



## Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 12:05 am GMT

PDB ID : 6R84  
EMDB ID : EMD-4751  
Title : Yeast Vms1 (Q295L)-60S ribosomal subunit complex (pre-state with Arb1)  
Authors : Su, T.; Izawa, T.; Cheng, J.; Yamashita, Y.; Berninghausen, O.; Inada, T.;  
Neupert, W.; Beckmann, R.  
Deposited on : 2019-03-31  
Resolution : 3.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

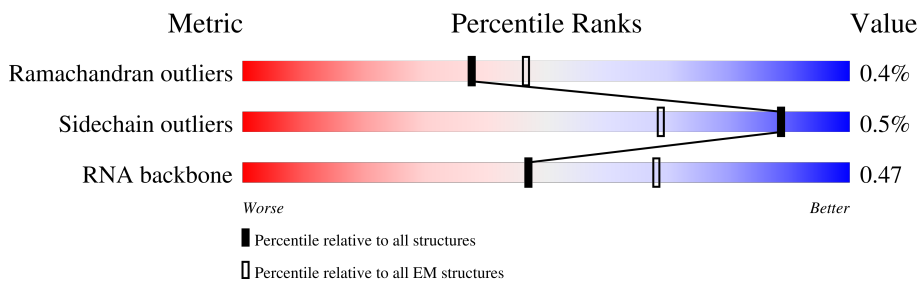
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 Å.

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



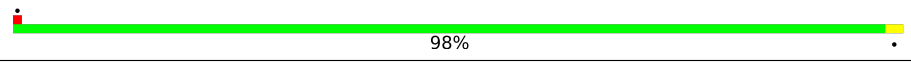
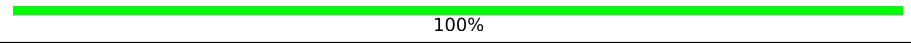
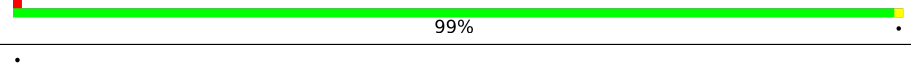
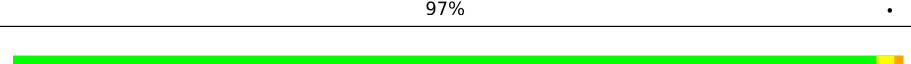
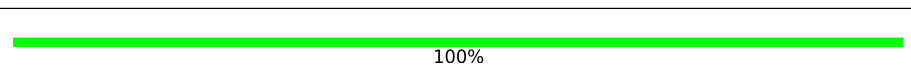
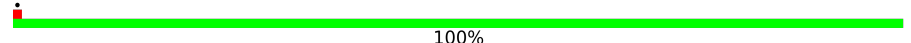
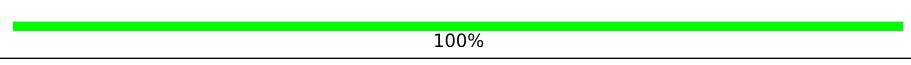
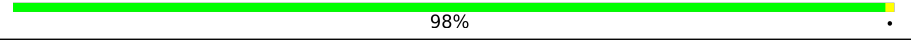
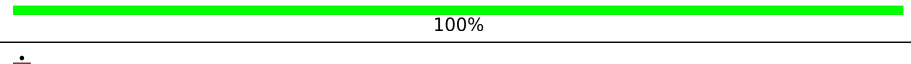
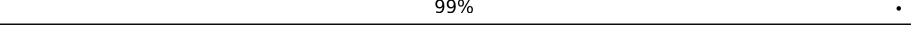
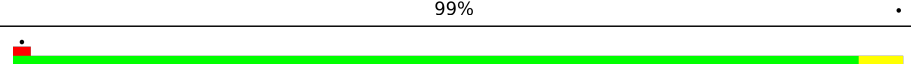
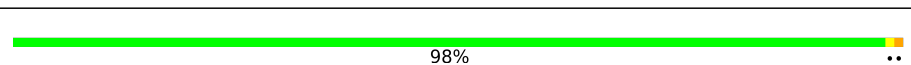
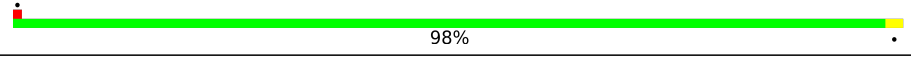
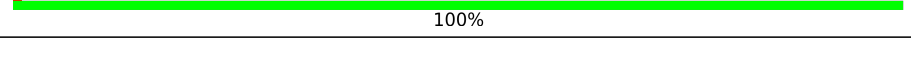
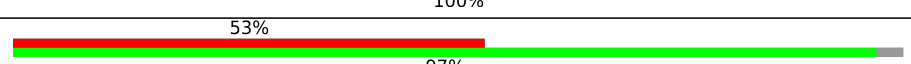

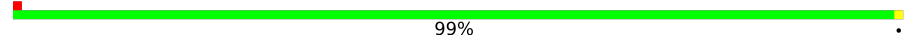

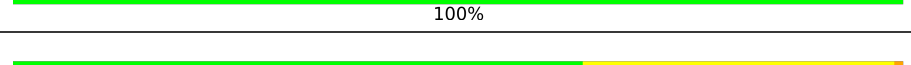
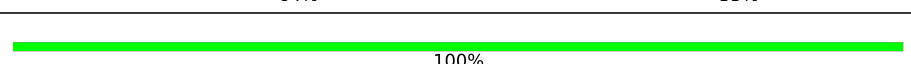
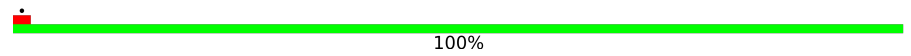



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	519	
2	R	433	
3	X	224	
4	i	112	
5	J	222	
6	j	119	
7	K	233	
8	k	99	


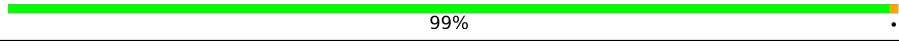
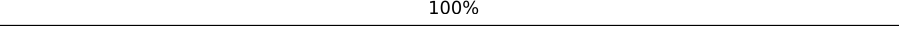
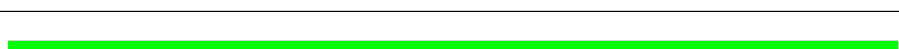
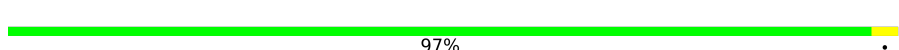
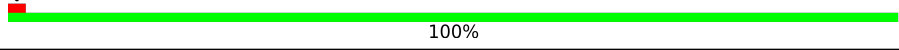
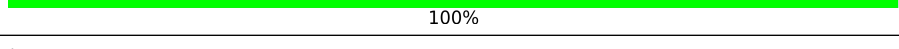
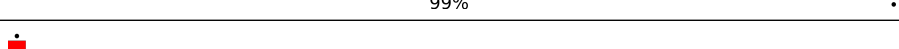

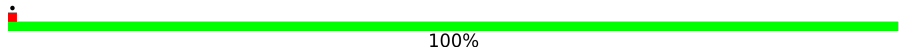
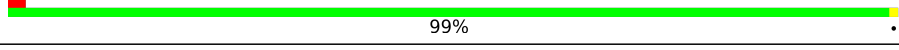
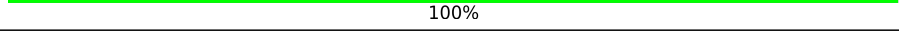

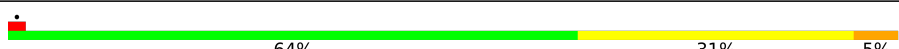



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Mol	Chain	Length	Quality of chain
9	7	191	 98%
10	l	87	 100%
11	M	169	 99%
12	m	77	 97%
13	N	193	 97%
14	n	50	 100%
15	O	136	 100%
16	o	52	 100%
17	p	203	 98%
18	Q	197	 100%
19	5	183	 99%
20	S	185	 99%
21	s	220	 95% 5%
22	T	152	 98%
23	U	172	 98%
24	V	159	 100%
25	W	100	 100%
26	P	155	 53% 97%
27	r	197	 14% 61% 39%
28	x	136	 99%
29	3	121	 73% 24%
30	Y	62	 100%
31	4	158	 64% 35%
32	Z	121	 100%
33	a	126	100%

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Mol	Chain	Length	Quality of chain
34	B	76	 79% 18%
35	b	135	 99%
36	C	105	 100%
37	c	148	 97%
38	D	91	 100%
39	d	58	 97%
40	E	252	 100%
41	e	97	 100%
42	F	386	 99%
43	f	109	 100%
44	G	361	 99%
45	g	127	 100%
46	H	296	 99%
47	h	106	 100%
48	I	175	 88% 11%
49	L	204	 41% 98%
50	1	3316	 64% 31% 5%

## 2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 138804 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 protein called ABC transporter ATP-binding protein ARB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	446	3522	2232	610	668	12	0	0

- Molecule 2 is a protein called Protein VMS1,Vms1,Protein VMS1,Vms1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	S	Se		
2	R	360	2804	1788	499	504	12	1	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	PHE	deletion	UNP Q04311
R	?	-	ASP	deletion	UNP Q04311
R	?	-	SER	deletion	UNP Q04311
R	?	-	THR	deletion	UNP Q04311
R	?	-	LEU	deletion	UNP Q04311
R	?	-	ARG	deletion	UNP Q04311
R	?	-	GLU	deletion	UNP Q04311
R	?	-	VAL	deletion	UNP Q04311
R	?	-	GLU	deletion	UNP Q04311
R	?	-	VAL	deletion	UNP Q04311
R	?	-	GLU	deletion	UNP Q04311
R	?	-	LYS	deletion	UNP Q04311
R	?	-	THR	deletion	UNP Q04311
R	?	-	SER	deletion	UNP Q04311
R	?	-	ASP	deletion	UNP Q04311
R	?	-	ASN	deletion	UNP Q04311
R	?	-	ASP	deletion	UNP Q04311
R	?	-	ARG	deletion	UNP Q04311
R	?	-	ASN	deletion	UNP Q04311
R	?	-	LYS	deletion	UNP Q04311
R	?	-	GLU	deletion	UNP Q04311

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Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	SER	deletion	UNP Q04311
R	?	-	GLY	deletion	UNP Q04311
R	?	-	ASP	deletion	UNP Q04311
R	?	-	LEU	deletion	UNP Q04311
R	?	-	GLN	deletion	UNP Q04311
R	?	-	ILE	deletion	UNP Q04311
R	?	-	ALA	deletion	UNP Q04311
R	?	-	ARG	deletion	UNP Q04311
R	?	-	LYS	deletion	UNP Q04311
R	?	-	LYS	deletion	UNP Q04311
R	?	-	VAL	deletion	UNP Q04311
R	?	-	THR	deletion	UNP Q04311
R	?	-	SER	deletion	UNP Q04311
R	?	-	ASN	deletion	UNP Q04311
R	?	-	VAL	deletion	UNP Q04311
R	?	-	MET	deletion	UNP Q04311
R	?	-	ARG	deletion	UNP Q04311
R	?	-	PHE	deletion	UNP Q04311
R	?	-	ASP	deletion	UNP Q04311
R	?	-	SER	deletion	UNP Q04311
R	?	-	ARG	deletion	UNP Q04311
R	?	-	ASN	deletion	UNP Q04311
R	?	-	GLU	deletion	UNP Q04311
R	?	-	GLN	deletion	UNP Q04311
R	?	-	LYS	deletion	UNP Q04311
R	?	-	ALA	deletion	UNP Q04311
R	187	SER	-	linker	UNP Q04311

- Molecule 3 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	X	224	1633	1019	279	328	7	0	0

- Molecule 4 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	i	112	880	545	179	152	4	0	0

- Molecule 5 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 6 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	j	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 7 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 8 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 9 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	7	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 10 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 11 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 12 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	m	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 13 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	N	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 14 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 16 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	o	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 17 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	p	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 18 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 19 is a protein called 60S ribosomal protein L17-A.



