22	A	1193	C	C2-N1-C1'	6.03	125.43	118.80
1	a	536	G	P-O3'-C3'	6.02	126.92	119.70
1	a	1305	G	C4-N9-C1'	6.01	134.32	126.50
22	A	94	U	N3-C2-O2	-6.01	117.99	122.20
22	A	2007	U	C2-N1-C1'	6.01	124.91	117.70
22	A	1388	U	N3-C2-O2	-6.01	117.99	122.20
22	A	1620	C	C2-N1-C1'	6.01	125.41	118.80
22	A	1502	G	C2-N3-C4	6.01	114.90	111.90
1	a	585	G	N3-C4-N9	6.00	129.60	126.00
22	A	1919	C	N1-C2-O2	5.99	122.50	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	410	C	C2-N1-C1'	5.99	125.39	118.80
1	a	37	C	O4'-C1'-N1	5.99	112.99	108.20
22	A	586	A	N1-C6-N6	-5.99	115.01	118.60
22	A	638	C	C5-C6-N1	5.98	123.99	121.00
22	A	1317	G	C4-N9-C1'	5.98	134.27	126.50
22	A	897	G	C4-N9-C1'	-5.97	118.73	126.50
22	A	2826	C	C2-N1-C1'	5.97	125.37	118.80
1	a	635	C	N3-C2-O2	-5.97	117.72	121.90
22	A	1551	U	C5-C6-N1	5.97	125.68	122.70
22	A	1293	G	C4-N9-C1'	5.95	134.23	126.50
1	a	427	A	P-O3'-C3'	5.94	126.83	119.70
24	C	83	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	a	1240	A	O5'-P-OP1	-5.94	100.36	105.70
22	A	925	C	N3-C2-O2	-5.94	117.74	121.90
22	A	1399	C	N1-C2-O2	5.94	122.46	118.90
22	A	1574	C	N1-C2-O2	5.93	122.46	118.90
22	A	1812	U	N3-C2-O2	-5.93	118.05	122.20
1	a	1049	G	C8-N9-C1'	5.93	134.71	127.00
1	a	1328	G	C8-N9-C1'	-5.93	119.30	127.00
1	a	578	A	C4-N9-C1'	5.92	136.96	126.30
22	A	602	C	N1-C2-O2	5.92	122.45	118.90
22	A	602	C	N3-C2-O2	-5.92	117.76	121.90
22	A	499	U	N3-C2-O2	-5.92	118.06	122.20
1	a	878	C	C6-N1-C1'	-5.91	113.70	120.80
22	A	1948	C	N1-C2-O2	5.91	122.45	118.90
3	d	2	SER	CA-CB-OG	5.91	127.14	111.20
1	a	613	U	N1-C2-O2	5.90	126.93	122.80
22	A	1115	C	C6-N1-C2	-5.90	117.94	120.30
22	A	40	C	C6-N1-C2	-5.90	117.94	120.30
1	a	331	C	C6-N1-C2	-5.90	117.94	120.30
22	A	1157	C	C6-N1-C2	-5.90	117.94	120.30
22	A	2262	C	N1-C2-O2	5.90	122.44	118.90
22	A	2794	G	C8-N9-C1'	-5.89	119.34	127.00
22	A	892	U	N1-C2-O2	5.89	126.92	122.80
22	A	2008	C	N3-C2-O2	-5.89	117.78	121.90
22	A	2881	C	N3-C2-O2	-5.89	117.78	121.90
22	A	1502	G	C8-N9-C1'	-5.89	119.35	127.00
22	A	1148	U	C5-C6-N1	5.88	125.64	122.70
22	A	926	C	C5-C6-N1	5.88	123.94	121.00
22	A	1148	U	N3-C2-O2	-5.88	118.09	122.20
22	A	1497	U	N1-C2-O2	5.88	126.91	122.80
23	B	85	U	C5-C6-N1	5.88	125.64	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1029	G	C4-N9-C1'	5.87	134.13	126.50
39	U	3	LEU	CA-CB-CG	5.87	128.81	115.30
22	A	1622	U	N3-C2-O2	-5.87	118.09	122.20
22	A	823	A	N3-C4-C5	-5.85	122.70	126.80
1	a	952	C	N3-C2-O2	-5.85	117.81	121.90
20	u	43	C	C6-N1-C2	-5.85	117.96	120.30
1	a	952	C	C2-N1-C1'	5.85	125.23	118.80
22	A	849	G	C8-N9-C4	-5.83	104.07	106.40
22	A	2455	C	C2-N1-C1'	5.83	125.22	118.80
22	A	105	C	C2-N1-C1'	5.82	125.20	118.80
22	A	2008	C	C6-N1-C2	-5.81	117.97	120.30
22	A	549	C	C2-N1-C1'	5.81	125.19	118.80
22	A	1394	G	N3-C4-N9	5.81	129.49	126.00
22	A	114	U	C2-N1-C1'	5.80	124.67	117.70
22	A	293	U	N3-C2-O2	-5.80	118.14	122.20
1	a	115	C	C6-N1-C2	-5.80	117.98	120.30
22	A	992	G	C6-C5-N7	-5.80	126.92	130.40
1	a	348	C	C2-N1-C1'	5.80	125.18	118.80
1	a	988	C	C6-N1-C2	-5.80	117.98	120.30
22	A	1369	C	C6-N1-C2	-5.79	117.98	120.30
1	a	659	U	N3-C2-O2	-5.79	118.15	122.20
1	a	752	C	C6-N1-C2	-5.79	117.98	120.30
22	A	1147	G	N7-C8-N9	5.79	116.00	113.10
22	A	1144	C	C6-N1-C2	-5.79	117.99	120.30
22	A	2208	C	N1-C2-O2	5.79	122.37	118.90
22	A	621	C	C6-N1-C2	-5.78	117.99	120.30
1	a	1218	C	N1-C2-O2	5.78	122.37	118.90
20	u	49	C	C5-C6-N1	5.78	123.89	121.00
20	u	75	C	C6-N1-C1'	-5.78	113.86	120.80
22	A	1726	C	C5-C6-N1	5.78	123.89	121.00
1	a	521	G	C4-C5-N7	5.77	113.11	110.80
1	a	559	G	P-O3'-C3'	5.77	126.63	119.70
1	a	1308	U	N1-C2-O2	5.77	126.84	122.80
1	a	551	C	N3-C2-O2	-5.77	117.86	121.90
22	A	1831	G	N3-C4-C5	-5.77	125.72	128.60
22	A	1511	C	N3-C2-O2	-5.76	117.87	121.90
22	A	2317	G	P-O3'-C3'	5.76	126.61	119.70
22	A	1092	C	C6-N1-C2	-5.76	118.00	120.30
22	A	1399	C	C5-C6-N1	5.76	123.88	121.00
22	A	2240	C	N1-C2-O2	5.76	122.35	118.90
1	a	39	G	P-O3'-C3'	5.75	126.60	119.70
1	a	1173	C	C6-N1-C2	-5.75	118.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	784	C	C6-N1-C2	-5.75	118.00	120.30
22	A	1369	C	C2-N1-C1'	5.75	125.12	118.80
23	B	58	C	C2-N1-C1'	5.75	125.12	118.80
22	A	1479	C	C2-N1-C1'	5.75	125.12	118.80
1	a	907	U	N3-C2-O2	-5.74	118.18	122.20
1	a	952	C	C5-C6-N1	5.74	123.87	121.00
1	a	559	G	C5-C6-O6	5.74	132.04	128.60
22	A	2801	C	C6-N1-C2	-5.74	118.01	120.30
22	A	1157	C	C2-N1-C1'	5.73	125.10	118.80
22	A	1758	C	C6-N1-C2	-5.73	118.01	120.30
22	A	311	A	P-O3'-C3'	5.73	126.57	119.70
23	B	28	C	N1-C2-O2	5.72	122.33	118.90
1	a	1142	U	N3-C2-O2	-5.72	118.19	122.20
22	A	1689	A	N3-C4-N9	5.72	131.98	127.40
22	A	2077	C	N1-C2-O2	5.71	122.33	118.90
22	A	476	C	N3-C2-O2	-5.71	117.90	121.90
22	A	2226	A	C5-N7-C8	-5.71	101.05	103.90
22	A	823	A	C8-N9-C4	-5.70	103.52	105.80
22	A	1120	A	N7-C8-N9	5.70	116.65	113.80
22	A	1574	C	C2-N1-C1'	5.70	125.07	118.80
1	a	419	G	C4-N9-C1'	5.70	133.91	126.50
22	A	293	U	N1-C2-O2	5.70	126.79	122.80
22	A	897	G	N3-C4-C5	5.69	131.45	128.60
22	A	1632	A	C2-N3-C4	5.69	113.44	110.60
22	A	2262	C	C2-N1-C1'	5.68	125.05	118.80
20	u	41	C	C2-N1-C1'	5.68	125.05	118.80
22	A	2209	U	N3-C2-O2	-5.68	118.22	122.20
1	a	415	C	C5-C6-N1	5.67	123.83	121.00
22	A	1394	G	C5-C6-N1	5.67	114.34	111.50
22	A	272	C	C6-N1-C2	-5.67	118.03	120.30
1	a	1305	G	N3-C4-N9	5.66	129.40	126.00
22	A	1379	G	N3-C4-N9	5.66	129.40	126.00
22	A	2457	U	N3-C2-O2	-5.66	118.24	122.20
20	u	72	C	N1-C2-O2	5.65	122.29	118.90
22	A	1790	G	N3-C4-N9	5.65	129.39	126.00
22	A	48	C	N1-C2-O2	5.65	122.29	118.90
22	A	1885	C	C2-N1-C1'	5.64	125.01	118.80
22	A	2044	A	O4'-C1'-N9	5.64	112.71	108.20
22	A	573	U	C5-C6-N1	5.64	125.52	122.70
22	A	848	G	N1-C6-O6	-5.64	116.52	119.90
22	A	2479	C	C6-N1-C2	-5.63	118.05	120.30
22	A	1304	U	N1-C2-O2	5.63	126.74	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1591	A	C2-N3-C4	5.63	113.41	110.60
22	A	1492	G	N3-C4-C5	5.62	131.41	128.60
33	O	41	ARG	CB-CG-CD	-5.62	96.99	111.60
22	A	1501	A	C2-N3-C4	5.62	113.41	110.60
22	A	994	G	P-O3'-C3'	5.62	126.44	119.70
1	a	383	U	C2-N1-C1'	5.62	124.44	117.70
22	A	1885	C	N3-C2-O2	-5.62	117.97	121.90
22	A	1955	C	N3-C2-O2	-5.62	117.97	121.90
22	A	246	U	N3-C2-O2	-5.61	118.28	122.20
22	A	2568	U	C6-N1-C2	-5.61	117.64	121.00
22	A	926	C	C6-N1-C2	-5.60	118.06	120.30
22	A	169	A	O4'-C1'-N9	5.60	112.68	108.20
22	A	1350	C	C6-N1-C2	-5.59	118.06	120.30
22	A	2854	G	N3-C4-N9	5.59	129.36	126.00
22	A	1790	G	C4-N9-C1'	5.59	133.77	126.50
22	A	902	A	C8-N9-C4	-5.59	103.56	105.80
22	A	1293	G	C8-N9-C1'	-5.59	119.73	127.00
1	a	38	G	C8-N9-C1'	-5.59	119.74	127.00
22	A	2127	C	C2-N1-C1'	5.59	124.95	118.80
22	A	1304	U	N3-C2-O2	-5.59	118.29	122.20
23	B	24	U	N3-C2-O2	-5.58	118.29	122.20
1	a	1049	G	N3-C4-N9	-5.58	122.65	126.00
22	A	284	C	N3-C2-O2	-5.58	117.99	121.90
22	A	1407	G	C6-C5-N7	-5.58	127.05	130.40
22	A	2734	U	N1-C2-O2	5.58	126.71	122.80
22	A	693	U	OP1-P-O3'	5.58	117.47	105.20
22	A	2145	A	C4-N9-C1'	5.58	136.34	126.30
22	A	2057	C	C6-N1-C2	-5.58	118.07	120.30
22	A	1435	C	N1-C2-O2	5.57	122.24	118.90
22	A	2307	C	C2-N1-C1'	5.57	124.93	118.80
22	A	1379	G	N3-C4-C5	-5.57	125.82	128.60
1	a	1082	C	C6-N1-C1'	-5.57	114.12	120.80
22	A	716	A	O4'-C1'-N9	5.57	112.65	108.20
22	A	905	G	C8-N9-C1'	-5.57	119.77	127.00
1	a	1040	U	C2-N1-C1'	5.56	124.37	117.70
1	a	1152	U	N3-C2-O2	-5.56	118.31	122.20
22	A	2717	C	N1-C2-O2	5.56	122.24	118.90
1	a	1306	C	C2-N1-C1'	5.56	124.92	118.80
1	a	763	A	P-O3'-C3'	5.56	126.37	119.70
22	A	114	U	N3-C2-O2	-5.56	118.31	122.20
22	A	1362	U	N1-C2-O2	5.55	126.69	122.80
1	a	559	G	N9-C4-C5	5.55	107.62	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1049	G	C4-N9-C1'	-5.55	119.29	126.50
22	A	33	C	N1-C2-O2	5.55	122.23	118.90
23	B	28	C	C6-N1-C2	-5.55	118.08	120.30
1	a	310	C	C6-N1-C2	-5.54	118.08	120.30
22	A	751	C	C5-C6-N1	5.54	123.77	121.00
1	a	1142	U	N1-C2-O2	5.54	126.67	122.80
22	A	164	U	C5-C6-N1	-5.54	119.93	122.70
22	A	823	A	N1-C6-N6	-5.53	115.28	118.60
1	a	863	C	N1-C2-O2	5.53	122.22	118.90
22	A	1758	C	C6-N1-C1'	-5.53	114.17	120.80
1	a	643	G	N3-C4-C5	5.52	131.36	128.60
1	a	1183	C	C2-N1-C1'	5.52	124.88	118.80
22	A	47	C	C6-N1-C2	-5.52	118.09	120.30
23	B	29	C	C6-N1-C1'	-5.51	114.18	120.80
22	A	2801	C	N3-C2-O2	-5.51	118.04	121.90
1	a	1018	U	N3-C2-O2	-5.51	118.34	122.20
1	a	1421	U	C2-N1-C1'	5.51	124.31	117.70
22	A	849	G	N9-C4-C5	5.50	107.60	105.40
22	A	1408	U	N3-C2-O2	-5.49	118.36	122.20
22	A	2553	C	N1-C2-O2	5.49	122.19	118.90
1	a	1152	U	C2-N1-C1'	5.49	124.29	117.70
22	A	1217	G	C2-N3-C4	5.49	114.64	111.90
22	A	2229	G	N3-C4-N9	5.49	129.29	126.00
1	a	426	A	N9-C4-C5	-5.49	103.61	105.80
22	A	1397	G	N7-C8-N9	5.49	115.84	113.10
1	a	444	U	C5-C4-O4	-5.48	122.61	125.90
1	a	1308	U	C2-N1-C1'	5.48	124.28	117.70
22	A	310	G	C4-N9-C1'	5.48	133.62	126.50
1	a	1305	G	C8-N9-C1'	-5.48	119.88	127.00
39	U	49	LYS	C-N-CA	5.47	135.37	121.70
1	a	826	C	C2-N1-C1'	5.47	124.81	118.80
1	a	625	G	C8-N9-C1'	-5.46	119.90	127.00
22	A	1029	G	C8-N9-C1'	-5.46	119.90	127.00
22	A	1945	U	N3-C2-O2	-5.46	118.38	122.20
22	A	1804	C	C6-N1-C2	-5.46	118.12	120.30
22	A	958	A	C5-C6-N1	5.46	120.43	117.70
22	A	1379	G	C8-N9-C1'	-5.45	119.91	127.00
22	A	156	U	C5-C6-N1	5.45	125.42	122.70
22	A	2175	C	C6-N1-C2	-5.45	118.12	120.30
22	A	1092	C	C6-N1-C1'	-5.45	114.27	120.80
22	A	1632	A	C4-N9-C1'	5.45	136.10	126.30
1	a	101	A	N7-C8-N9	5.44	116.52	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	2226	A	N7-C8-N9	5.44	116.52	113.80
22	A	499	U	N1-C2-O2	5.44	126.61	122.80
22	A	925	C	C6-N1-C2	-5.44	118.12	120.30
22	A	2819	U	N3-C2-O2	-5.44	118.39	122.20
22	A	1948	C	C6-N1-C1'	-5.44	114.27	120.80
22	A	561	G	C4-N9-C1'	5.44	133.57	126.50
22	A	1435	C	C2-N1-C1'	5.43	124.78	118.80
22	A	2303	G	C8-N9-C4	-5.43	104.23	106.40
22	A	2651	U	N3-C2-O2	-5.43	118.40	122.20
1	a	1084	G	N3-C4-N9	5.43	129.26	126.00
22	A	2819	U	N1-C2-O2	5.43	126.60	122.80
22	A	2479	C	C2-N1-C1'	5.42	124.77	118.80