Mol	Chain	Residues	Atoms				AltConf	Trace
19	5	183	Total	C	N	O	0	0
			1420	882	281	257		

- Molecule 20 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 21 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	s	220	Total	C	N	O	S	0	0
			1770	1121	335	307	7		

- Molecule 22 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	T	152	Total	C	N	O	0	0
			1228	763	260	205		

- Molecule 23 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 24 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 25 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	W	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 26 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	P	150	Total	C	N	O	0	0
			737	437	150	150		

- Molecule 27 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	r	121	Total	C	N	O	S	0	0
			967	621	170	173	3		

- Molecule 28 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	x	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 29 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 30 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	62	Total	C	N	O	S	0	0
			513	330	101	81	1		

- Molecule 31 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 32 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 33 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	a	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 34 is a RNA chain called tRNA-Ala.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B	76	Total	C	N	O	P	0	0
			1622	721	285	540	76		

- Molecule 35 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	b	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 36 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	C	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 37 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 38 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	D	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 39 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	d	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 40 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	E	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 41 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	e	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 42 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	F	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 43 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	f	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 44 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	G	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 45 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	g	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 46 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	H	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 47 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	h	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 48 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	I	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 49 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	L	204	Total	C	N	O	S	0	0
			1609	1031	279	290	9		

- Molecule 50 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1	3316	Total	C	N	O	P	0	0
			70924	31675	12770	23163	3316		

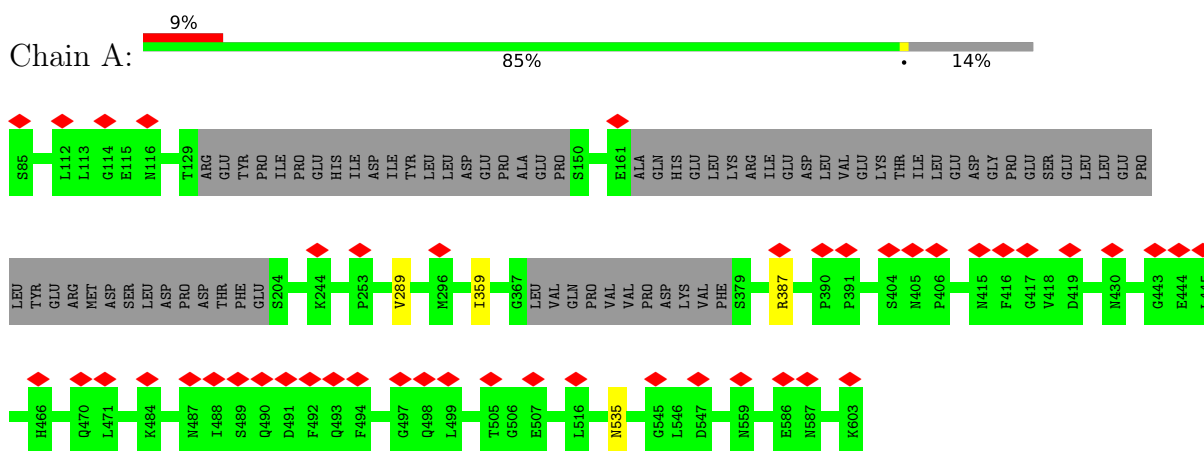
- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
51	R	1	Total	Zn	0
			1	1	

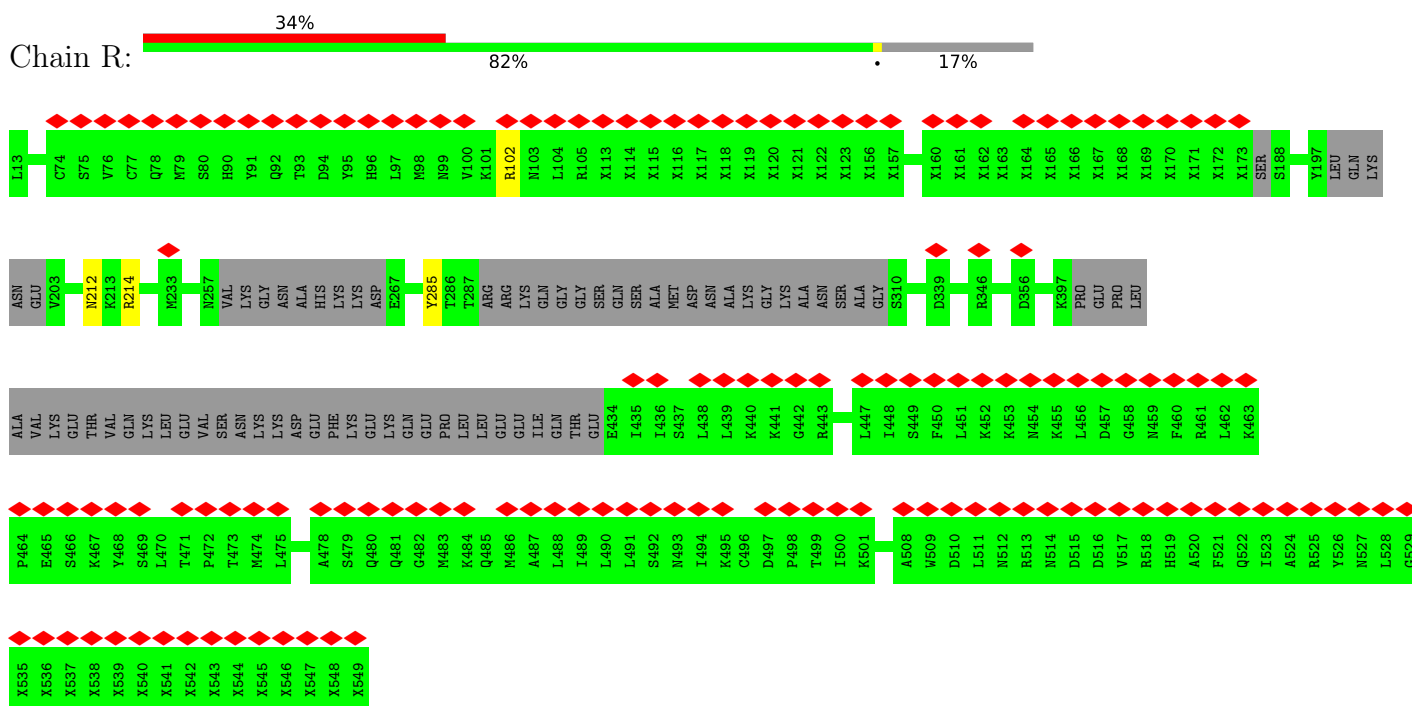
### 3 Residue-property plots

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.

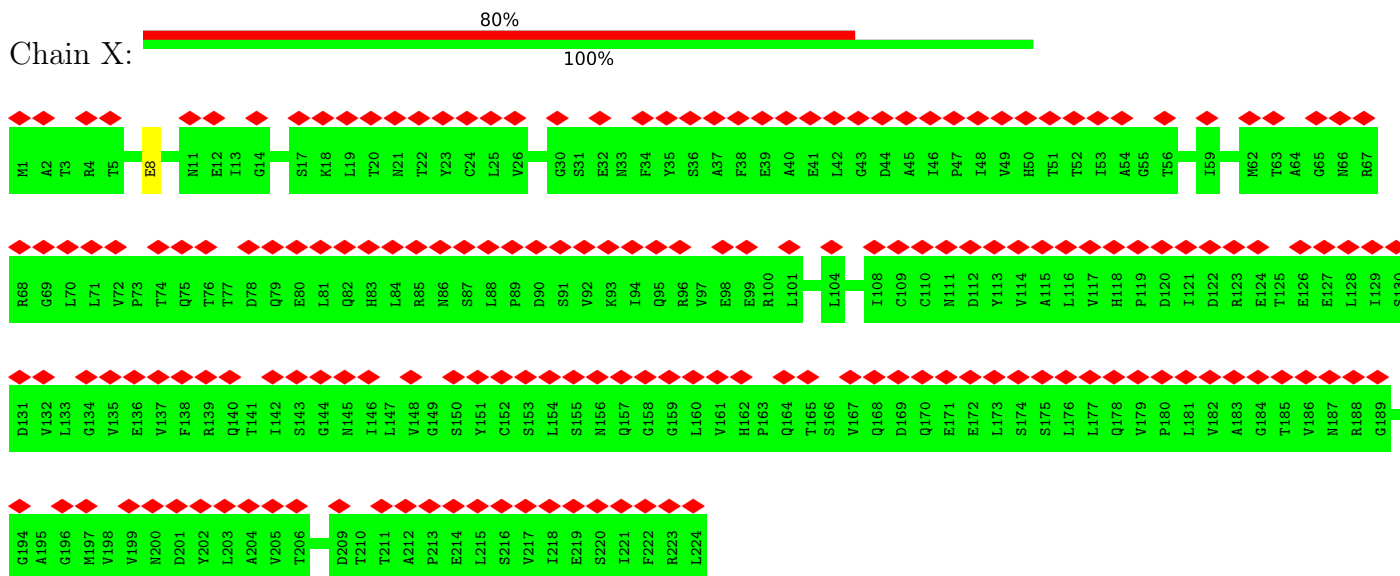
- Molecule 1: ABC transporter ATP-binding protein ARB1



- Molecule 2: Protein VMS1,Vms1,Protein VMS1,Vms1



- Molecule 3: Eukaryotic translation initiation factor 6



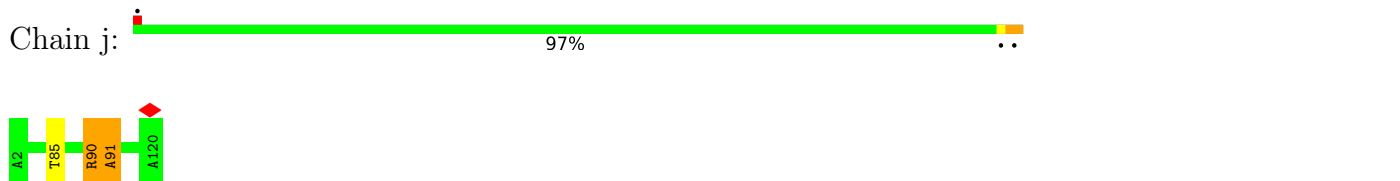
- Molecule 4: 60S ribosomal protein L34-A



- Molecule 5: 60S ribosomal protein L7-A



- Molecule 6: 60S ribosomal protein L35-A

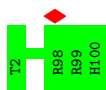


- Molecule 7: 60S ribosomal protein L8-A

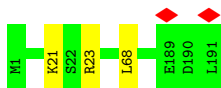


- Molecule 8: 60S ribosomal protein L36-A





- Molecule 9: 60S ribosomal protein L9-A

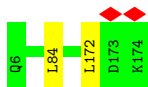


- Molecule 10: 60S ribosomal protein L37-A

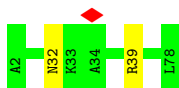


There are no outlier residues recorded for this chain.

- Molecule 11: 60S ribosomal protein L11-B



- Molecule 12: 60S ribosomal protein L38



- Molecule 13: 60S ribosomal protein L13-A



- Molecule 14: 60S ribosomal protein L39



There are no outlier residues recorded for this chain.

- Molecule 15: 60S ribosomal protein L14-A







- Molecule 16: Ubiquitin-60S ribosomal protein L40

Chain o: 100%

There are no outlier residues recorded for this chain.

- Molecule 17: 60S ribosomal protein L15-A

Chain p: 98%



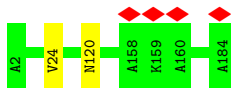
- Molecule 18: 60S ribosomal protein L16-A

Chain Q: 100%

There are no outlier residues recorded for this chain.

- Molecule 19: 60S ribosomal protein L17-A

Chain 5: 99%



- Molecule 20: 60S ribosomal protein L18-A

Chain S: 99%



- Molecule 21: 60S ribosomal protein L10

Chain s: 95% 5%



- Molecule 22: 60S ribosomal protein L19-A

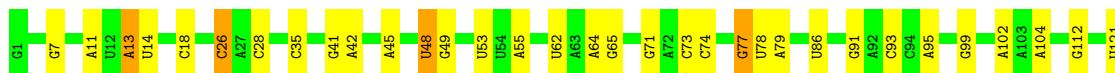
Chain T: 98%





- Molecule 29: 5S rRNA

Chain 3:  73% 24%



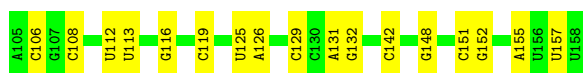
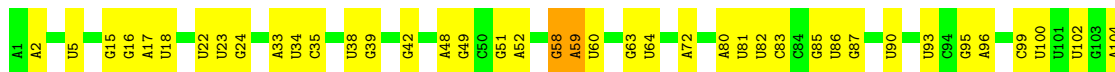
- Molecule 30: 60S ribosomal protein L24-A

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 31: 5.8S rRNA

Chain 4:  64% 35%



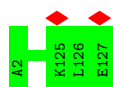
- Molecule 32: 60S ribosomal protein L25

Chain Z:  100%


There are no outlier residues recorded for this chain.

- Molecule 33: 60S ribosomal protein L26-A

Chain a:  100%



- Molecule 34: tRNA-Ala

Chain B:  79% 18%



- Molecule 35: 60S ribosomal protein L27-A

Chain b:  99%



- Molecule 36: 60S ribosomal protein L42-A

Chain C:  100%



- Molecule 37: 60S ribosomal protein L28

Chain c:  97%



- Molecule 38: 60S ribosomal protein L43-A

Chain D:  100%

There are no outlier residues recorded for this chain.

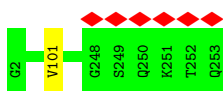
- Molecule 39: 60S ribosomal protein L29

Chain d:  97%



- Molecule 40: 60S ribosomal protein L2-A

Chain E:  100%



- Molecule 41: 60S ribosomal protein L30

Chain e:  100%



- Molecule 42: 60S ribosomal protein L3

Chain F:  99%



- Molecule 43: 60S ribosomal protein L31-A

Chain f:  100%



- Molecule 44: 60S ribosomal protein L4-A

Chain G:  99%



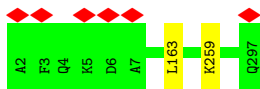
- Molecule 45: 60S ribosomal protein L32

Chain g:  100%



- Molecule 46: 60S ribosomal protein L5

Chain H:  99%




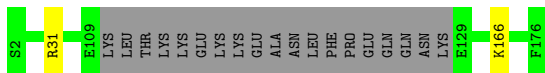
- Molecule 47: 60S ribosomal protein L33-A

Chain h:  100%

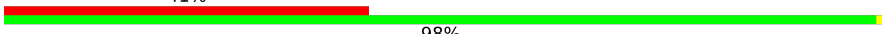
There are no outlier residues recorded for this chain.

- Molecule 48: 60S ribosomal protein L6-A

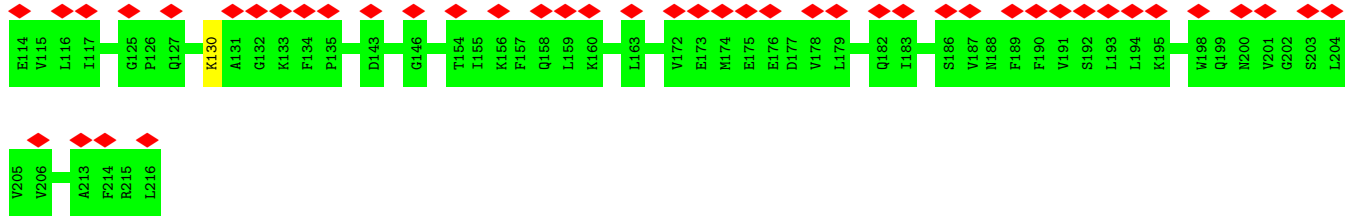
Chain I:  88% 11%



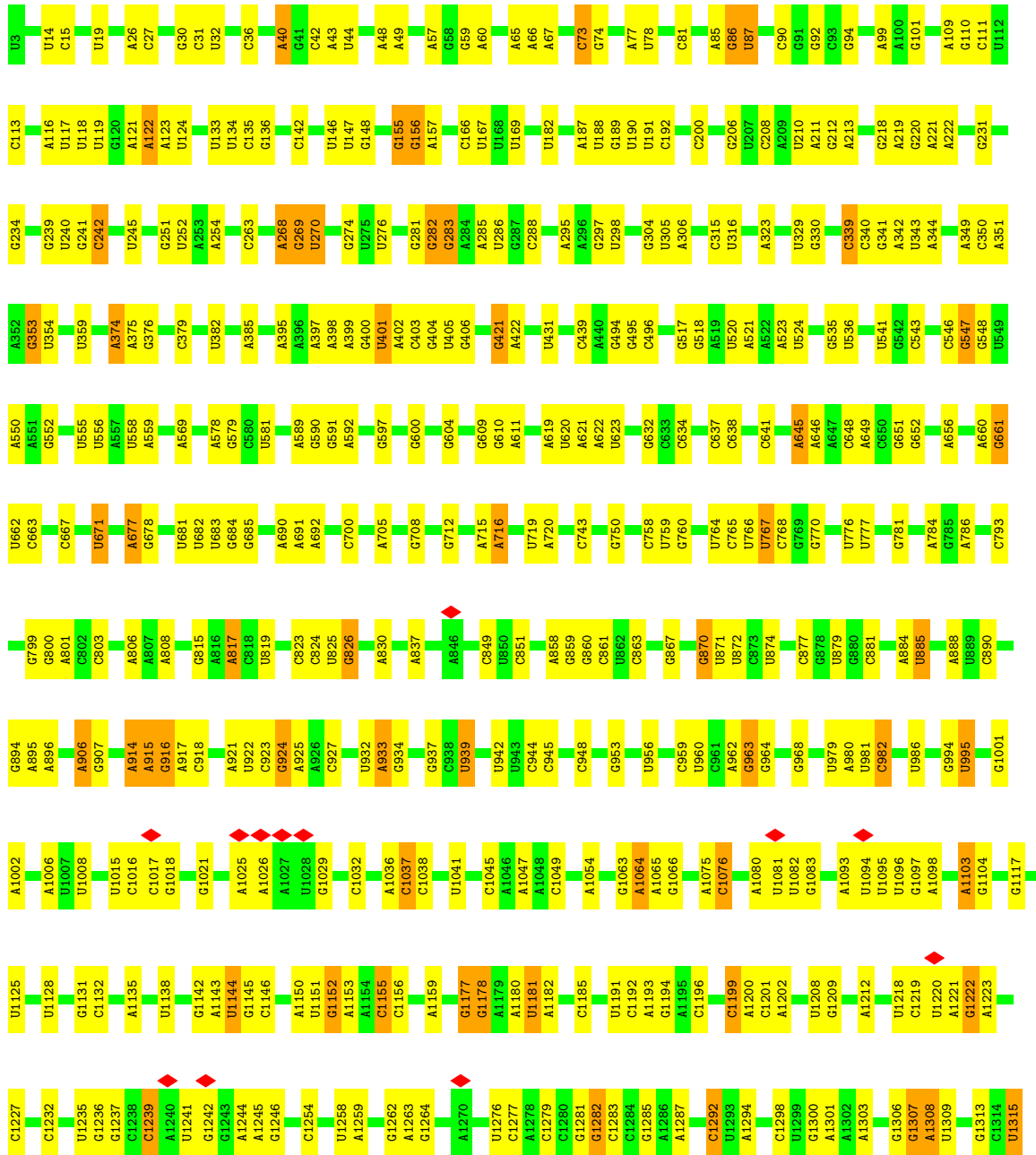
- Molecule 49: 60S ribosomal protein L1-A