22	A	2334	A	C2-N3-C4	5.42	113.31	110.60
22	A	1408	U	N1-C2-O2	5.41	126.59	122.80
22	A	2257	U	N1-C2-O2	5.41	126.59	122.80
1	a	585	G	N3-C4-C5	-5.41	125.89	128.60
22	A	903	G	C4-N9-C1'	-5.41	119.47	126.50
22	A	947	G	OP2-P-O3'	5.41	117.10	105.20
22	A	897	G	C6-C5-N7	5.41	133.64	130.40
22	A	1902	G	O4'-C1'-N9	5.41	112.52	108.20
1	a	1086	U	N3-C2-O2	-5.40	118.42	122.20
22	A	1882	C	C6-N1-C2	-5.40	118.14	120.30
22	A	2057	C	C2-N1-C1'	5.40	124.74	118.80
1	a	996	C	N3-C2-O2	-5.39	118.12	121.90
1	a	416	C	C6-N1-C2	-5.39	118.14	120.30
1	a	688	G	C6-C5-N7	-5.39	127.17	130.40
1	a	383	U	N1-C2-O2	5.39	126.57	122.80
22	A	396	C	C6-N1-C2	-5.39	118.15	120.30
22	A	2174	G	N3-C4-N9	-5.38	122.77	126.00
22	A	1114	G	C5-C6-O6	5.38	131.83	128.60
22	A	1236	U	C2-N1-C1'	5.38	124.16	117.70
22	A	1147	G	C5-N7-C8	-5.38	101.61	104.30
1	a	415	C	C6-N1-C2	-5.38	118.15	120.30
22	A	2651	U	C6-N1-C1'	-5.38	113.67	121.20
22	A	104	U	N3-C2-O2	-5.38	118.44	122.20
22	A	2240	C	N3-C2-O2	-5.37	118.14	121.90
22	A	890	A	P-O3'-C3'	5.37	126.14	119.70
22	A	644	U	C2-N1-C1'	5.37	124.14	117.70
22	A	1689	A	C4-N9-C1'	5.37	135.96	126.30
22	A	1501	A	N3-C4-N9	5.37	131.69	127.40
22	A	2278	C	N3-C2-O2	-5.36	118.15	121.90
22	A	1831	G	C8-N9-C1'	-5.36	120.03	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	492	C	C2-N1-C1'	5.36	124.69	118.80
22	A	209	U	C2-N1-C1'	5.36	124.13	117.70
22	A	1317	G	C8-N9-C1'	-5.36	120.03	127.00
22	A	2746	G	C4-N9-C1'	5.35	133.46	126.50
1	a	672	U	C6-N1-C1'	5.35	128.69	121.20
20	u	49	C	C6-N1-C1'	-5.35	114.38	120.80
22	A	1102	G	N1-C6-O6	5.35	123.11	119.90
22	A	1349	U	C6-N1-C1'	-5.35	113.71	121.20
23	B	68	C	C6-N1-C2	-5.35	118.16	120.30
22	A	823	A	C4-N9-C1'	5.35	135.93	126.30
22	A	293	U	C2-N1-C1'	5.34	124.11	117.70
1	a	1089	U	N1-C2-O2	5.34	126.54	122.80
1	a	1094	U	N3-C2-O2	-5.34	118.47	122.20
22	A	2568	U	N1-C2-N3	5.34	118.10	114.90
22	A	602	C	C5-C6-N1	5.33	123.67	121.00
22	A	2753	U	C2-N1-C1'	5.33	124.10	117.70
1	a	340	A	C4-C5-N7	5.33	113.37	110.70
1	a	584	C	C6-N1-C2	-5.33	118.17	120.30
22	A	1210	C	C6-N1-C2	-5.33	118.17	120.30
1	a	1318	C	C6-N1-C1'	-5.32	114.41	120.80
22	A	309	C	N1-C2-O2	5.32	122.09	118.90
22	A	1589	G	N3-C4-C5	-5.32	125.94	128.60
22	A	2287	A	C4-C5-C6	5.32	119.66	117.00
22	A	2469	G	C4-N9-C1'	5.32	133.41	126.50
22	A	1928	C	N1-C2-O2	5.31	122.09	118.90
1	a	720	U	N1-C2-O2	5.31	126.52	122.80
22	A	1882	C	C5-C6-N1	5.31	123.65	121.00
22	A	784	C	C2-N1-C1'	5.31	124.64	118.80
22	A	1831	G	N3-C4-N9	5.30	129.18	126.00
1	a	71	U	N3-C2-O2	-5.30	118.49	122.20
1	a	369	G	C4-N9-C1'	5.30	133.39	126.50
22	A	2568	U	C6-N1-C1'	5.30	128.62	121.20
1	a	383	U	N3-C2-O2	-5.30	118.49	122.20
22	A	549	C	N3-C2-O2	-5.30	118.19	121.90
22	A	943	U	N3-C2-O2	-5.30	118.49	122.20
22	A	1479	C	N1-C2-O2	5.30	122.08	118.90
22	A	796	C	C6-N1-C2	-5.29	118.18	120.30
1	a	561	A	C4-C5-C6	5.29	119.65	117.00
1	a	1240	A	C4-N9-C1'	5.29	135.83	126.30
22	A	1317	G	C6-C5-N7	-5.29	127.22	130.40
23	B	68	C	O4'-C1'-N1	5.29	112.43	108.20
1	a	639	C	C6-N1-C2	-5.29	118.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	958	A	N3-C4-N9	5.29	131.63	127.40
1	a	308	A	N9-C4-C5	-5.29	103.69	105.80
22	A	1292	U	OP1-P-O3'	5.29	116.83	105.20
22	A	2128	A	C4-N9-C1'	5.28	135.80	126.30
22	A	2552	C	C6-N1-C2	-5.28	118.19	120.30
1	a	635	C	C2-N1-C1'	5.28	124.60	118.80
1	a	497	A	C4-N9-C1'	5.27	135.79	126.30
1	a	424	U	N1-C2-O2	5.27	126.49	122.80
1	a	769	C	C2-N1-C1'	5.27	124.60	118.80
22	A	561	G	C4-C5-N7	5.27	112.91	110.80
22	A	1045	C	N3-C2-O2	-5.27	118.21	121.90
22	A	1399	C	N3-C2-O2	-5.27	118.21	121.90
22	A	1622	U	N1-C2-O2	5.27	126.49	122.80
22	A	2077	C	N3-C2-O2	-5.27	118.21	121.90
20	u	57	G	N3-C2-N2	-5.26	116.22	119.90
22	A	721	U	N3-C2-O2	-5.26	118.52	122.20
22	A	949	U	C6-N1-C2	-5.26	117.84	121.00
22	A	2825	C	C6-N1-C2	-5.26	118.19	120.30
22	A	2670	U	N3-C2-O2	-5.26	118.52	122.20
1	a	590	G	N3-C2-N2	-5.26	116.22	119.90
22	A	2670	U	N1-C2-O2	5.26	126.48	122.80
22	A	2565	C	N3-C2-O2	-5.26	118.22	121.90
1	a	468	C	C5-C6-N1	5.25	123.63	121.00
22	A	1768	C	C6-N1-C2	-5.25	118.20	120.30
22	A	2020	C	C2-N1-C1'	5.25	124.58	118.80
22	A	831	C	N3-C2-O2	-5.24	118.23	121.90
22	A	1210	C	C5-C6-N1	5.24	123.62	121.00
1	a	712	U	N1-C2-O2	5.24	126.47	122.80
22	A	1024	G	C2-N3-C4	5.24	114.52	111.90
22	A	957	G	N3-C4-N9	5.24	129.15	126.00
22	A	2061	C	C6-N1-C2	-5.24	118.20	120.30
1	a	1043	C	C6-N1-C2	-5.24	118.20	120.30
22	A	2175	C	C6-N1-C1'	5.24	127.08	120.80
22	A	104	U	N1-C2-O2	5.23	126.46	122.80
22	A	1024	G	C8-N9-C1'	-5.23	120.20	127.00
22	A	1197	G	N9-C4-C5	-5.23	103.31	105.40
22	A	1882	C	N3-C2-O2	-5.23	118.24	121.90
1	a	995	C	C6-N1-C2	-5.23	118.21	120.30
1	a	643	G	C4-N9-C1'	-5.22	119.71	126.50
1	a	720	U	N3-C2-O2	-5.22	118.54	122.20
22	A	1765	C	C6-N1-C2	-5.22	118.21	120.30
1	a	927	U	N3-C2-O2	-5.22	118.55	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	893	C	N1-C2-O2	5.22	122.03	118.90
22	A	1718	C	C6-N1-C2	-5.22	118.21	120.30
22	A	2801	C	C2-N1-C1'	5.22	124.54	118.80
1	a	38	G	C2-N3-C4	5.22	114.51	111.90
22	A	1511	C	C6-N1-C2	-5.21	118.21	120.30
22	A	2035	G	C8-N9-C1'	-5.21	120.22	127.00
1	a	6	G	O4'-C1'-N9	5.21	112.37	108.20
1	a	1374	C	O4'-C1'-N1	5.21	112.36	108.20
22	A	1902	G	C4-N9-C1'	5.21	133.27	126.50
22	A	2700	G	N3-C4-C5	-5.21	126.00	128.60
1	a	1382	C	C6-N1-C2	-5.21	118.22	120.30
22	A	638	C	N1-C2-O2	5.20	122.02	118.90
1	a	971	U	N3-C2-O2	-5.20	118.56	122.20
22	A	2724	C	N3-C2-O2	-5.20	118.26	121.90
22	A	1069	A	N7-C8-N9	5.20	116.40	113.80
22	A	2794	G	N3-C4-N9	5.20	129.12	126.00
22	A	2589	C	C6-N1-C2	-5.20	118.22	120.30
22	A	607	G	N3-C4-N9	5.20	129.12	126.00
22	A	958	A	C4-N9-C1'	5.19	135.65	126.30
22	A	1025	C	C2-N1-C1'	5.19	124.51	118.80
1	a	659	U	N1-C2-O2	5.19	126.43	122.80
22	A	621	C	C2-N1-C1'	5.19	124.51	118.80
1	a	419	G	C8-N9-C1'	-5.19	120.25	127.00
22	A	77	C	C2-N1-C1'	5.19	124.51	118.80
22	A	2417	C	N1-C2-O2	5.19	122.01	118.90
22	A	77	C	C6-N1-C2	-5.18	118.23	120.30
22	A	561	G	C8-N9-C1'	-5.18	120.27	127.00
20	u	8	U	N1-C2-O2	5.18	126.43	122.80
22	A	897	G	N1-C6-O6	-5.18	116.79	119.90
22	A	1827	U	N3-C2-O2	-5.18	118.58	122.20
1	a	537	C	N3-C2-O2	-5.17	118.28	121.90
1	a	159	C	N1-C2-O2	5.17	122.00	118.90
1	a	340	A	N9-C4-C5	-5.17	103.73	105.80
22	A	2629	U	C2-N1-C1'	5.17	123.90	117.70
1	a	108	U	N1-C2-O2	5.17	126.42	122.80
22	A	413	U	N1-C2-O2	5.17	126.42	122.80
22	A	1351	C	N1-C2-O2	5.17	122.00	118.90
22	A	931	C	N1-C2-O2	5.16	122.00	118.90
20	u	49	C	N1-C2-O2	5.16	122.00	118.90
1	a	688	G	C4-N9-C1'	5.16	133.21	126.50
22	A	897	G	C5-C6-O6	5.16	131.69	128.60
1	a	406	C	C5-C6-N1	5.16	123.58	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1520	G	C4-N9-C1'	5.16	133.20	126.50
22	A	1045	C	N1-C2-O2	5.16	121.99	118.90
22	A	2779	A	C2-N3-C4	5.16	113.18	110.60
1	a	21	U	N3-C2-O2	-5.15	118.59	122.20
22	A	2114	U	N3-C2-O2	-5.15	118.59	122.20
20	u	76	A	N3-C4-C5	5.15	130.41	126.80
22	A	246	U	N1-C2-O2	5.15	126.40	122.80
22	A	1948	C	C5-C6-N1	5.15	123.57	121.00
1	a	1001	C	C6-N1-C2	-5.14	118.24	120.30
22	A	370	G	C4-N9-C1'	5.14	133.19	126.50
20	u	51	U	N3-C2-O2	-5.14	118.60	122.20
22	A	2114	U	N1-C2-O2	5.14	126.40	122.80
1	a	893	C	C6-N1-C2	-5.13	118.25	120.30
22	A	1584	G	OP2-P-O3'	5.13	116.50	105.20
23	B	73	U	O4'-C1'-N1	-5.13	104.09	108.20
22	A	1381	C	C2-N1-C1'	5.13	124.44	118.80
1	a	927	U	N1-C2-O2	5.13	126.39	122.80
22	A	1216	G	P-O3'-C3'	5.13	125.85	119.70
23	B	95	U	C2-N1-C1'	5.13	123.85	117.70
22	A	1955	C	C2-N1-C1'	5.12	124.44	118.80
20	u	49	C	C6-N1-C2	-5.12	118.25	120.30
22	A	1075	U	N1-C2-O2	5.12	126.39	122.80
22	A	164	U	C2-N1-C1'	-5.12	111.56	117.70
1	a	752	C	C5-C6-N1	5.12	123.56	121.00
22	A	549	C	C5-C6-N1	5.11	123.56	121.00
22	A	649	C	C5-C6-N1	5.11	123.56	121.00
22	A	730	C	C5-C6-N1	5.11	123.56	121.00
22	A	422	A	C5-N7-C8	-5.11	101.35	103.90
22	A	2417	C	N3-C2-O2	-5.10	118.33	121.90
1	a	1308	U	N3-C2-O2	-5.10	118.63	122.20
22	A	1293	G	N3-C4-N9	5.10	129.06	126.00
22	A	1102	G	C8-N9-C1'	-5.09	120.38	127.00
22	A	1785	C	C6-N1-C2	-5.09	118.26	120.30
1	a	340	A	C5-C6-N6	-5.09	119.63	123.70
1	a	491	C	C6-N1-C2	-5.09	118.26	120.30
22	A	1407	G	C4-N9-C1'	5.09	133.11	126.50
1	a	1176	C	N1-C2-O2	5.08	121.95	118.90
1	a	1144	C	C5-C6-N1	5.08	123.54	121.00
20	u	26	A	N9-C4-C5	-5.08	103.77	105.80
22	A	1885	C	C5-C6-N1	5.08	123.54	121.00
1	a	862	C	N1-C2-O2	5.07	121.94	118.90
22	A	2114	U	C2-N1-C1'	5.07	123.78	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	138	C	N1-C2-O2	5.06	121.94	118.90
1	a	1054	A	C5-N7-C8	-5.06	101.37	103.90
22	A	2474	U	N3-C2-O2	-5.06	118.66	122.20
22	A	2565	C	N1-C2-O2	5.06	121.94	118.90
22	A	2145	A	N3-C4-N9	5.05	131.44	127.40
1	a	159	C	N3-C2-O2	-5.05	118.37	121.90
1	a	540	C	C5-C6-N1	5.05	123.52	121.00
22	A	892	U	C2-N1-C1'	5.05	123.76	117.70
22	A	2794	G	C6-C5-N7	-5.05	127.37	130.40
1	a	658	C	C6-N1-C2	-5.04	118.28	120.30
22	A	1075	U	N3-C2-O2	-5.04	118.67	122.20
7	h	74	ILE	CG1-CB-CG2	-5.04	100.31	111.40
22	A	660	A	C5-N7-C8	-5.04	101.38	103.90
22	A	1453	U	C2-N1-C1'	5.04	123.75	117.70
20	u	32	U	N1-C2-O2	5.03	126.32	122.80
22	A	2007	U	C6-N1-C2	-5.03	117.98	121.00
22	A	1569	G	N3-C4-C5	5.03	131.12	128.60
22	A	2127	C	N3-C2-O2	-5.03	118.38	121.90
22	A	2326	U	C5-C6-N1	5.03	125.22	122.70
1	a	71	U	N1-C2-O2	5.03	126.32	122.80
1	a	401	C	N3-C2-O2	-5.03	118.38	121.90
1	a	474	C	C6-N1-C2	-5.03	118.29	120.30
22	A	751	C	C6-N1-C2	-5.03	118.29	120.30
22	A	310	G	C8-N9-C1'	-5.02	120.47	127.00
22	A	447	C	C6-N1-C2	-5.02	118.29	120.30
22	A	1157	C	C5-C6-N1	5.02	123.51	121.00
23	B	28	C	N3-C2-O2	-5.02	118.39	121.90
22	A	805	G	N3-C4-C5	-5.02	126.09	128.60
22	A	423	C	C6-N1-C2	-5.01	118.29	120.30
22	A	1713	C	C5-C6-N1	5.01	123.51	121.00
22	A	2885	C	N1-C2-O2	5.01	121.91	118.90
1	a	539	G	C4-N9-C1'	5.01	133.01	126.50
22	A	2417	C	C6-N1-C2	-5.01	118.30	120.30
22	A	1114	G	N1-C6-O6	-5.01	116.89	119.90
22	A	272	C	N3-C2-O2	-5.01	118.39	121.90
20	u	57	G	C8-N9-C1'	5.00	133.51	127.00