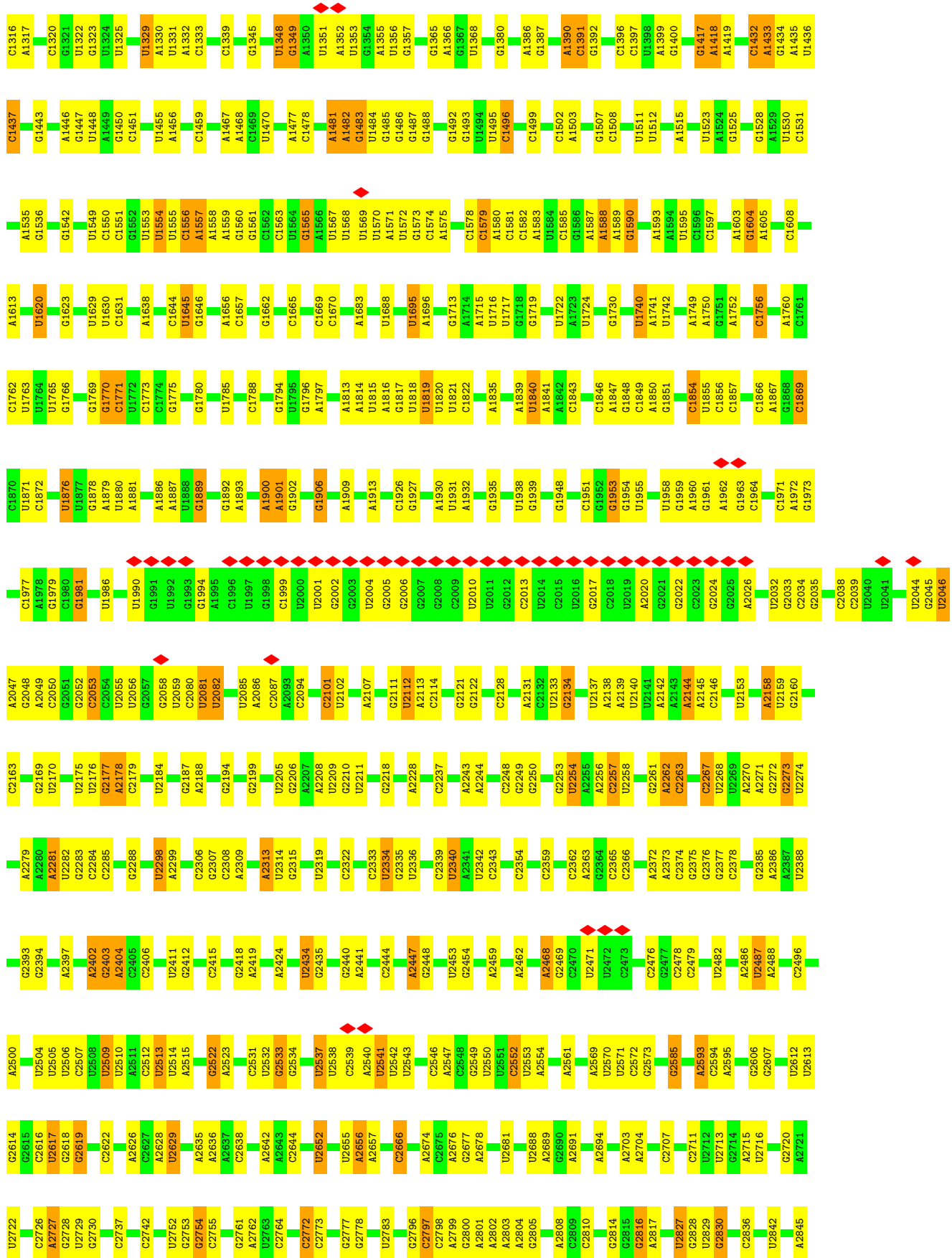
Chain L:  41% 98%

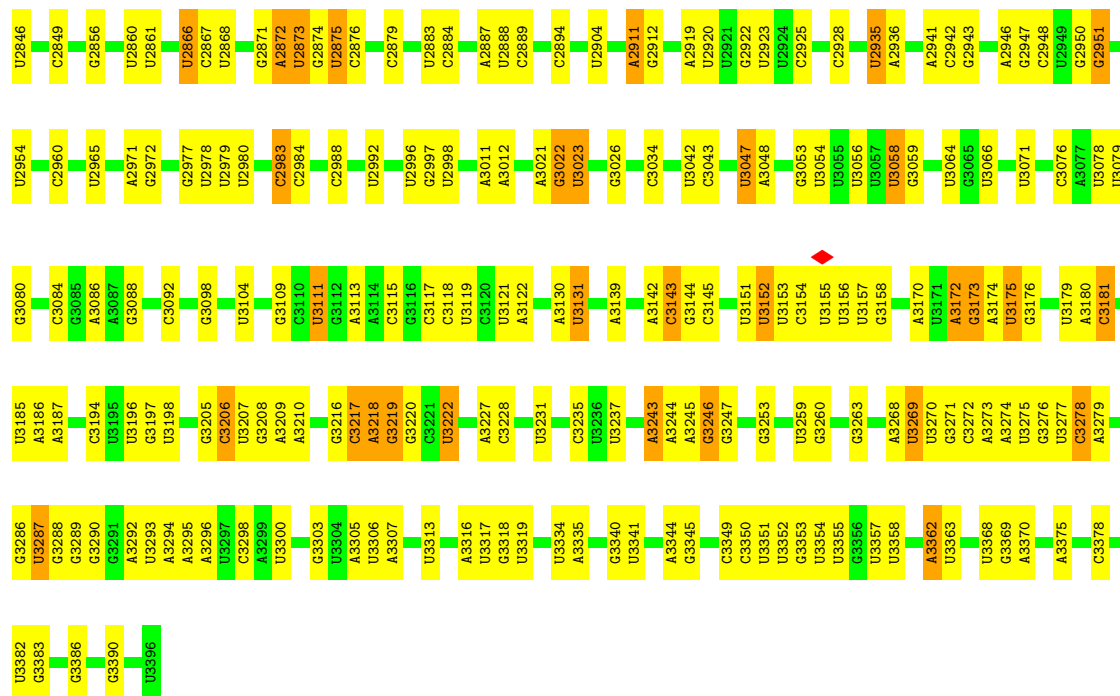




• Molecule 50: 25S rRNA









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31832	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.560	Depositor
Minimum map value	-0.382	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.025	Depositor
Map size ( $\text{\AA}$ )	429.264, 429.264, 429.264	wwPDB
Map dimensions	396, 396, 396	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.084, 1.084, 1.084	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	0.28	0/3583	0.51	0/4831
2	R	0.30	0/2631	0.50	0/3532
3	X	0.27	0/1653	0.50	0/2255
4	i	0.58	0/890	0.64	0/1189
5	J	0.48	0/1821	0.59	0/2451
6	j	0.39	0/978	0.63	0/1301
7	K	0.42	0/1836	0.62	0/2481
8	k	0.40	0/778	0.61	0/1034
9	7	0.46	0/1539	0.59	0/2073
10	l	0.58	0/696	0.72	0/923
11	M	0.33	0/1374	0.60	0/1842
12	m	0.38	0/618	0.61	0/826
13	N	0.44	0/1568	0.66	1/2106 (0.0%)
14	n	0.58	0/443	0.73	0/588
15	O	0.44	0/1068	0.60	0/1438
16	o	0.45	0/423	0.61	0/562
17	p	0.61	0/1757	0.72	1/2354 (0.0%)
18	Q	0.55	0/1585	0.62	0/2128
19	5	0.52	0/1443	0.68	0/1944
20	S	0.41	0/1465	0.63	1/1965 (0.1%)
21	s	0.45	0/1807	0.71	2/2425 (0.1%)
22	T	0.47	0/1245	0.66	1/1661 (0.1%)
23	U	0.55	1/1481 (0.1%)	0.65	0/1990
24	V	0.47	0/1300	0.61	0/1743
25	W	0.43	0/812	0.56	0/1099
26	P	0.25	0/734	0.53	0/1015
27	r	0.27	0/982	0.57	0/1320
28	x	0.48	0/1018	0.62	0/1369
29	3	0.75	0/2883	1.17	14/4491 (0.3%)
30	Y	0.46	0/525	0.58	0/696
31	4	0.97	0/3746	1.16	15/5832 (0.3%)
32	Z	0.50	0/979	0.60	0/1321

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	a	0.40	0/1004	0.60	0/1341
34	B	0.43	0/1810	1.06	2/2821 (0.1%)
35	b	0.44	0/1118	0.59	0/1497
36	C	0.43	0/860	0.63	0/1136
37	c	0.46	0/1204	0.68	0/1612
38	D	0.54	0/701	0.66	0/934
39	d	0.37	0/473	0.54	0/629
40	E	0.58	0/1948	0.70	0/2617
41	e	0.42	0/751	0.58	0/1008
42	F	0.58	1/3146 (0.0%)	0.69	1/4228 (0.0%)
43	f	0.54	0/890	0.62	0/1196
44	G	0.47	0/2800	0.66	0/3790
45	g	0.48	0/1041	0.60	0/1394
46	H	0.36	0/2425	0.57	1/3271 (0.0%)
47	h	0.57	0/868	0.60	0/1168
48	I	0.38	0/1260	0.55	0/1694
49	L	0.28	0/1634	0.59	0/2195
50	1	0.95	4/79382 (0.0%)	1.26	679/123763 (0.5%)
All	All	0.78	6/148976 (0.0%)	1.05	718/219079 (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
1	A	0	1
3	X	0	1
5	J	0	2
6	j	0	2
7	K	0	3
9	7	0	1
11	M	0	1
12	m	0	1
13	N	0	3
21	s	0	2
23	U	0	1
35	b	0	1
37	c	0	1
39	d	0	1
42	F	0	1
44	G	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
46	H	0	1
All	All	0	27

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	F	237	LYS	C-N	-8.92	1.13	1.34
50	1	2828	G	N7-C5	-5.89	1.35	1.39
50	1	2951	G	N7-C5	-5.38	1.36	1.39
50	1	2911	A	N9-C4	-5.16	1.34	1.37
50	1	3047	U	N3-C4	-5.11	1.33	1.38
23	U	59	VAL	CB-CG2	-5.04	1.42	1.52

All (718) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	2080	C	N1-C2-O2	14.11	127.37	118.90
50	1	2080	C	N3-C2-O2	-13.39	112.52	121.90
50	1	3278	C	N1-C2-O2	13.38	126.93	118.90
50	1	1432	C	C2-N1-C1'	13.14	133.25	118.80
50	1	3278	C	C2-N1-C1'	12.02	132.03	118.80
50	1	2875	U	N3-C2-O2	-10.48	114.86	122.20
50	1	2875	U	C2-N1-C1'	10.11	129.84	117.70
50	1	2875	U	N1-C2-O2	9.97	129.78	122.80
50	1	1496	C	C2-N1-C1'	9.90	129.69	118.80
50	1	3278	C	N3-C2-O2	-9.84	115.01	121.90
50	1	1432	C	C6-N1-C1'	-9.84	109.00	120.80
50	1	2080	C	C2-N1-C1'	9.42	129.16	118.80
50	1	1530	U	N3-C2-O2	-9.25	115.73	122.20
50	1	3278	C	C6-N1-C1'	-9.22	109.73	120.80
50	1	2827	U	N3-C2-O2	-9.20	115.76	122.20
50	1	1283	C	N3-C2-O2	-9.19	115.47	121.90
50	1	3047	U	N3-C2-O2	-9.14	115.81	122.20
50	1	1493	G	N1-C6-O6	-9.09	114.45	119.90
50	1	2550	U	N3-C2-O2	-8.94	115.94	122.20
50	1	2951	G	C6-C5-N7	-8.90	125.06	130.40
50	1	270	U	N1-C2-O2	8.90	129.03	122.80
50	1	2366	C	C5-C6-N1	8.89	125.44	121.00
50	1	663	C	C6-N1-C2	-8.84	116.77	120.30
50	1	1871	U	N3-C2-O2	-8.84	116.01	122.20
50	1	823	C	C6-N1-C2	-8.79	116.78	120.30
50	1	1530	U	N1-C2-O2	8.71	128.90	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	1283	C	N1-C2-O2	8.69	124.11	118.90
50	1	2080	C	C6-N1-C2	-8.64	116.84	120.30
50	1	2415	C	C5-C6-N1	8.63	125.31	121.00
50	1	2366	C	C6-N1-C2	-8.58	116.87	120.30
50	1	2550	U	N1-C2-O2	8.53	128.77	122.80
50	1	27	C	C2-N1-C1'	8.50	128.15	118.80
50	1	2257	C	N1-C2-O2	8.35	123.91	118.90
50	1	3143	C	N1-C2-O2	8.31	123.89	118.90
50	1	1432	C	N1-C2-O2	8.29	123.88	118.90
50	1	78	U	N3-C2-O2	-8.28	116.41	122.20
50	1	2883	U	C5-C6-N1	8.23	126.82	122.70
50	1	2378	C	C5-C6-N1	8.19	125.10	121.00
50	1	800	G	C4-N9-C1'	8.19	137.14	126.50
50	1	27	C	N1-C2-O2	8.18	123.81	118.90
50	1	1550	C	C6-N1-C2	-8.17	117.03	120.30
50	1	2257	C	C2-N1-C1'	8.12	127.73	118.80
50	1	2666	C	C2-N1-C1'	8.10	127.71	118.80
50	1	1556	C	C6-N1-C2	-8.09	117.06	120.30
50	1	2797	C	C2-N1-C1'	8.09	127.70	118.80
50	1	270	U	N3-C2-O2	-8.07	116.55	122.20
50	1	651	G	C6-C5-N7	-8.00	125.60	130.40
50	1	933	A	P-O3'-C3'	7.93	129.22	119.70
50	1	2415	C	N1-C2-O2	7.93	123.66	118.90
50	1	1496	C	N1-C2-O2	7.81	123.59	118.90
50	1	2153	U	N3-C2-O2	-7.80	116.74	122.20
50	1	1349	G	N3-C4-C5	-7.76	124.72	128.60
50	1	1872	C	N1-C2-O2	7.76	123.56	118.90
50	1	2298	U	N1-C2-O2	7.75	128.23	122.80
50	1	1437	C	C2-N1-C1'	7.74	127.31	118.80
50	1	1525	G	C4-N9-C1'	7.73	136.55	126.50
50	1	1185	C	C6-N1-C2	-7.72	117.21	120.30
50	1	2415	C	C6-N1-C2	-7.72	117.21	120.30
50	1	3047	U	C2-N1-C1'	7.71	126.95	117.70
50	1	663	C	C5-C6-N1	7.68	124.84	121.00
50	1	1645	U	C2-N1-C1'	7.67	126.90	117.70
50	1	122	A	C2-N3-C4	7.67	114.43	110.60
50	1	700	C	C6-N1-C2	-7.62	117.25	120.30
50	1	2797	C	N1-C2-O2	7.62	123.47	118.90
50	1	2478	C	N1-C2-O2	7.59	123.45	118.90
50	1	3047	U	N1-C2-N3	7.57	119.44	114.90
50	1	2541	U	P-O3'-C3'	7.56	128.77	119.70
50	1	1432	C	C5-C6-N1	7.54	124.77	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	2797	C	C5-C6-N1	7.53	124.76	121.00
50	1	2666	C	C6-N1-C2	-7.52	117.29	120.30
50	1	1349	G	N3-C4-N9	7.51	130.50	126.00
50	1	1585	C	C6-N1-C2	-7.48	117.31	120.30
50	1	823	C	C5-C6-N1	7.47	124.73	121.00
50	1	1530	U	C2-N1-C1'	7.46	126.66	117.70
50	1	3217	C	N1-C2-O2	7.46	123.37	118.90
50	1	1550	C	C5-C6-N1	7.44	124.72	121.00
50	1	1432	C	C6-N1-C2	-7.43	117.33	120.30
50	1	922	U	C2-N1-C1'	7.41	126.59	117.70
50	1	1496	C	C5-C6-N1	7.39	124.69	121.00
50	1	700	C	C5-C6-N1	7.38	124.69	121.00
50	1	2925	C	C6-N1-C2	-7.36	117.36	120.30
13	N	48	PRO	C-N-CA	7.31	139.97	121.70
50	1	1495	U	N1-C2-N3	7.28	119.27	114.90
20	S	41	ASP	CB-CG-OD1	7.26	124.84	118.30
50	1	2988	C	C6-N1-C2	-7.26	117.40	120.30
50	1	2177	G	P-O3'-C3'	7.24	128.38	119.70
50	1	638	C	C5-C6-N1	7.22	124.61	121.00
50	1	1155	C	C6-N1-C2	-7.22	117.41	120.30
50	1	2764	C	N1-C2-O2	7.20	123.22	118.90
50	1	2509	U	P-O3'-C3'	7.18	128.31	119.70
50	1	2468	A	P-O3'-C3'	7.17	128.31	119.70
50	1	906	A	P-O3'-C3'	7.13	128.25	119.70
50	1	1604	G	C4-N9-C1'	7.13	135.76	126.50
50	1	2447	A	P-O3'-C3'	7.13	128.25	119.70
50	1	2334	U	N3-C2-O2	-7.10	117.23	122.20
50	1	1277	C	N1-C2-O2	7.10	123.16	118.90
50	1	2951	G	C4-C5-N7	7.10	113.64	110.80
50	1	793	C	C5-C6-N1	7.09	124.55	121.00
50	1	1872	C	C6-N1-C2	-7.09	117.46	120.30
50	1	2153	U	N1-C2-N3	7.09	119.15	114.90
50	1	3084	C	C6-N1-C2	-7.09	117.47	120.30
50	1	1770	G	C4-N9-C1'	7.08	135.71	126.50
50	1	2298	U	N3-C2-O2	-7.08	117.24	122.20
50	1	2836	C	N3-C2-O2	-7.08	116.95	121.90
50	1	645	A	C2-N3-C4	7.07	114.14	110.60
50	1	421	G	N3-C4-N9	7.07	130.24	126.00
50	1	2984	C	C2-N1-C1'	7.06	126.57	118.80
50	1	524	U	N3-C2-O2	-7.05	117.26	122.20
50	1	1604	G	N3-C4-N9	7.04	130.22	126.00
50	1	3023	U	N3-C2-O2	-7.04	117.27	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	3350	C	C5-C6-N1	7.03	124.51	121.00
50	1	288	C	C6-N1-C2	-7.02	117.49	120.30
50	1	793	C	C6-N1-C2	-7.01	117.50	120.30
50	1	651	G	N3-C4-N9	7.01	130.20	126.00
50	1	3306	U	C2-N1-C1'	6.98	126.08	117.70
50	1	2362	C	C6-N1-C2	-6.97	117.51	120.30
50	1	1556	C	N1-C2-O2	6.95	123.07	118.90
50	1	2298	U	C2-N1-C1'	6.93	126.01	117.70
50	1	1298	C	C6-N1-C2	-6.92	117.53	120.30
50	1	1277	C	N3-C2-O2	-6.91	117.06	121.90
50	1	1493	G	N3-C4-C5	-6.90	125.15	128.60
50	1	3306	U	N3-C2-O2	-6.90	117.37	122.20
50	1	282	G	C8-N9-C4	-6.90	103.64	106.40
50	1	2359	C	C6-N1-C2	-6.89	117.54	120.30
50	1	1496	C	C6-N1-C1'	-6.88	112.54	120.80
50	1	2343	C	C6-N1-C2	-6.88	117.55	120.30
50	1	1840	U	P-O3'-C3'	6.85	127.92	119.70
50	1	3350	C	C6-N1-C2	-6.84	117.56	120.30
50	1	3349	C	C6-N1-C2	-6.83	117.57	120.30
50	1	2619	G	C5-C6-O6	-6.83	124.50	128.60
50	1	2404	A	O4'-C1'-N9	6.83	113.66	108.20
50	1	1496	C	C6-N1-C2	-6.83	117.57	120.30
50	1	1507	G	N3-C4-N9	6.83	130.10	126.00
50	1	3111	U	N1-C2-O2	6.82	127.57	122.80
50	1	800	G	N3-C4-C5	-6.81	125.20	128.60
50	1	1103	A	O4'-C1'-N9	6.80	113.64	108.20
50	1	1871	U	N1-C2-O2	6.80	127.56	122.80
50	1	2298	U	O4'-C1'-N1	6.79	113.64	108.20
50	1	800	G	C8-N9-C1'	-6.78	118.18	127.00
50	1	1349	G	C4-N9-C1'	6.78	135.31	126.50
50	1	2616	C	C2-N1-C1'	6.77	126.25	118.80
17	p	75	VAL	CA-CB-CG2	6.74	121.01	110.90
50	1	3071	U	N3-C2-O2	-6.74	117.49	122.20
50	1	918	C	C6-N1-C2	-6.73	117.61	120.30
50	1	2134	G	C4-C5-N7	6.73	113.49	110.80
50	1	2133	U	N3-C2-O2	-6.72	117.50	122.20
50	1	3023	U	N1-C2-O2	6.71	127.50	122.80
50	1	1037	C	C2-N1-C1'	6.70	126.17	118.80
50	1	1437	C	C6-N1-C2	-6.70	117.62	120.30
50	1	2237	C	N1-C2-O2	6.68	122.91	118.90