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
46	1	48	VAL	Peptide

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Mol	Chain	Res	Type	Group
49	4	3	ARG	Peptide
24	C	154	LEU	Peptide
24	C	198	GLU	Peptide
24	C	83	TYR	Peptide
25	D	53	TYR	Peptide
25	D	89	GLY	Peptide
26	E	80	SER	Peptide
27	F	3	ARG	Peptide
28	G	47	GLY	Peptide
29	K	45	PHE	Peptide
31	M	30	THR	Peptide
31	M	85	PHE	Peptide
32	N	101	LYS	Peptide
32	N	133	LYS	Peptide
32	N	24	GLY	Peptide
32	N	7	VAL	Peptide
32	N	8	LYS	Peptide
33	O	60	ARG	Peptide
35	Q	49	LYS	Peptide
37	S	49	GLY	Peptide
40	V	72	ASP	Peptide
40	V	87	ASP	Peptide
40	V	97	THR	Peptide
42	X	49	GLN	Peptide
43	Y	21	ALA	Peptide
2	c	22	TRP	Peptide
3	d	187	TYR	Peptide
3	d	188	PRO	Peptide
3	d	189	GLU	Peptide
11	l	133	LYS	Peptide
11	l	37	ASN	Peptide
18	s	41	PHE	Peptide
19	t	66	ILE	Peptide

5.2 Too-close contacts

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	c	202/204 (99%)	178 (88%)	24 (12%)	0	100	100
3	d	199/201 (99%)	169 (85%)	30 (15%)	0	100	100
4	e	161/163 (99%)	142 (88%)	19 (12%)	0	100	100
5	f	95/97 (98%)	86 (90%)	9 (10%)	0	100	100
6	g	152/154 (99%)	137 (90%)	15 (10%)	0	100	100
7	h	129/131 (98%)	118 (92%)	11 (8%)	0	100	100
8	i	126/128 (98%)	109 (86%)	16 (13%)	1 (1%)	19	60
9	j	97/99 (98%)	83 (86%)	14 (14%)	0	100	100
10	k	115/117 (98%)	95 (83%)	20 (17%)	0	100	100
11	l	134/136 (98%)	103 (77%)	30 (22%)	1 (1%)	22	62
12	m	110/112 (98%)	85 (77%)	25 (23%)	0	100	100
13	n	58/60 (97%)	51 (88%)	7 (12%)	0	100	100
14	o	86/88 (98%)	76 (88%)	10 (12%)	0	100	100
15	p	87/89 (98%)	72 (83%)	15 (17%)	0	100	100
16	q	81/83 (98%)	67 (83%)	14 (17%)	0	100	100
17	r	64/66 (97%)	52 (81%)	12 (19%)	0	100	100
18	s	76/78 (97%)	59 (78%)	17 (22%)	0	100	100
19	t	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
24	C	269/275 (98%)	241 (90%)	28 (10%)	0	100	100
25	D	205/207 (99%)	178 (87%)	27 (13%)	0	100	100
26	E	204/206 (99%)	174 (85%)	30 (15%)	0	100	100
27	F	175/177 (99%)	150 (86%)	25 (14%)	0	100	100
28	G	172/176 (98%)	141 (82%)	29 (17%)	2 (1%)	13	52
29	K	141/145 (97%)	124 (88%)	17 (12%)	0	100	100
30	L	120/122 (98%)	104 (87%)	16 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	M	144/146 (99%)	102 (71%)	40 (28%)	2 (1%)	11	48
32	N	139/141 (99%)	115 (83%)	24 (17%)	0	100	100
33	O	121/123 (98%)	96 (79%)	25 (21%)	0	100	100
34	P	108/117 (92%)	92 (85%)	16 (15%)	0	100	100
35	Q	110/114 (96%)	101 (92%)	9 (8%)	0	100	100
36	R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
37	S	98/102 (96%)	89 (91%)	9 (9%)	0	100	100
38	T	110/112 (98%)	98 (89%)	12 (11%)	0	100	100
39	U	87/89 (98%)	68 (78%)	18 (21%)	1 (1%)	14	54
40	V	98/101 (97%)	71 (72%)	24 (24%)	3 (3%)	4	32
41	W	92/94 (98%)	73 (79%)	18 (20%)	1 (1%)	14	54
42	X	74/76 (97%)	64 (86%)	10 (14%)	0	100	100
43	Y	52/54 (96%)	42 (81%)	10 (19%)	0	100	100
44	Z	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
45	0	54/58 (93%)	50 (93%)	4 (7%)	0	100	100
46	1	57/59 (97%)	42 (74%)	15 (26%)	0	100	100
47	2	54/56 (96%)	48 (89%)	6 (11%)	0	100	100
48	3	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
49	4	42/44 (96%)	37 (88%)	5 (12%)	0	100	100
50	5	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	9	46
51	6	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
All	All	5097/5211 (98%)	4343 (85%)	742 (15%)	12 (0%)	50	80