50	1	3298	C	C6-N1-C2	-6.66	117.64	120.30
50	1	800	G	N3-C4-N9	6.64	129.99	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	1872	C	N3-C2-O2	-6.63	117.26	121.90
50	1	3043	C	C6-N1-C2	-6.63	117.65	120.30
50	1	2550	U	C2-N1-C1'	6.59	125.61	117.70
50	1	421	G	N3-C4-C5	-6.59	125.30	128.60
50	1	2512	C	C2-N1-C1'	6.58	126.04	118.80
50	1	1645	U	N1-C2-O2	6.58	127.41	122.80
50	1	2727	A	P-O3'-C3'	6.58	127.60	119.70
50	1	2378	C	C6-N1-C2	-6.58	117.67	120.30
50	1	2726	C	C2-N1-C1'	6.58	126.03	118.80
50	1	524	U	N1-C2-O2	6.57	127.39	122.80
50	1	87	U	N3-C2-O2	-6.56	117.61	122.20
50	1	1645	U	N3-C2-O2	-6.56	117.61	122.20
50	1	1770	G	C8-N9-C1'	-6.56	118.47	127.00
50	1	3143	C	N3-C2-O2	-6.54	117.32	121.90
50	1	156	G	P-O3'-C3'	6.54	127.55	119.70
50	1	2846	U	C2-N1-C1'	6.53	125.53	117.70
50	1	3042	U	C5-C6-N1	6.52	125.96	122.70
31	4	64	U	N3-C2-O2	-6.51	117.65	122.20
50	1	1556	C	N3-C2-O2	-6.51	117.34	121.90
50	1	1900	A	P-O3'-C3'	6.51	127.51	119.70
50	1	3058	U	N1-C2-O2	6.49	127.34	122.80
50	1	87	U	N1-C2-O2	6.49	127.34	122.80
50	1	2153	U	C6-N1-C2	-6.49	117.11	121.00
50	1	1478	C	C6-N1-C2	-6.49	117.71	120.30
50	1	1493	G	C2-N3-C4	6.48	115.14	111.90
50	1	282	G	N7-C8-N9	6.48	116.34	113.10
50	1	968	G	C4-N9-C1'	6.48	134.92	126.50
50	1	1604	G	C8-N9-C1'	-6.48	118.58	127.00
50	1	1329	U	OP1-P-O3'	6.46	119.41	105.20
50	1	27	C	C6-N1-C1'	-6.45	113.06	120.80
50	1	677	A	P-O3'-C3'	6.45	127.44	119.70
50	1	2146	C	C5-C6-N1	6.45	124.22	121.00
50	1	2873	U	N3-C2-O2	-6.44	117.69	122.20
50	1	3076	C	C6-N1-C2	-6.44	117.72	120.30
50	1	2585	G	N3-C4-N9	6.43	129.86	126.00
50	1	2487	U	P-O3'-C3'	6.42	127.40	119.70
50	1	1064	A	P-O3'-C3'	6.42	127.40	119.70
50	1	2875	U	C6-N1-C1'	-6.41	112.22	121.20
50	1	3066	U	C5-C6-N1	6.41	125.91	122.70
50	1	877	C	N1-C2-O2	6.41	122.75	118.90
50	1	3350	C	C2-N1-C1'	6.41	125.85	118.80
50	1	339	C	N1-C2-O2	6.41	122.75	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	2479	C	N1-C2-O2	6.41	122.74	118.90
50	1	2796	G	C4-N9-C1'	6.40	134.82	126.50
50	1	2257	C	N3-C2-O2	-6.40	117.42	121.90
29	3	26	C	N1-C2-O2	6.39	122.74	118.90
50	1	2884	C	C6-N1-C2	-6.39	117.74	120.30
50	1	3058	U	N3-C2-O2	-6.39	117.73	122.20
50	1	3181	C	N1-C2-O2	6.39	122.73	118.90
50	1	2827	U	N1-C2-O2	6.37	127.26	122.80
50	1	3058	U	C2-N1-C1'	6.37	125.34	117.70
31	4	108	C	C5-C6-N1	6.36	124.18	121.00
50	1	2434	U	N1-C2-O2	6.36	127.25	122.80
31	4	59	A	O4'-C1'-N9	6.35	113.28	108.20
50	1	1977	C	C5-C6-N1	6.35	124.17	121.00
50	1	359	U	N3-C2-O2	-6.34	117.76	122.20
50	1	767	U	P-O3'-C3'	6.34	127.30	119.70
50	1	933	A	OP1-P-O3'	6.34	119.14	105.20
50	1	2796	G	N3-C4-N9	6.32	129.79	126.00
50	1	2652	U	N1-C2-O2	6.32	127.22	122.80
50	1	3344	A	N7-C8-N9	6.32	116.96	113.80
31	4	100	U	C2-N1-C1'	6.32	125.28	117.70
50	1	3047	U	C5-C4-O4	6.32	129.69	125.90
50	1	27	C	C5-C6-N1	6.31	124.16	121.00
50	1	2177	G	OP2-P-O3'	6.30	119.07	105.20
50	1	283	G	N3-C4-N9	6.30	129.78	126.00
50	1	353	G	P-O3'-C3'	6.30	127.26	119.70
50	1	3047	U	O5'-P-OP2	-6.29	100.04	105.70
50	1	1155	C	N3-C2-O2	-6.29	117.50	121.90
50	1	543	C	C2-N1-C1'	6.28	125.71	118.80
50	1	3235	C	C2-N1-C1'	6.28	125.71	118.80
29	3	18	C	C2-N1-C1'	6.27	125.70	118.80
50	1	2836	C	N1-C2-O2	6.27	122.66	118.90
50	1	1432	C	N3-C2-O2	-6.27	117.51	121.90
50	1	40	A	O4'-C1'-N9	6.27	113.21	108.20
50	1	3104	U	N3-C2-O2	-6.26	117.82	122.20
50	1	803	C	C5-C6-N1	6.26	124.13	121.00
29	3	28	C	N1-C2-O2	6.26	122.65	118.90
50	1	986	U	N3-C2-O2	-6.26	117.82	122.20
50	1	2537	U	P-O3'-C3'	6.24	127.18	119.70
50	1	885	U	N3-C2-O2	-6.23	117.84	122.20
50	1	2619	G	C4-C5-N7	6.23	113.29	110.80
50	1	2711	C	N3-C2-O2	-6.23	117.54	121.90
50	1	3181	C	C2-N1-C1'	6.22	125.64	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	3053	G	N3-C4-N9	6.21	129.73	126.00
50	1	2415	C	C2-N1-C1'	6.21	125.63	118.80
50	1	133	U	N1-C2-O2	6.21	127.15	122.80
50	1	359	U	N1-C2-O2	6.21	127.15	122.80
50	1	1307	G	P-O3'-C3'	6.21	127.15	119.70
50	1	1604	G	N3-C4-C5	-6.20	125.50	128.60
50	1	3071	U	N1-C2-O2	6.20	127.14	122.80
50	1	1770	G	C6-C5-N7	-6.20	126.68	130.40
50	1	543	C	N1-C2-O2	6.20	122.62	118.90
50	1	1695	U	P-O3'-C3'	6.19	127.13	119.70
50	1	2666	C	N1-C2-O2	6.19	122.62	118.90
50	1	3217	C	C2-N1-C1'	6.19	125.61	118.80
50	1	824	C	C6-N1-C2	-6.19	117.82	120.30
50	1	2334	U	N1-C2-O2	6.19	127.13	122.80
50	1	2199	G	C4-N9-C1'	6.17	134.52	126.50
50	1	315	C	N3-C2-O2	-6.17	117.58	121.90
50	1	1669	C	C6-N1-C2	-6.17	117.83	120.30
50	1	122	A	O4'-C1'-N9	6.16	113.13	108.20
50	1	2960	C	C6-N1-C2	-6.16	117.84	120.30
50	1	1339	C	C6-N1-C2	-6.15	117.84	120.30
50	1	242	C	N1-C2-O2	6.14	122.58	118.90
50	1	421	G	C2-N3-C4	6.14	114.97	111.90
50	1	1349	G	C2-N3-C4	6.12	114.96	111.90
50	1	2257	C	C6-N1-C2	-6.12	117.85	120.30
42	F	168	LYS	C-N-CA	6.12	137.00	121.70
50	1	1525	G	C8-N9-C1'	-6.12	119.05	127.00
50	1	78	U	N1-C2-O2	6.12	127.08	122.80
50	1	155	G	P-O3'-C3'	6.11	127.03	119.70
50	1	1433	A	P-O3'-C3'	6.11	127.03	119.70
50	1	948	C	C6-N1-C2	-6.11	117.86	120.30
50	1	1333	C	N1-C2-O2	6.10	122.56	118.90
50	1	2267	C	P-O3'-C3'	6.10	127.02	119.70
50	1	956	U	C6-N1-C2	-6.08	117.35	121.00
50	1	1481	A	N3-C4-N9	6.08	132.27	127.40
50	1	1951	C	C2-N1-C1'	6.08	125.49	118.80
50	1	2984	C	N1-C2-O2	6.08	122.55	118.90
50	1	3047	U	C4-C5-C6	6.08	123.35	119.70
50	1	2830	G	C4-N9-C1'	6.08	134.40	126.50
50	1	825	U	C5-C6-N1	6.07	125.74	122.70
50	1	3231	U	N1-C2-O2	6.07	127.05	122.80
31	4	142	C	C6-N1-C2	-6.06	117.88	120.30
50	1	2094	C	N3-C2-O2	-6.06	117.66	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	2585	G	N3-C4-C5	-6.06	125.57	128.60
50	1	3231	U	N3-C2-O2	-6.06	117.96	122.20
50	1	2796	G	C8-N9-C1'	-6.04	119.14	127.00
50	1	3231	U	C2-N1-C1'	6.04	124.95	117.70
29	3	77	G	P-O3'-C3'	6.04	126.95	119.70
50	1	1418	A	P-O3'-C3'	6.04	126.94	119.70
50	1	3217	C	N3-C2-O2	-6.03	117.68	121.90
50	1	122	A	N3-C4-N9	6.03	132.22	127.40
50	1	269	G	P-O3'-C3'	6.03	126.94	119.70
50	1	1990	U	N1-C2-O2	6.03	127.02	122.80
50	1	2872	A	O4'-C1'-N9	6.03	113.02	108.20
50	1	2726	C	N1-C2-O2	6.02	122.51	118.90
50	1	3219	G	P-O3'-C3'	6.02	126.92	119.70
50	1	2894	C	C6-N1-C2	-6.02	117.89	120.30
50	1	87	U	C2-N1-C1'	6.01	124.92	117.70
50	1	2617	U	N3-C2-O2	-6.01	117.99	122.20
50	1	270	U	C2-N1-C1'	6.01	124.91	117.70
50	1	2652	U	N3-C2-O2	-6.01	117.99	122.20
50	1	3287	U	C2-N1-C1'	6.01	124.91	117.70
31	4	52	A	N7-C8-N9	6.00	116.80	113.80
50	1	634	C	C6-N1-C2	-6.00	117.90	120.30
50	1	915	A	C4-N9-C1'	6.00	137.11	126.30
50	1	2406	C	C6-N1-C2	-6.00	117.90	120.30
50	1	2925	C	N1-C2-O2	6.00	122.50	118.90