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	G	48	ASN
40	V	73	PRO
8	i	41	HIS
28	G	47	GLY
31	M	95	VAL
40	V	88	GLY
41	W	16	SER
31	M	98	GLU
39	U	50	VAL

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Mol	Chain	Res	Type
50	5	32	ARG
11	l	39	ASN
40	V	72	ASP

5.3.2 Protein sidechains [i](#)

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	c	162/162 (100%)	162 (100%)	0	100	100
3	d	175/175 (100%)	173 (99%)	2 (1%)	73	88
4	e	126/126 (100%)	125 (99%)	1 (1%)	81	92
5	f	86/86 (100%)	86 (100%)	0	100	100
6	g	131/131 (100%)	131 (100%)	0	100	100
7	h	112/112 (100%)	111 (99%)	1 (1%)	78	90
8	i	101/101 (100%)	99 (98%)	2 (2%)	55	79
9	j	90/90 (100%)	88 (98%)	2 (2%)	52	78
10	k	91/91 (100%)	91 (100%)	0	100	100
11	l	118/118 (100%)	117 (99%)	1 (1%)	81	92
12	m	95/95 (100%)	95 (100%)	0	100	100
13	n	51/51 (100%)	50 (98%)	1 (2%)	55	79
14	o	78/78 (100%)	77 (99%)	1 (1%)	69	87
15	p	79/79 (100%)	78 (99%)	1 (1%)	69	87
16	q	76/76 (100%)	74 (97%)	2 (3%)	46	75
17	r	57/57 (100%)	55 (96%)	2 (4%)	36	68
18	s	68/68 (100%)	67 (98%)	1 (2%)	65	84
19	t	62/62 (100%)	62 (100%)	0	100	100
24	C	225/225 (100%)	225 (100%)	0	100	100
25	D	169/170 (99%)	167 (99%)	2 (1%)	71	87
26	E	171/172 (99%)	169 (99%)	2 (1%)	71	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	F	153/154 (99%)	153 (100%)	0	100	100
28	G	146/146 (100%)	146 (100%)	0	100	100
29	K	122/122 (100%)	121 (99%)	1 (1%)	81	92
30	L	98/98 (100%)	98 (100%)	0	100	100
31	M	111/112 (99%)	111 (100%)	0	100	100
32	N	112/112 (100%)	109 (97%)	3 (3%)	44	74
33	O	104/105 (99%)	104 (100%)	0	100	100
34	P	86/91 (94%)	85 (99%)	1 (1%)	71	87
35	Q	97/97 (100%)	97 (100%)	0	100	100
36	R	94/94 (100%)	93 (99%)	1 (1%)	73	88
37	S	83/83 (100%)	83 (100%)	0	100	100
38	T	94/95 (99%)	94 (100%)	0	100	100
39	U	80/80 (100%)	79 (99%)	1 (1%)	69	87
40	V	84/85 (99%)	84 (100%)	0	100	100
41	W	85/85 (100%)	85 (100%)	0	100	100
42	X	60/61 (98%)	60 (100%)	0	100	100
43	Y	47/47 (100%)	45 (96%)	2 (4%)	29	63
44	Z	55/55 (100%)	54 (98%)	1 (2%)	59	81
45	0	49/49 (100%)	49 (100%)	0	100	100
46	1	55/55 (100%)	55 (100%)	0	100	100
47	2	46/46 (100%)	46 (100%)	0	100	100
48	3	49/49 (100%)	49 (100%)	0	100	100
49	4	39/39 (100%)	39 (100%)	0	100	100
50	5	51/51 (100%)	51 (100%)	0	100	100
51	6	35/35 (100%)	35 (100%)	0	100	100
All	All	4358/4371 (100%)	4327 (99%)	31 (1%)	84	93

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	d	58	ARG
3	d	66	ARG
4	e	149	ARG

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Mol	Chain	Res	Type
7	h	74	ILE
8	i	14	ASN
8	i	130	ARG
9	j	5	LYS
9	j	16	ARG
11	l	32	LYS
13	n	26	ARG
14	o	54	ARG
15	p	90	LYS
16	q	5	ARG
16	q	6	ASN
17	r	13	LYS
17	r	65	ARG
18	s	6	LYS
25	D	119	PHE
25	D	168	ARG
26	E	74	ARG
26	E	169	ASN
29	K	45	PHE
32	N	17	MET
32	N	74	TYR
32	N	99	ARG
34	P	103	ARG
36	R	47	PHE
39	U	48	VAL
43	Y	17	ASN
43	Y	32	ASN
44	Z	2	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
2	c	85	ASN
4	e	8	HIS
5	f	87	ASN
6	g	106	ASN
7	h	57	GLN
9	j	56	HIS
9	j	97	ASN
10	k	118	HIS
11	l	90	HIS
11	l	125	GLN

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Mol	Chain	Res	Type
13	n	52	GLN
14	o	62	HIS
15	p	88	ASN
16	q	6	ASN
17	r	56	GLN
18	s	22	GLN
19	t	72	ASN
24	C	95	HIS
24	C	134	ASN
24	C	230	HIS
25	D	14	GLN
25	D	37	GLN
26	E	14	ASN
26	E	20	ASN
26	E	29	ASN
26	E	49	HIS
26	E	75	GLN
26	E	145	ASN
26	E	169	ASN
27	F	2	ASN
27	F	37	ASN
28	G	73	ASN
31	M	38	GLN
34	P	114	ASN
36	R	38	GLN
36	R	81	HIS
38	T	65	ASN
40	V	75	ASN
41	W	58	ASN
41	W	78	GLN
43	Y	17	ASN
43	Y	23	ASN
43	Y	32	ASN
45	0	40	ASN
47	2	40	HIS
48	3	26	ASN
50	5	4	GLN
50	5	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1519/1523 (99%)	413 (27%)	0
20	u	75/76 (98%)	26 (34%)	0
21	v	4/5 (80%)	1 (25%)	0
22	A	2900/2903 (99%)	713 (24%)	21 (0%)
23	B	115/116 (99%)	38 (33%)	3 (2%)
All	All	4613/4623 (99%)	1191 (25%)	24 (0%)

All (1191) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	5	A
1	a	6	G
1	a	7	A
1	a	19	G
1	a	24	G
1	a	25	G
1	a	26	A
1	a	27	C
1	a	28	G
1	a	29	A
1	a	30	A
1	a	31	C
1	a	32	G
1	a	33	C
1	a	35	G
1	a	36	G
1	a	37	C
1	a	38	G
1	a	40	C
1	a	44	C
1	a	45	C
1	a	47	A
1	a	48	A
1	a	51	C
1	a	53	U
1	a	56	A
1	a	60	C
1	a	65	G
1	a	66	C
1	a	68	U
1	a	70	U
1	a	71	U
1	a	114	A

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Mol	Chain	Res	Type
1	a	126	C
1	a	132	G
1	a	135	A
1	a	136	A
1	a	137	C
1	a	140	A
1	a	141	C
1	a	142	C
1	a	148	G
1	a	150	G
1	a	152	G
1	a	154	G
1	a	165	G
1	a	169	C
1	a	179	U
1	a	180	A
1	a	183	G
1	a	185	A
1	a	186	U
1	a	189	C
1	a	192	U
1	a	202	A
1	a	203	U
1	a	204	G
1	a	211	G
1	a	212	A
1	a	215	G
1	a	218	A
1	a	219	G
1	a	222	G
1	a	225	U
1	a	226	U
1	a	228	G
1	a	231	U
1	a	235	G
1	a	240	U
1	a	241	G
1	a	243	A
1	a	255	U
1	a	256	G
1	a	259	U
1	a	262	G

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Mol	Chain	Res	Type
1	a	266	G
1	a	278	A
1	a	281	G
1	a	282	C
1	a	284	C
1	a	288	A
1	a	290	G
1	a	294	A
1	a	295	C
1	a	296	G
1	a	304	G
1	a	309	C
1	a	310	C
1	a	311	U
1	a	313	A
1	a	315	A
1	a	318	G
1	a	319	U
1	a	320	G
1	a	321	A
1	a	323	C
1	a	336	A
1	a	342	A
1	a	343	C
1	a	344	A
1	a	359	A
1	a	361	G
1	a	362	G
1	a	367	C
1	a	369	G
1	a	378	A
1	a	379	A
1	a	381	C
1	a	382	U
1	a	383	U
1	a	384	C
1	a	387	C
1	a	388	A
1	a	393	A
1	a	397	A
1	a	399	G
1	a	403	G

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Mol	Chain	Res	Type
1	a	407	G
1	a	412	A
1	a	414	G
1	a	415	C
1	a	416	C
1	a	417	G
1	a	418	C
1	a	421	G
1	a	425	G
1	a	427	A
1	a	428	G
1	a	429	A
1	a	430	A
1	a	438	G
1	a	443	G
1	a	444	U
1	a	446	A
1	a	447	A
1	a	455	U
1	a	456	G
1	a	463	A
1	a	469	A
1	a	470	A
1	a	474	C
1	a	475	G
1	a	476	U
1	a	477	U
1	a	478	A
1	a	480	U
1	a	481	A
1	a	483	C
1	a	484	U
1	a	488	C
1	a	489	G
1	a	490	U
1	a	493	C
1	a	497	A
1	a	498	C
1	a	499	G
1	a	500	G
1	a	501	U
1	a	512	A

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Mol	Chain	Res	Type
1	a	514	A
1	a	515	G
1	a	516	C
1	a	521	G
1	a	522	C
1	a	523	U
1	a	524	A
1	a	525	A
1	a	526	C
1	a	532	G
1	a	533	C
1	a	534	C
1	a	535	A
1	a	536	G
1	a	537	C
1	a	538	A
1	a	539	G
1	a	542	G
1	a	546	U
1	a	547	A
1	a	548	A
1	a	550	A
1	a	555	G
1	a	556	G
1	a	560	C
1	a	561	A
1	a	562	A
1	a	564	C
1	a	583	G
1	a	584	C
1	a	585	G
1	a	586	U
1	a	587	A
1	a	588	A
1	a	590	G
1	a	591	C
1	a	592	G
1	a	594	G
1	a	596	G
1	a	603	G
1	a	625	G
1	a	633	C

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Mol	Chain	Res	Type
1	a	634	U
1	a	635	C
1	a	637	A
1	a	638	C
1	a	643	G
1	a	644	A
1	a	646	G
1	a	647	G
1	a	648	U
1	a	649	C
1	a	668	U
1	a	671	G
1	a	680	A
1	a	681	G
1	a	701	U
1	a	702	A
1	a	710	A
1	a	718	G
1	a	725	G
1	a	736	A
1	a	739	G
1	a	744	A
1	a	749	G
1	a	764	A
1	a	765	C
1	a	767	G
1	a	770	G
1	a	773	G
1	a	775	G
1	a	802	A
1	a	808	U
1	a	814	G
1	a	832	C
1	a	835	U
1	a	836	G
1	a	843	A
1	a	847	G
1	a	851	G
1	a	858	U
1	a	859	C
1	a	860	C
1	a	861	G

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Mol	Chain	Res	Type
1	a	862	C
1	a	868	A
1	a	869	G
1	a	876	A
1	a	878	C
1	a	879	A
1	a	881	A
1	a	883	G
1	a	886	U
1	a	887	U
1	a	888	A
1	a	892	A
1	a	901	G
1	a	905	A
1	a	906	G
1	a	930	A
1	a	943	G
1	a	950	C
1	a	951	A
1	a	966	U
1	a	967	G
1	a	973	U
1	a	974	A
1	a	975	A
1	a	976	U
1	a	977	U
1	a	978	C
1	a	982	G
1	a	984	A
1	a	985	A
1	a	987	G
1	a	992	G
1	a	993	A
1	a	994	A
1	a	995	C
1	a	998	U
1	a	999	A
1	a	1000	C
1	a	1001	C
1	a	1002	A
1	a	1008	U
1	a	1009	G

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Mol	Chain	Res	Type
1	a	1018	U
1	a	1020	A
1	a	1022	C
1	a	1027	U
1	a	1030	A
1	a	1031	G
1	a	1036	A
1	a	1038	C
1	a	1039	U
1	a	1040	U
1	a	1042	C
1	a	1043	C
1	a	1044	C
1	a	1046	U
1	a	1047	C
1	a	1048	G
1	a	1051	G
1	a	1052	A
1	a	1055	A
1	a	1061	C
1	a	1069	G
1	a	1077	G
1	a	1080	G
1	a	1081	U
1	a	1095	G
1	a	1097	G
1	a	1102	U
1	a	1110	G
1	a	1111	U
1	a	1117	A
1	a	1124	G
1	a	1140	G
1	a	1141	U
1	a	1146	A
1	a	1147	U
1	a	1149	A
1	a	1153	A
1	a	1154	G
1	a	1155	U
1	a	1156	U
1	a	1157	G
1	a	1161	A

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Mol	Chain	Res	Type
1	a	1172	A
1	a	1173	C
1	a	1174	U
1	a	1183	C
1	a	1196	G
1	a	1199	G
1	a	1202	G
1	a	1208	G
1	a	1211	A
1	a	1212	A
1	a	1227	U
1	a	1228	A
1	a	1229	U
1	a	1237	G
1	a	1238	C
1	a	1239	U
1	a	1240	A
1	a	1241	C
1	a	1242	A
1	a	1255	U
1	a	1256	G
1	a	1268	G
1	a	1272	C
1	a	1275	U
1	a	1276	A
1	a	1293	A
1	a	1295	A
1	a	1300	U
1	a	1301	U
1	a	1302	A
1	a	1303	A
1	a	1305	G
1	a	1312	U
1	a	1313	C
1	a	1314	A
1	a	1315	G
1	a	1316	U
1	a	1317	U
1	a	1318	C
1	a	1320	G
1	a	1328	G
1	a	1330	U

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Mol	Chain	Res	Type
1	a	1334	A
1	a	1335	C
1	a	1336	U
1	a	1337	C
1	a	1338	G
1	a	1355	A
1	a	1361	A
1	a	1362	G
1	a	1372	A
1	a	1374	C
1	a	1375	A
1	a	1376	G
1	a	1378	A
1	a	1379	C
1	a	1388	G
1	a	1389	A
1	a	1391	U
1	a	1396	U
1	a	1409	A
1	a	1412	C
1	a	1413	A
1	a	1415	C
1	a	1434	G
1	a	1438	G
1	a	1440	A
1	a	1441	A
1	a	1448	A
1	a	1457	A
1	a	1461	A
1	a	1465	U
1	a	1467	U
1	a	1468	U
1	a	1500	U
1	a	1503	G
1	a	1508	A
1	a	1514	U
1	a	1515	A
1	a	1518	A
1	a	1519	A
1	a	1520	G
1	a	1521	G
1	a	1522	U

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Mol	Chain	Res	Type
1	a	1545	G
1	a	1546	G
20	u	4	C
20	u	8	U
20	u	9	A
20	u	13	C
20	u	15	G
20	u	17	C
20	u	18	G
20	u	19	G
20	u	20	U
20	u	21	A
20	u	24	G
20	u	26	A
20	u	44	G
20	u	46	G
20	u	47	U
20	u	48	C
20	u	49	C
20	u	54	U
20	u	55	U
20	u	56	C
20	u	57	G
20	u	58	A
20	u	59	U
20	u	74	C
20	u	75	C
20	u	76	A
21	v	17	U
22	A	10	G
22	A	13	U
22	A	14	A
22	A	15	A
22	A	16	G
22	A	26	U
22	A	29	A
22	A	35	U
22	A	49	G
22	A	50	A
22	A	52	G
22	A	62	A
22	A	65	A

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Mol	Chain	Res	Type
22	A	72	A
22	A	75	U
22	A	76	G
22	A	89	G
22	A	97	G
22	A	100	A
22	A	102	G
22	A	103	A
22	A	110	G
22	A	117	G
22	A	118	A
22	A	119	A
22	A	120	U
22	A	125	G
22	A	131	A
22	A	151	A
22	A	155	U
22	A	156	U
22	A	162	A
22	A	165	A
22	A	166	C
22	A	168	U
22	A	169	A
22	A	177	A
22	A	180	G
22	A	181	G
22	A	182	U
22	A	184	G
22	A	185	A
22	A	189	A
22	A	199	A
22	A	202	A
22	A	204	C
22	A	207	A
22	A	218	G
22	A	219	A
22	A	224	A
22	A	225	A
22	A	229	A
22	A	231	A
22	A	232	U
22	A	233	U

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Mol	Chain	Res	Type
22	A	235	G
22	A	244	A
22	A	250	G
22	A	251	G
22	A	253	G
22	A	254	A
22	A	255	G
22	A	268	A
22	A	270	C
22	A	279	A
22	A	284	C
22	A	285	U
22	A	286	U
22	A	288	C
22	A	289	U
22	A	294	G
22	A	298	U
22	A	300	G
22	A	301	U
22	A	302	A
22	A	309	C
22	A	310	G
22	A	312	U
22	A	313	A
22	A	318	A
22	A	321	C
22	A	322	U
22	A	332	G
22	A	339	G
22	A	344	G
22	A	348	A
22	A	352	C
22	A	367	A
22	A	368	A
22	A	383	A
22	A	386	G
22	A	389	G
22	A	393	A
22	A	397	C
22	A	399	A
22	A	400	G
22	A	414	A

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Mol	Chain	Res	Type
22	A	421	A
22	A	426	G
22	A	451	G
22	A	452	A
22	A	471	U
22	A	476	C
22	A	487	A
22	A	488	U
22	A	494	A
22	A	496	C
22	A	497	A
22	A	507	G
22	A	516	G
22	A	517	A
22	A	521	G
22	A	533	G
22	A	543	U
22	A	544	A
22	A	547	U
22	A	548	C
22	A	549	C
22	A	551	G
22	A	561	G
22	A	566	C
22	A	567	A
22	A	569	C
22	A	570	A
22	A	571	A
22	A	572	G
22	A	584	U
22	A	585	A
22	A	586	A
22	A	588	G
22	A	600	G
22	A	610	G
22	A	611	A
22	A	612	A
22	A	623	A
22	A	632	U
22	A	640	A
22	A	653	G
22	A	654	A

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Mol	Chain	Res	Type
22	A	655	G
22	A	660	A
22	A	669	G
22	A	670	A
22	A	673	G
22	A	676	A
22	A	677	G
22	A	684	U
22	A	685	A
22	A	690	G
22	A	692	A
22	A	693	U
22	A	694	G
22	A	708	A
22	A	709	G
22	A	710	A
22	A	711	C
22	A	712	C
22	A	722	G
22	A	726	U
22	A	741	G
22	A	750	G
22	A	753	G
22	A	757	A
22	A	759	C
22	A	766	G
22	A	769	G
22	A	770	A
22	A	787	U
22	A	788	G
22	A	792	A
22	A	804	A
22	A	805	G
22	A	808	G
22	A	815	G
22	A	816	C
22	A	817	G
22	A	822	A
22	A	823	A
22	A	824	U
22	A	825	U
22	A	832	G

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Mol	Chain	Res	Type
22	A	833	A
22	A	840	A
22	A	845	G
22	A	846	C
22	A	849	G
22	A	851	U
22	A	852	C
22	A	867	U
22	A	868	U
22	A	886	U
22	A	887	G
22	A	888	A
22	A	891	A
22	A	892	U
22	A	900	G
22	A	901	U
22	A	902	A
22	A	903	G
22	A	905	G
22	A	907	A
22	A	908	C
22	A	909	U
22	A	910	G
22	A	919	A
22	A	920	G
22	A	921	G
22	A	923	G
22	A	924	C
22	A	925	C
22	A	927	A
22	A	928	U
22	A	932	G
22	A	933	G
22	A	934	G
22	A	935	U
22	A	936	U
22	A	939	C
22	A	943	U
22	A	944	U
22	A	945	C
22	A	946	A
22	A	947	G

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Mol	Chain	Res	Type
22	A	948	A
22	A	950	A
22	A	951	A
22	A	952	A
22	A	955	C
22	A	956	C
22	A	957	G
22	A	958	A
22	A	959	A
22	A	960	U
22	A	961	G
22	A	964	A
22	A	966	U
22	A	967	C
22	A	981	A
22	A	983	U
22	A	985	A
22	A	986	G
22	A	991	C
22	A	992	G
22	A	993	A
22	A	994	G
22	A	995	U
22	A	997	A
22	A	998	U
22	A	1001	G
22	A	1007	U
22	A	1014	A
22	A	1016	G
22	A	1023	A
22	A	1026	C
22	A	1028	A
22	A	1029	G
22	A	1036	A
22	A	1037	G
22	A	1045	C
22	A	1048	A
22	A	1051	A
22	A	1053	A
22	A	1057	G
22	A	1061	A
22	A	1062	G

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Mol	Chain	Res	Type
22	A	1063	U
22	A	1064	G
22	A	1065	G
22	A	1066	A
22	A	1073	U
22	A	1079	G
22	A	1085	C
22	A	1087	G
22	A	1092	C
22	A	1093	U
22	A	1094	A
22	A	1096	G
22	A	1097	A
22	A	1098	U
22	A	1100	U
22	A	1101	U
22	A	1104	C
22	A	1106	U
22	A	1107	A
22	A	1111	G
22	A	1112	C
22	A	1113	A
22	A	1114	G
22	A	1116	C
22	A	1117	A
22	A	1118	C
22	A	1120	A
22	A	1121	U
22	A	1122	U
22	A	1125	A
22	A	1127	G
22	A	1128	A
22	A	1129	G
22	A	1130	U
22	A	1131	G
22	A	1134	U
22	A	1135	A
22	A	1137	U
22	A	1138	A
22	A	1139	G
22	A	1140	C
22	A	1141	U

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Mol	Chain	Res	Type
22	A	1142	C
22	A	1143	A
22	A	1144	C
22	A	1145	U
22	A	1146	A
22	A	1147	G
22	A	1148	U
22	A	1149	C
22	A	1150	G
22	A	1151	A
22	A	1152	G
22	A	1157	C
22	A	1166	A
22	A	1167	A
22	A	1168	A
22	A	1171	G
22	A	1172	U
22	A	1174	C
22	A	1175	C
22	A	1179	G
22	A	1181	U
22	A	1182	A
22	A	1212	A
22	A	1214	U
22	A	1215	A
22	A	1217	G
22	A	1224	G
22	A	1244	G
22	A	1249	G
22	A	1257	A
22	A	1272	G
22	A	1273	G
22	A	1275	G
22	A	1277	G
22	A	1285	G
22	A	1287	G
22	A	1290	A
22	A	1292	U
22	A	1293	G
22	A	1302	A
22	A	1308	G
22	A	1309	A

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Mol	Chain	Res	Type
22	A	1310	A
22	A	1311	A
22	A	1336	U
22	A	1337	A
22	A	1338	U
22	A	1350	C
22	A	1357	A
22	A	1365	U
22	A	1366	C
22	A	1373	G
22	A	1376	U
22	A	1377	U
22	A	1388	U
22	A	1394	G
22	A	1396	G
22	A	1397	G
22	A	1401	A
22	A	1404	G
22	A	1407	G
22	A	1411	G
22	A	1415	U
22	A	1416	G
22	A	1417	G
22	A	1420	A
22	A	1428	G
22	A	1429	A
22	A	1431	A
22	A	1432	U
22	A	1436	U
22	A	1439	A
22	A	1443	G
22	A	1448	U
22	A	1449	U
22	A	1450	U
22	A	1451	U
22	A	1452	G
22	A	1453	U
22	A	1455	U
22	A	1456	G
22	A	1457	A
22	A	1461	A
22	A	1462	U

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Mol	Chain	Res	Type
22	A	1469	A
22	A	1470	C
22	A	1471	G
22	A	1475	U
22	A	1487	U
22	A	1488	G
22	A	1489	C
22	A	1491	U
22	A	1492	G
22	A	1493	C
22	A	1494	G
22	A	1495	A
22	A	1496	U
22	A	1497	U
22	A	1500	A
22	A	1501	A
22	A	1502	G
22	A	1503	U
22	A	1504	G
22	A	1509	U
22	A	1510	C
22	A	1519	G
22	A	1521	G
22	A	1525	U
22	A	1531	G
22	A	1535	U
22	A	1536	A
22	A	1539	U
22	A	1551	U
22	A	1552	A
22	A	1559	A
22	A	1566	A
22	A	1567	C
22	A	1568	G
22	A	1573	G
22	A	1576	A
22	A	1584	G
22	A	1585	U
22	A	1586	A
22	A	1589	G
22	A	1590	A
22	A	1592	G