50	1	2144	A	O4'-C1'-N9	6.00	113.00	108.20
50	1	86	G	P-O3'-C3'	6.00	126.90	119.70
50	1	3143	C	C2-N1-C1'	5.99	125.39	118.80
50	1	1819	U	N3-C2-O2	-5.99	118.01	122.20
50	1	2478	C	N3-C2-O2	-5.99	117.71	121.90
22	T	99	LEU	CB-CG-CD2	-5.99	100.82	111.00
50	1	1309	U	N3-C2-O2	-5.99	118.01	122.20
50	1	1819	U	N1-C2-O2	5.99	126.99	122.80
31	4	59	A	O5'-P-OP2	-5.98	100.32	105.70
50	1	2666	C	C5-C6-N1	5.98	123.99	121.00
50	1	2313	A	P-O3'-C3'	5.97	126.87	119.70
50	1	939	U	N1-C2-O2	5.97	126.98	122.80
50	1	2622	C	C6-N1-C2	-5.96	117.92	120.30
50	1	1178	G	N7-C8-N9	5.96	116.08	113.10
50	1	1695	U	OP2-P-O3'	5.96	118.31	105.20
50	1	3022	G	P-O3'-C3'	5.96	126.85	119.70
50	1	1144	U	P-O3'-C3'	5.96	126.85	119.70
50	1	1239	C	O5'-P-OP1	5.94	117.82	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	1771	C	N1-C2-O2	5.93	122.46	118.90
50	1	2772	C	P-O3'-C3'	5.93	126.82	119.70
50	1	3175	U	P-O3'-C3'	5.93	126.82	119.70
50	1	1670	C	N1-C2-O2	5.92	122.45	118.90
50	1	1854	C	C6-N1-C2	-5.92	117.93	120.30
50	1	2112	U	P-O3'-C3'	5.92	126.80	119.70
50	1	3287	U	N1-C2-O2	5.92	126.94	122.80
50	1	1977	C	C6-N1-C2	-5.92	117.93	120.30
50	1	3064	U	N3-C2-O2	-5.91	118.06	122.20
50	1	1144	U	N3-C4-O4	5.91	123.53	119.40
50	1	2873	U	N1-C2-O2	5.91	126.93	122.80
50	1	2273	G	P-O3'-C3'	5.90	126.78	119.70
50	1	2983	C	N1-C2-O2	5.90	122.44	118.90
50	1	2612	U	N3-C2-O2	-5.90	118.07	122.20
50	1	1478	C	C5-C6-N1	5.89	123.95	121.00
50	1	3344	A	C5-N7-C8	-5.89	100.95	103.90
50	1	1103	A	P-O3'-C3'	5.89	126.77	119.70
50	1	924	G	P-O3'-C3'	5.89	126.77	119.70
50	1	2772	C	N1-C2-O2	5.88	122.43	118.90
34	B	75	C	C6-N1-C2	-5.88	117.95	120.30
50	1	1308	A	C5-C6-N1	5.88	120.64	117.70
50	1	1208	U	N3-C2-O2	-5.87	118.09	122.20
50	1	1178	G	C8-N9-C4	-5.87	104.05	106.40
50	1	2828	G	C8-N9-C4	-5.87	104.05	106.40
50	1	2333	C	C6-N1-C2	-5.86	117.96	120.30
50	1	1953	G	P-O3'-C3'	5.85	126.72	119.70
50	1	1194	G	N7-C8-N9	5.85	116.02	113.10
50	1	1770	G	N3-C4-N9	5.84	129.50	126.00
50	1	1670	C	N3-C2-O2	-5.83	117.82	121.90
50	1	1368	U	N3-C2-O2	-5.83	118.12	122.20
50	1	81	C	N3-C2-O2	-5.82	117.83	121.90
50	1	3300	U	N3-C2-O2	-5.82	118.13	122.20
50	1	1177	G	P-O3'-C3'	5.81	126.67	119.70
50	1	1397	C	C5-C6-N1	5.80	123.90	121.00
50	1	1155	C	N1-C2-O2	5.80	122.38	118.90
50	1	2178	A	P-O3'-C3'	5.80	126.66	119.70
50	1	1556	C	C5-C6-N1	5.79	123.89	121.00
21	s	175	LEU	CA-CB-CG	5.79	128.61	115.30
50	1	2593	A	P-O3'-C3'	5.78	126.64	119.70
50	1	2447	A	OP1-P-O3'	5.78	117.91	105.20
50	1	2943	G	C4-N9-C1'	5.77	134.01	126.50
50	1	2830	G	N3-C4-C5	-5.77	125.71	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	2237	C	N3-C2-O2	-5.77	117.86	121.90
50	1	3043	C	C5-C6-N1	5.76	123.88	121.00
50	1	1597	C	C5-C6-N1	5.76	123.88	121.00
50	1	3047	U	C6-N1-C2	-5.76	117.54	121.00
50	1	1530	U	C6-N1-C2	-5.75	117.55	121.00
50	1	288	C	C5-C6-N1	5.75	123.88	121.00
50	1	2988	C	C5-C6-N1	5.75	123.88	121.00
31	4	119	C	C6-N1-C2	-5.75	118.00	120.30
50	1	1227	C	N1-C2-O2	5.75	122.35	118.90
50	1	1620	U	N3-C2-O2	-5.75	118.18	122.20
50	1	1492	G	N3-C4-N9	5.74	129.45	126.00
50	1	282	G	P-O3'-C3'	5.74	126.59	119.70
50	1	1292	C	N1-C2-O2	5.74	122.34	118.90
50	1	1740	U	P-O3'-C3'	5.74	126.58	119.70
50	1	2935	U	C2-N1-C1'	5.73	124.58	117.70
50	1	245	U	N1-C2-O2	5.73	126.81	122.80
50	1	1349	G	C8-N9-C1'	-5.73	119.55	127.00
50	1	2434	U	C2-N1-C1'	5.73	124.58	117.70
50	1	1208	U	N1-C2-O2	5.72	126.81	122.80
50	1	1499	C	C6-N1-C2	-5.72	118.01	120.30
50	1	2158	A	P-O3'-C3'	5.72	126.57	119.70
50	1	2552	C	C2-N1-C1'	5.72	125.10	118.80
50	1	1199	C	P-O3'-C3'	5.71	126.55	119.70
50	1	2943	G	C8-N9-C1'	-5.71	119.58	127.00
50	1	1554	U	P-O3'-C3'	5.70	126.54	119.70
50	1	2925	C	C5-C6-N1	5.70	123.85	121.00
50	1	3278	C	C5-C6-N1	5.70	123.85	121.00
50	1	339	C	N3-C2-O2	-5.69	117.92	121.90
50	1	651	G	C4-C5-N7	5.69	113.08	110.80
50	1	1417	G	P-O3'-C3'	5.69	126.53	119.70
50	1	3246	G	P-O3'-C3'	5.69	126.53	119.70
31	4	108	C	C6-N1-C2	-5.68	118.03	120.30
50	1	2080	C	C6-N1-C1'	-5.68	113.98	120.80
50	1	3111	U	N3-C2-O2	-5.68	118.22	122.20
50	1	3298	C	C5-C6-N1	5.68	123.84	121.00
50	1	1218	U	N3-C2-O2	-5.68	118.22	122.20
50	1	2764	C	N3-C2-O2	-5.68	117.92	121.90
50	1	918	C	C5-C6-N1	5.68	123.84	121.00
50	1	2638	C	C6-N1-C2	-5.67	118.03	120.30
50	1	2666	C	N3-C2-O2	-5.67	117.93	121.90
50	1	2797	C	C6-N1-C1'	-5.67	113.99	120.80
50	1	1317	A	O4'-C1'-N9	5.67	112.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	2522	G	C4-N9-C1'	5.66	133.86	126.50
50	1	2836	C	C2-N1-C1'	5.66	125.03	118.80
50	1	2911	A	P-O3'-C3'	5.66	126.49	119.70
50	1	870	G	P-O3'-C3'	5.66	126.49	119.70
50	1	1990	U	N3-C2-O2	-5.64	118.25	122.20
50	1	1144	U	C5-C4-O4	-5.64	122.51	125.90
50	1	2943	G	C6-C5-N7	-5.64	127.02	130.40
50	1	3173	G	O5'-P-OP1	5.64	117.47	110.70
50	1	3350	C	N1-C2-O2	5.63	122.28	118.90
50	1	2616	C	N1-C2-O2	5.63	122.28	118.90
50	1	2163	C	C6-N1-C2	-5.63	118.05	120.30
50	1	2403	G	OP1-P-O3'	5.63	117.58	105.20
50	1	1152	G	C4-N9-C1'	5.62	133.81	126.50
50	1	2053	C	N1-C2-O2	5.62	122.27	118.90
50	1	1368	U	N1-C2-O2	5.62	126.73	122.80
50	1	3269	U	P-O3'-C3'	5.61	126.44	119.70
50	1	800	G	C2-N3-C4	5.61	114.70	111.90
50	1	2513	U	P-O3'-C3'	5.61	126.43	119.70
50	1	1889	G	C4-C5-N7	5.60	113.04	110.80
50	1	3104	U	N1-C2-O2	5.60	126.72	122.80
50	1	1348	U	C5-C6-N1	5.60	125.50	122.70
50	1	1871	U	C6-N1-C2	-5.60	117.64	121.00
50	1	2677	G	C4-N9-C1'	5.60	133.78	126.50
50	1	3306	U	N1-C2-O2	5.59	126.72	122.80
50	1	1525	G	C8-N9-C4	-5.59	104.16	106.40
50	1	2783	U	N3-C2-O2	-5.59	118.29	122.20
50	1	1620	U	N1-C2-O2	5.59	126.71	122.80
50	1	2722	U	N3-C2-O2	-5.59	118.29	122.20
50	1	1496	C	N3-C2-O2	-5.58	117.99	121.90
50	1	1037	C	N1-C2-O2	5.58	122.25	118.90
50	1	2478	C	C2-N1-C1'	5.58	124.94	118.80
50	1	31	C	C6-N1-C2	-5.58	118.07	120.30
50	1	1876	U	C5-C6-N1	5.58	125.49	122.70
50	1	1574	C	C5-C6-N1	5.57	123.78	121.00
50	1	1222	G	O4'-C1'-N9	5.57	112.66	108.20
50	1	963	G	C6-C5-N7	-5.57	127.06	130.40
50	1	1771	C	N3-C2-O2	-5.57	118.00	121.90
50	1	1493	G	C5-C6-N1	5.56	114.28	111.50
50	1	2866	U	OP1-P-O3'	5.56	117.42	105.20
50	1	656	A	N7-C8-N9	5.55	116.58	113.80
50	1	2772	C	C2-N1-C1'	5.55	124.91	118.80
31	4	58	G	OP1-P-O3'	5.54	117.39	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	1315	U	C5-C6-N1	-5.54	119.93	122.70
50	1	2797	C	C6-N1-C2	-5.54	118.08	120.30
50	1	2925	C	N3-C2-O2	-5.54	118.02	121.90
50	1	3054	U	C5-C6-N1	5.54	125.47	122.70
50	1	122	A	N3-C4-C5	-5.54	122.93	126.80
50	1	1597	C	C6-N1-C2	-5.54	118.09	120.30