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Mol	Chain	Res	Type
22	A	1600	C
22	A	1601	G
22	A	1603	C
22	A	1604	A
22	A	1605	C
22	A	1606	A
22	A	1612	A
22	A	1613	A
22	A	1615	A
22	A	1623	C
22	A	1629	A
22	A	1630	G
22	A	1631	A
22	A	1632	A
22	A	1633	A
22	A	1634	A
22	A	1635	C
22	A	1645	U
22	A	1646	A
22	A	1650	U
22	A	1651	A
22	A	1653	A
22	A	1673	A
22	A	1677	U
22	A	1689	A
22	A	1690	G
22	A	1691	C
22	A	1717	G
22	A	1718	C
22	A	1737	C
22	A	1738	G
22	A	1741	A
22	A	1747	G
22	A	1756	U
22	A	1757	U
22	A	1758	C
22	A	1770	G
22	A	1777	G
22	A	1778	G
22	A	1784	G
22	A	1787	A
22	A	1790	G

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Mol	Chain	Res	Type
22	A	1795	U
22	A	1796	C
22	A	1798	A
22	A	1799	A
22	A	1801	A
22	A	1814	C
22	A	1815	A
22	A	1821	G
22	A	1822	U
22	A	1823	A
22	A	1828	G
22	A	1829	A
22	A	1830	A
22	A	1842	G
22	A	1843	A
22	A	1872	G
22	A	1881	G
22	A	1882	C
22	A	1886	G
22	A	1896	A
22	A	1913	A
22	A	1917	G
22	A	1919	C
22	A	1920	G
22	A	1927	A
22	A	1928	C
22	A	1943	G
22	A	1944	G
22	A	1948	C
22	A	1952	A
22	A	1953	U
22	A	1969	U
22	A	1970	U
22	A	1977	C
22	A	1978	G
22	A	1979	C
22	A	1981	C
22	A	1984	A
22	A	1985	A
22	A	1986	G
22	A	1989	G
22	A	1990	U

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Mol	Chain	Res	Type
22	A	1996	U
22	A	2005	U
22	A	2006	G
22	A	2007	U
22	A	2011	A
22	A	2035	G
22	A	2036	U
22	A	2044	A
22	A	2045	A
22	A	2046	G
22	A	2047	A
22	A	2048	U
22	A	2057	C
22	A	2066	G
22	A	2069	C
22	A	2070	G
22	A	2074	A
22	A	2075	G
22	A	2076	A
22	A	2082	U
22	A	2083	G
22	A	2084	G
22	A	2107	G
22	A	2115	G
22	A	2125	U
22	A	2126	A
22	A	2127	C
22	A	2129	G
22	A	2130	G
22	A	2131	A
22	A	2132	U
22	A	2134	G
22	A	2139	G
22	A	2140	A
22	A	2141	G
22	A	2144	G
22	A	2145	A
22	A	2146	U
22	A	2148	A
22	A	2149	G
22	A	2155	A
22	A	2158	G

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Mol	Chain	Res	Type
22	A	2159	C
22	A	2160	U
22	A	2161	A
22	A	2162	G
22	A	2165	U
22	A	2166	C
22	A	2168	G
22	A	2170	G
22	A	2174	G
22	A	2178	U
22	A	2182	G
22	A	2183	G
22	A	2184	G
22	A	2186	U
22	A	2187	A
22	A	2198	G
22	A	2200	U
22	A	2213	A
22	A	2217	G
22	A	2218	C
22	A	2227	U
22	A	2228	C
22	A	2239	A
22	A	2252	G
22	A	2253	G
22	A	2280	A
22	A	2282	A
22	A	2283	A
22	A	2284	G
22	A	2297	C
22	A	2298	C
22	A	2301	A
22	A	2302	A
22	A	2317	G
22	A	2318	G
22	A	2319	U
22	A	2323	A
22	A	2325	A
22	A	2333	A
22	A	2334	A
22	A	2336	A
22	A	2337	G

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Mol	Chain	Res	Type
22	A	2339	G
22	A	2341	A
22	A	2348	G
22	A	2349	A
22	A	2350	A
22	A	2359	G
22	A	2361	C
22	A	2364	C
22	A	2372	A
22	A	2379	G
22	A	2390	A
22	A	2393	G
22	A	2397	G
22	A	2398	G
22	A	2399	C
22	A	2405	G
22	A	2406	A
22	A	2417	C
22	A	2420	C
22	A	2427	G
22	A	2433	U
22	A	2436	C
22	A	2437	U
22	A	2439	A
22	A	2442	G
22	A	2443	G
22	A	2445	U
22	A	2455	C
22	A	2461	G
22	A	2462	A
22	A	2469	G
22	A	2473	A
22	A	2488	C
22	A	2492	A
22	A	2498	G
22	A	2505	U
22	A	2517	A
22	A	2519	G
22	A	2532	A
22	A	2534	C
22	A	2543	G
22	A	2548	C

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Mol	Chain	Res	Type
22	A	2549	G
22	A	2557	G
22	A	2558	G
22	A	2561	U
22	A	2566	U
22	A	2580	A
22	A	2581	G
22	A	2586	A
22	A	2587	C
22	A	2588	G
22	A	2592	G
22	A	2596	G
22	A	2598	U
22	A	2599	U
22	A	2600	C
22	A	2616	A
22	A	2623	U
22	A	2624	C
22	A	2627	U
22	A	2629	U
22	A	2634	C
22	A	2643	U
22	A	2650	U
22	A	2651	U
22	A	2652	G
22	A	2667	U
22	A	2668	A
22	A	2677	G
22	A	2696	G
22	A	2703	U
22	A	2728	G
22	A	2746	G
22	A	2747	A
22	A	2749	G
22	A	2753	U
22	A	2762	A
22	A	2766	C
22	A	2770	U
22	A	2778	A
22	A	2779	A
22	A	2780	G
22	A	2789	A

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Mol	Chain	Res	Type
22	A	2791	G
22	A	2792	A
22	A	2793	U
22	A	2795	A
22	A	2804	A
22	A	2805	U
22	A	2809	U
22	A	2812	A
22	A	2813	A
22	A	2814	G
22	A	2819	U
22	A	2829	G
22	A	2831	G
22	A	2835	U
22	A	2836	G
22	A	2844	A
22	A	2845	G
22	A	2846	A
22	A	2847	U
22	A	2868	G
22	A	2869	U
22	A	2872	U
22	A	2878	G
22	A	2883	G
22	A	2891	C
22	A	2897	G
22	A	2902	A
22	A	2904	G
23	B	8	G
23	B	10	G
23	B	11	A
23	B	13	A
23	B	14	G
23	B	22	G
23	B	31	G
23	B	40	C
23	B	42	G
23	B	43	A
23	B	51	A
23	B	54	U
23	B	55	A
23	B	64	A

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Mol	Chain	Res	Type
23	B	65	G
23	B	70	G
23	B	71	A
23	B	73	U
23	B	74	G
23	B	75	U
23	B	76	A
23	B	77	G
23	B	79	G
23	B	80	A
23	B	81	A
23	B	82	G
23	B	84	G
23	B	85	U
23	B	86	U
23	B	87	U
23	B	91	U
23	B	92	U
23	B	94	G
23	B	97	A
23	B	98	G
23	B	99	A
23	B	101	U
23	B	107	G

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	A	179	A
22	A	311	A
22	A	427	A
22	A	559	G
22	A	654	A
22	A	693	U
22	A	890	A
22	A	934	G
22	A	949	U
22	A	963	C
22	A	994	G
22	A	1101	U
22	A	1147	G
22	A	1239	U

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Mol	Chain	Res	Type
22	A	1431	A
22	A	1584	G
22	A	1585	U
22	A	1604	A
22	A	1605	C
22	A	2317	G
22	A	2813	A
23	B	73	U
23	B	90	C
23	B	98	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	a	3
22	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	928:U	O3'	931:C	P	13.85
1	a	71:U	O3'	97:G	P	13.64
1	A	1579:U	O3'	1583:A	P	5.91
1	a	465:G	O3'	466:A	P	5.38
1	a	519:C	O3'	520:G	P	3.31

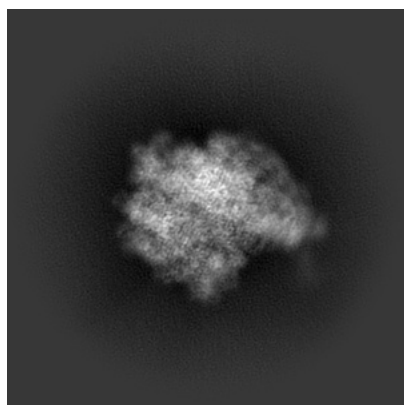
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0656. These allow visual inspection of the internal detail of the map and identification of artifacts.

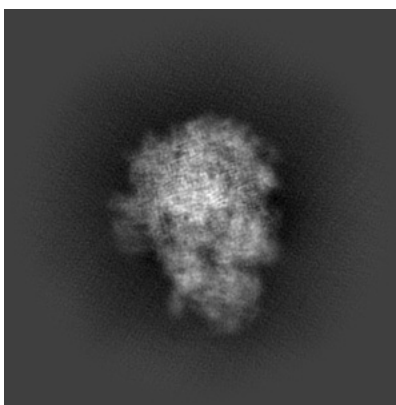
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

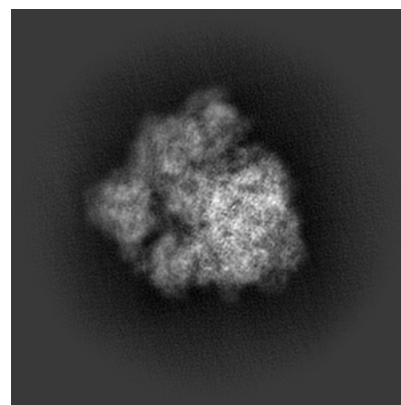
6.1.1 Primary map



X



Y

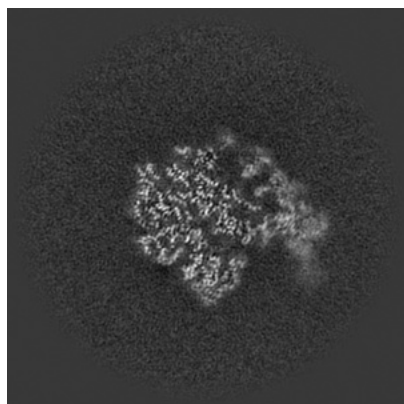


Z

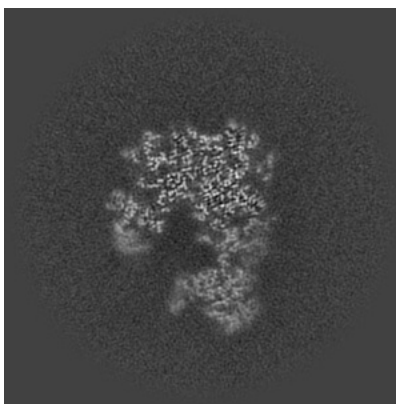
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

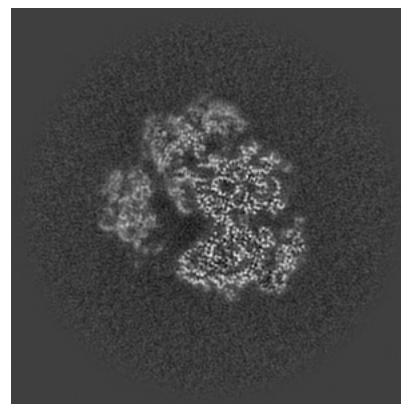
6.2.1 Primary map



X Index: 220



Y Index: 220

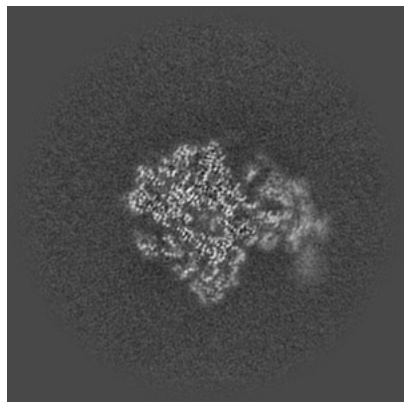


Z Index: 220

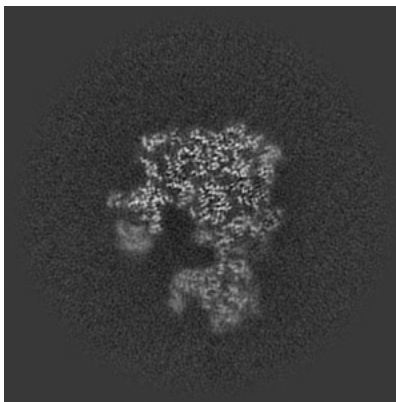
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

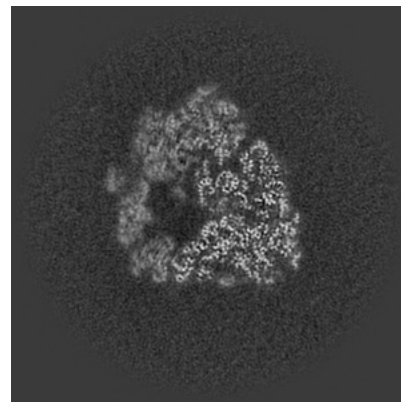
6.3.1 Primary map



X Index: 226



Y Index: 228

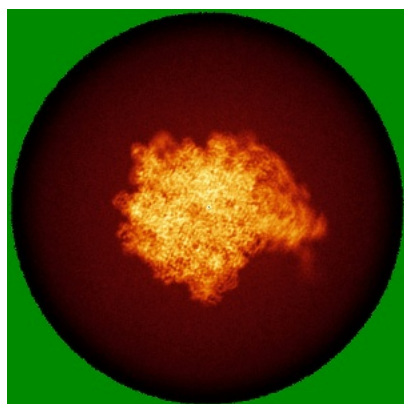


Z Index: 209

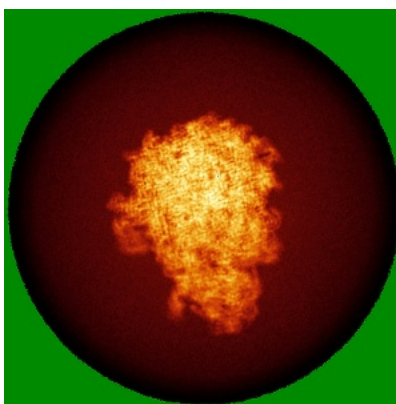
The images above show the largest variance slices of the map in three orthogonal directions.

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

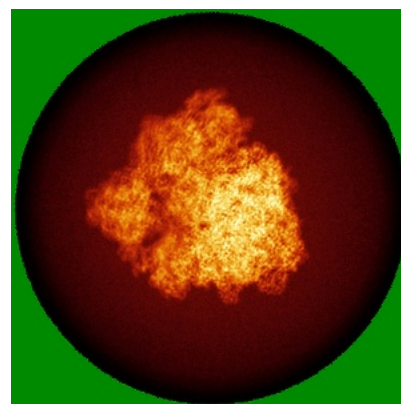
6.4.1 Primary map



X



Y



Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.238. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

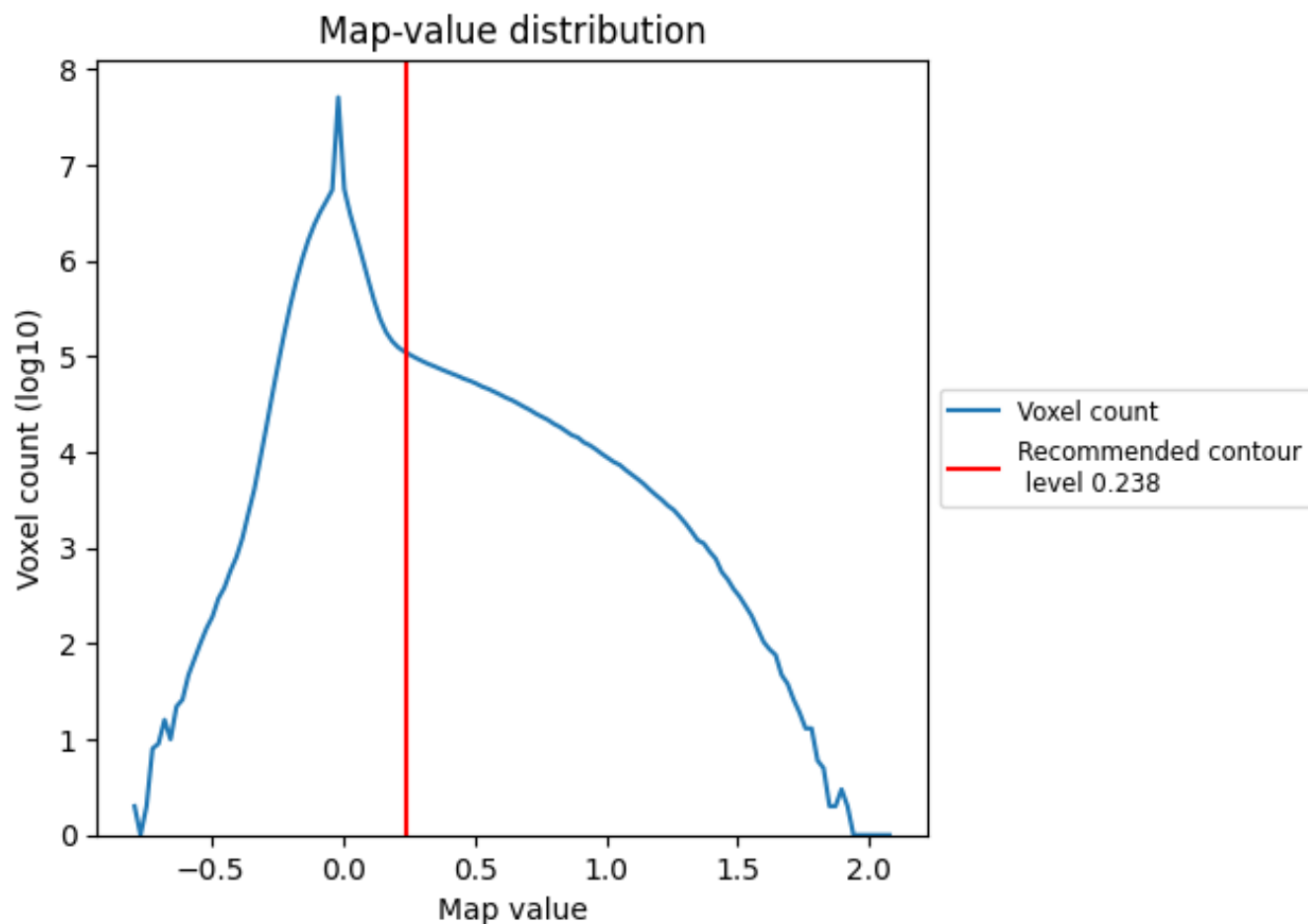
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

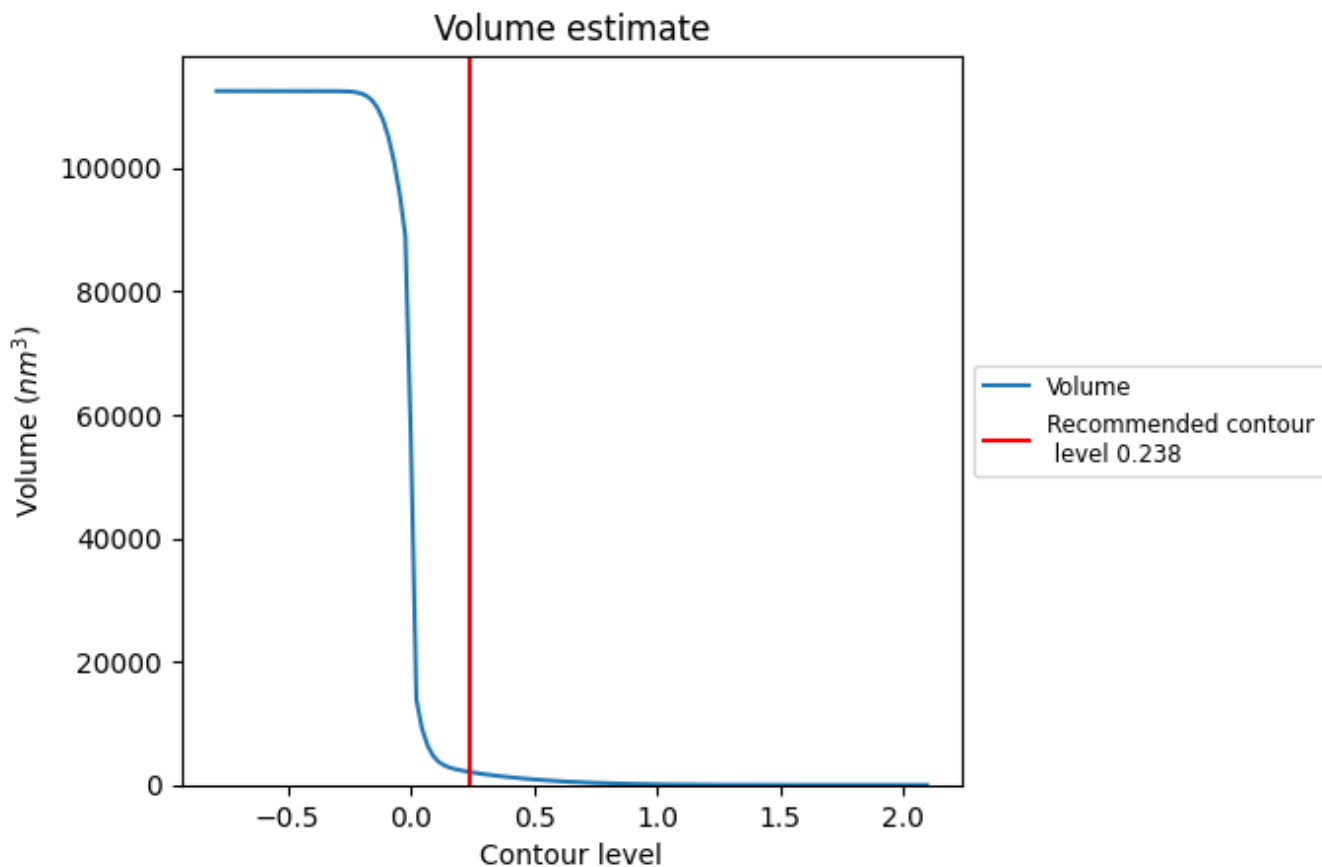
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

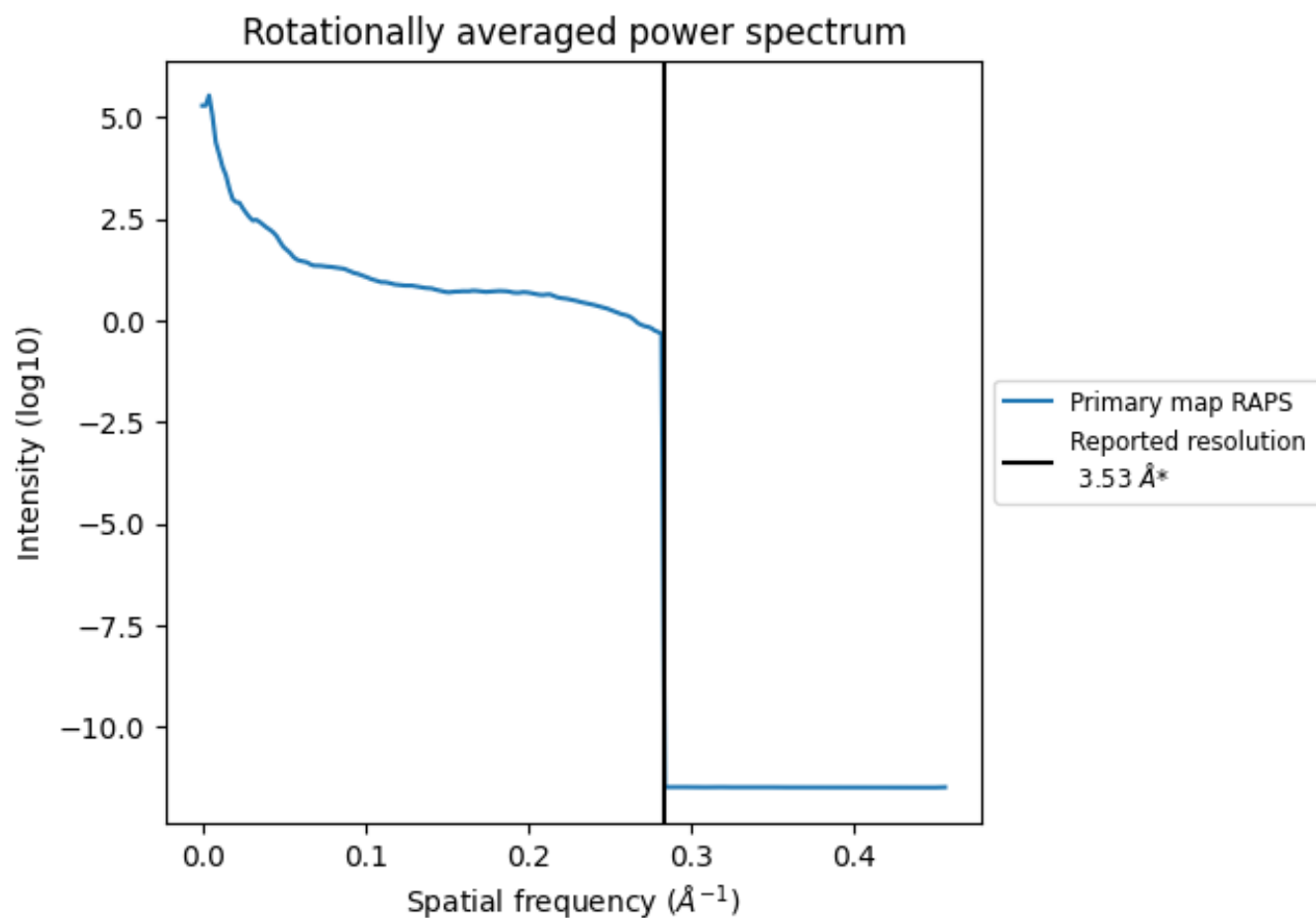
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2103 nm^3 ; this corresponds to an approximate mass of 1899 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.283\AA^{-1}

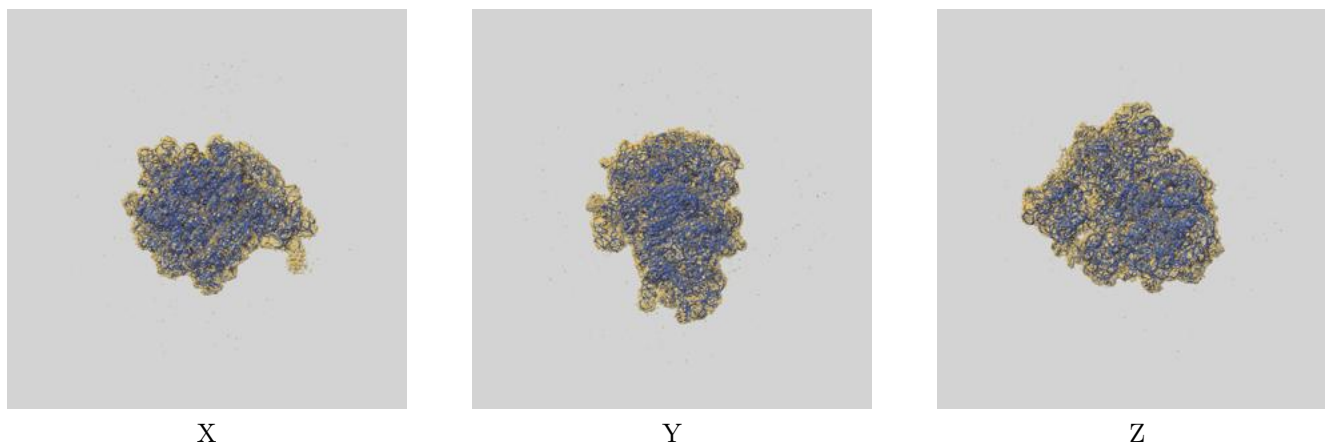
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

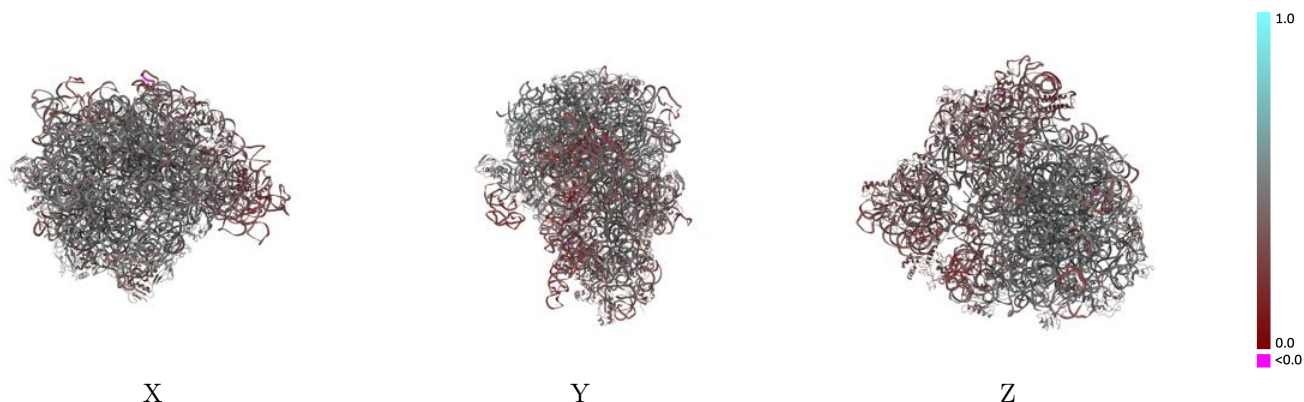
This section contains information regarding the fit between EMDB map EMD-0656 and PDB model 6O8W. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



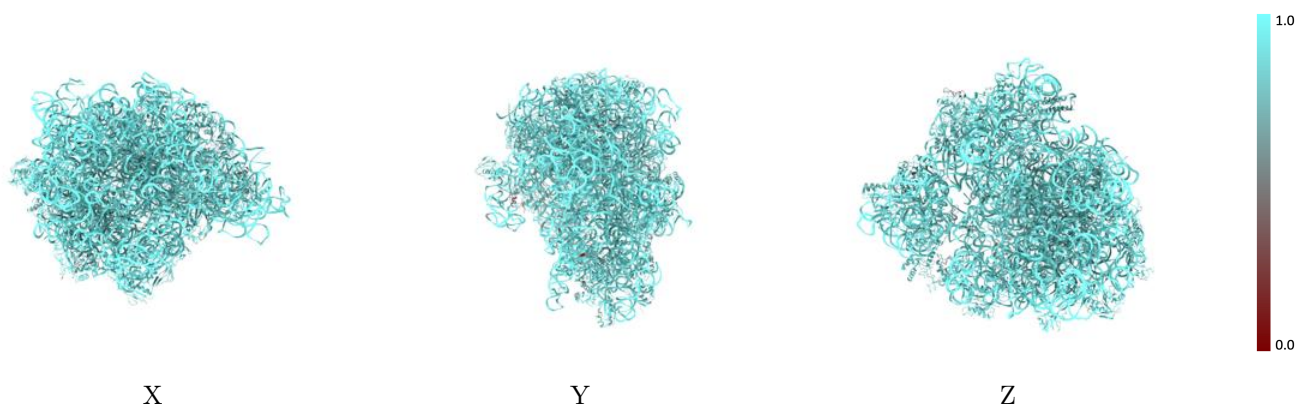
The images above show the 3D surface view of the map at the recommended contour level 0.238 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



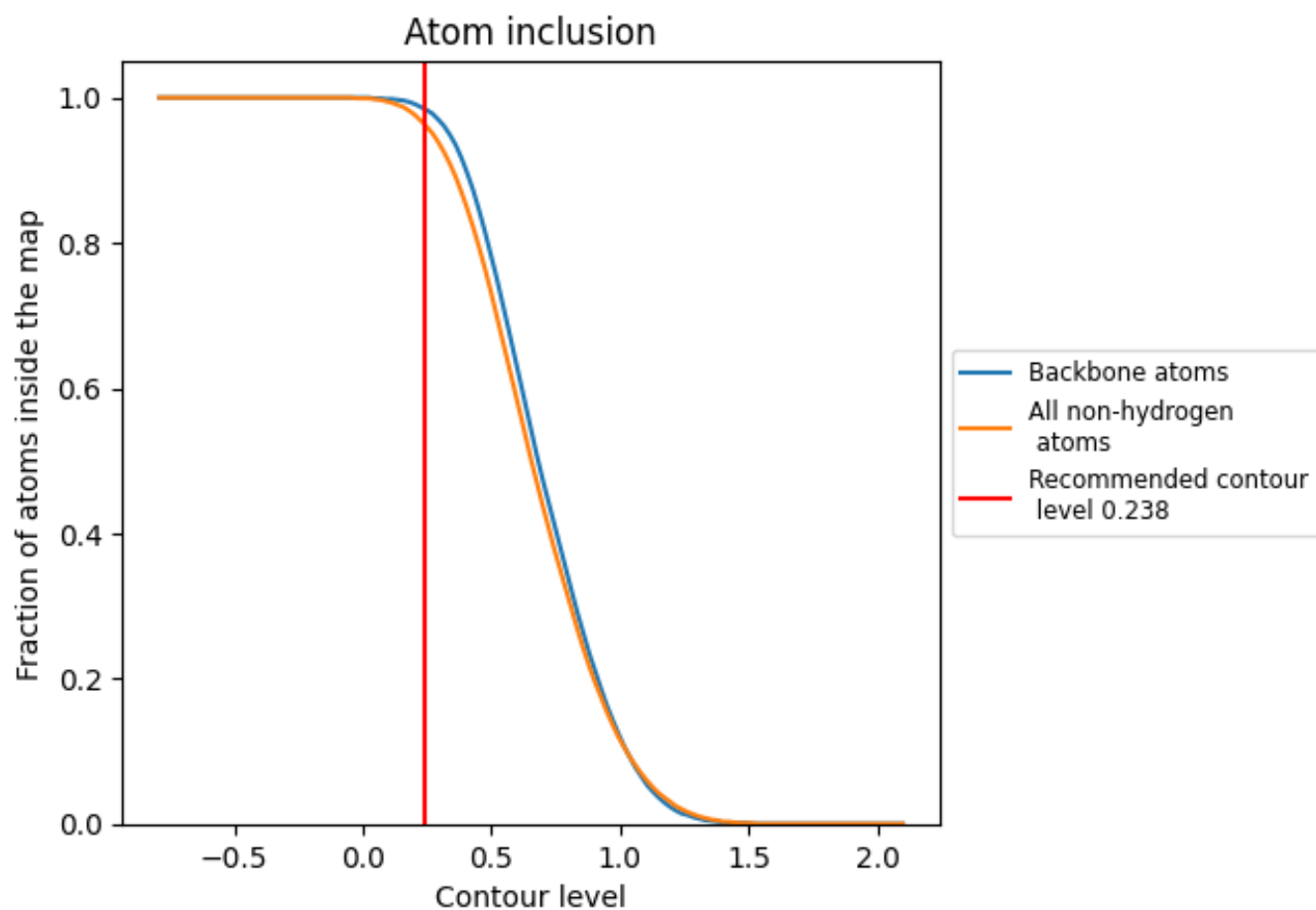
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.238).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary



































The table lists the average atom inclusion at the recommended contour level (0.238) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.4220
0	 0.9250	 0.4750
1	 0.9010	 0.2830
2	 0.9570	 0.4810
3	 0.9360	 0.4750
4	 0.9290	 0.4550
5	 0.9330	 0.4840
6	 0.9700	 0.4810
A	 0.9920	 0.4520
B	 0.9940	 0.4030
C	 0.9310	 0.4740
D	 0.9390	 0.4820
E	 0.9420	 0.4600
F	 0.8580	 0.3350
G	 0.9060	 0.4000
K	 0.9350	 0.4660
L	 0.9130	 0.4900
M	 0.9500	 0.4780
N	 0.8220	 0.4190
O	 0.9340	 0.4600
P	 0.9080	 0.3870
Q	 0.9130	 0.4650
R	 0.9120	 0.4460
S	 0.9230	 0.4770
T	 0.9460	 0.4730
U	 0.9300	 0.4470
V	 0.9070	 0.4290
W	 0.3690	 0.3130
X	 0.9400	 0.4890
Y	 0.9710	 0.4960
Z	 0.9040	 0.4170
a	 0.9910	 0.3860
c	 0.9000	 0.3740
d	 0.8350	 0.3200
e	 0.9020	 0.4160



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Chain	Atom inclusion	Q-score
f	 0.8760	 0.4240
g	 0.8500	 0.3170
h	 0.9150	 0.3940
i	 0.9400	 0.3680
j	 0.8680	 0.3610
k	 0.8820	 0.4040
l	 0.8670	 0.3440
m	 0.8920	 0.3050
n	 0.9580	 0.3810
o	 0.8850	 0.3800
p	 0.9030	 0.3150
q	 0.8540	 0.3660
r	 0.8790	 0.3940
s	 0.9000	 0.2810
t	 0.8380	 0.2850
u	 0.9900	 0.3890
v	 0.9800	 0.4700