50	1	2726	C	N3-C2-O2	-5.53	118.03	121.90
50	1	401	U	N1-C2-O2	5.53	126.67	122.80
50	1	496	C	C6-N1-C2	-5.52	118.09	120.30
50	1	1588	A	O4'-C1'-N9	5.52	112.62	108.20
50	1	1869	C	C5-C6-N1	5.52	123.76	121.00
50	1	1981	G	C4-N9-C1'	5.52	133.68	126.50
50	1	3243	A	C8-N9-C4	5.52	108.01	105.80
50	1	916	G	P-O3'-C3'	5.52	126.32	119.70
29	3	28	C	C2-N1-C1'	5.51	124.86	118.80
50	1	2879	C	C5-C6-N1	5.51	123.75	121.00
50	1	2359	C	C5-C6-N1	5.50	123.75	121.00
50	1	2873	U	O4'-C1'-N1	5.50	112.60	108.20
50	1	133	U	C2-N1-C1'	5.50	124.30	117.70
50	1	1194	G	C8-N9-C4	-5.50	104.20	106.40
50	1	1857	C	C6-N1-C2	-5.49	118.10	120.30
50	1	1298	C	C5-C6-N1	5.49	123.75	121.00
50	1	2415	C	N3-C2-O2	-5.49	118.06	121.90
50	1	2340	U	N3-C2-O2	-5.49	118.36	122.20
50	1	1276	U	N1-C2-O2	5.48	126.64	122.80
50	1	543	C	C5-C6-N1	5.48	123.74	121.00
50	1	1840	U	N1-C2-N3	5.48	118.19	114.90
50	1	2754	G	N9-C4-C5	-5.48	103.21	105.40
50	1	242	C	N3-C2-O2	-5.48	118.06	121.90
50	1	1276	U	N3-C2-O2	-5.48	118.36	122.20
50	1	2257	C	C5-C6-N1	5.48	123.74	121.00
50	1	31	C	C2-N1-C1'	5.48	124.82	118.80
50	1	401	U	N3-C2-O2	-5.48	118.37	122.20
50	1	1397	C	C6-N1-C2	-5.48	118.11	120.30
50	1	963	G	C4-C5-N7	5.47	112.99	110.80
50	1	32	U	C5-C6-N1	5.47	125.43	122.70
50	1	2546	C	N1-C2-O2	5.47	122.18	118.90
50	1	3034	C	N1-C2-O2	5.47	122.18	118.90
50	1	1587	A	C4-C5-C6	-5.46	114.27	117.00
50	1	2513	U	OP1-P-O3'	5.46	117.21	105.20
50	1	2257	C	C6-N1-C1'	-5.46	114.25	120.80
50	1	3023	U	C2-N1-C1'	5.46	124.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	28	U	C5-C6-N1	5.46	125.43	122.70
50	1	2983	C	N3-C2-O2	-5.45	118.08	121.90
50	1	863	C	C6-N1-C2	-5.45	118.12	120.30
50	1	1320	C	C6-N1-C2	-5.44	118.12	120.30
50	1	2199	G	C8-N9-C1'	-5.44	119.92	127.00
50	1	1872	C	C5-C6-N1	5.44	123.72	121.00
50	1	245	U	N3-C2-O2	-5.43	118.40	122.20
50	1	113	C	C2-N1-C1'	5.43	124.77	118.80
50	1	133	U	N3-C2-O2	-5.43	118.40	122.20
50	1	42	C	C5-C6-N1	5.43	123.71	121.00
50	1	1579	C	N3-C2-O2	-5.42	118.10	121.90
50	1	1482	A	C4-N9-C1'	5.42	136.06	126.30
50	1	2298	U	C6-N1-C1'	-5.42	113.61	121.20
50	1	2619	G	C6-C5-N7	-5.42	127.15	130.40
50	1	1889	G	C4-N9-C1'	5.42	133.54	126.50
50	1	1390	A	O4'-C1'-N9	5.41	112.53	108.20
50	1	1977	C	N1-C2-O2	5.41	122.14	118.90
50	1	1396	C	C6-N1-C2	-5.40	118.14	120.30
50	1	652	G	N3-C4-C5	-5.40	125.90	128.60
50	1	73	C	P-O3'-C3'	5.40	126.18	119.70
50	1	915	A	C8-N9-C1'	-5.40	117.98	127.70
50	1	401	U	C2-N1-C1'	5.39	124.17	117.70
50	1	3131	U	N1-C2-O2	5.39	126.58	122.80
50	1	914	A	P-O3'-C3'	5.38	126.16	119.70
50	1	3206	C	N1-C2-O2	5.37	122.12	118.90
50	1	1218	U	N1-C2-O2	5.37	126.56	122.80
50	1	379	C	C6-N1-C2	-5.37	118.15	120.30
50	1	1483	G	P-O3'-C3'	5.37	126.14	119.70
50	1	1418	A	C5-C6-N1	5.36	120.38	117.70
50	1	1977	C	C2-N1-C1'	5.36	124.70	118.80
50	1	276	U	C6-N1-C2	-5.36	117.78	121.00
50	1	343	U	OP2-P-O3'	5.36	117.00	105.20
50	1	825	U	C6-N1-C2	-5.36	117.78	121.00
50	1	2342	U	C6-N1-C2	-5.36	117.78	121.00
50	1	823	C	C2-N1-C1'	5.36	124.69	118.80
50	1	3298	C	C2-N1-C1'	5.35	124.69	118.80
50	1	268	A	N1-C2-N3	-5.35	126.62	129.30
50	1	2354	C	C6-N1-C2	-5.35	118.16	120.30
50	1	2875	U	C6-N1-C2	-5.35	117.79	121.00
50	1	942	U	O5'-P-OP1	-5.35	100.89	105.70
31	4	64	U	N1-C2-O2	5.34	126.54	122.80
50	1	2951	G	C4-N9-C1'	5.34	133.44	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	3	73	C	C6-N1-C2	-5.34	118.16	120.30
50	1	956	U	C5-C6-N1	5.34	125.37	122.70
50	1	1665	C	C6-N1-C2	-5.33	118.17	120.30
50	1	81	C	N1-C2-O2	5.33	122.10	118.90
50	1	1146	C	C6-N1-C2	-5.33	118.17	120.30
50	1	2629	U	N1-C2-O2	5.33	126.53	122.80
29	3	35	C	N1-C2-O2	5.33	122.10	118.90
46	H	163	LEU	CA-CB-CG	5.33	127.56	115.30
50	1	2585	G	C4-N9-C1'	5.33	133.43	126.50
50	1	3152	U	P-O3'-C3'	5.33	126.09	119.70
50	1	1481	A	C8-N9-C1'	-5.32	118.12	127.70
50	1	927	C	C6-N1-C2	-5.32	118.17	120.30
50	1	968	G	N3-C4-C5	-5.32	125.94	128.60
50	1	2948	C	C6-N1-C2	-5.32	118.17	120.30
50	1	2619	G	N1-C6-O6	5.31	123.09	119.90
50	1	2434	U	N3-C2-O2	-5.31	118.48	122.20
31	4	93	U	N3-C2-O2	-5.31	118.48	122.20
50	1	81	C	C6-N1-C2	-5.30	118.18	120.30
21	s	169	LYS	CA-CB-CG	5.30	125.06	113.40
50	1	1590	G	C4-N9-C1'	5.30	133.39	126.50
50	1	2133	U	N1-C2-O2	5.30	126.51	122.80
50	1	2553	U	N3-C2-O2	-5.29	118.49	122.20
50	1	2998	U	C2-N1-C1'	5.29	124.05	117.70
50	1	1125	U	C6-N1-C2	-5.29	117.83	121.00
31	4	18	U	C5-C6-N1	5.29	125.34	122.70
50	1	1620	U	C2-N1-C1'	5.29	124.04	117.70
50	1	933	A	C4-C5-N7	5.28	113.34	110.70
50	1	282	G	C2'-C3'-O3'	5.28	122.15	113.70
50	1	42	C	C6-N1-C2	-5.28	118.19	120.30
50	1	1348	U	C2-N1-C1'	5.28	124.03	117.70
50	1	1432	C	C5-C4-N4	-5.28	116.51	120.20
50	1	2081	U	N1-C2-O2	5.28	126.49	122.80
50	1	274	G	N3-C4-N9	5.27	129.16	126.00
50	1	945	C	C2-N1-C1'	5.27	124.60	118.80
50	1	2846	U	N3-C2-O2	-5.27	118.51	122.20
50	1	826	G	N3-C4-C5	-5.27	125.97	128.60
50	1	547	G	P-O3'-C3'	5.26	126.01	119.70
50	1	1177	G	OP1-P-O3'	5.26	116.76	105.20
50	1	1277	C	C6-N1-C2	-5.25	118.20	120.30
50	1	1181	U	C2-N1-C1'	-5.25	111.41	117.70
50	1	1958	U	N1-C2-O2	5.24	126.47	122.80
50	1	2376	G	N1-C6-O6	-5.24	116.75	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	3	28	C	N3-C2-O2	-5.24	118.23	121.90
50	1	36	C	N1-C2-O2	5.24	122.04	118.90
50	1	2263	C	C6-N1-C2	-5.24	118.21	120.30
50	1	3172	A	P-O3'-C3'	5.24	125.98	119.70
50	1	3145	C	N3-C2-O2	-5.23	118.24	121.90
50	1	1565	G	C4-N9-C1'	5.23	133.30	126.50
50	1	101	G	C8-N9-C1'	-5.23	120.20	127.00
50	1	819	U	C5-C4-O4	-5.23	122.76	125.90
50	1	1329	U	P-O3'-C3'	5.23	125.97	119.70
50	1	1756	C	C5-C6-N1	5.23	123.61	121.00
50	1	2052	G	C4-N9-C1'	5.23	133.29	126.50
50	1	3235	C	N1-C2-O2	5.23	122.04	118.90
50	1	743	C	N1-C2-O2	5.22	122.03	118.90
50	1	3344	A	C6-C5-N7	-5.22	128.65	132.30
50	1	1281	G	N3-C4-N9	5.21	129.13	126.00
50	1	716	A	O5'-P-OP1	-5.21	101.01	105.70
50	1	1459	C	C5-C6-N1	5.21	123.61	121.00
50	1	283	G	C6-C5-N7	-5.21	127.27	130.40
50	1	2146	C	C6-N1-C2	-5.21	118.22	120.30
50	1	2522	G	C8-N9-C1'	-5.21	120.23	127.00
29	3	13	A	C4-N9-C1'	5.21	135.67	126.30
50	1	167	U	N1-C2-O2	5.21	126.44	122.80
50	1	2868	U	N1-C2-O2	5.21	126.44	122.80
29	3	48	U	N3-C2-O2	-5.21	118.56	122.20
50	1	1557	A	OP1-P-O3'	5.21	116.65	105.20
50	1	982	C	C2-N1-C1'	5.20	124.52	118.80
50	1	1146	C	C5-C6-N1	5.20	123.60	121.00
50	1	1282	G	C4-N9-C1'	5.20	133.26	126.50
50	1	1481	A	C4-N9-C1'	5.20	135.66	126.30
50	1	208	C	C6-N1-C2	-5.20	118.22	120.30
50	1	1565	G	N3-C4-N9	5.20	129.12	126.00
50	1	1279	C	C5-C6-N1	5.20	123.60	121.00
50	1	2479	C	N3-C2-O2	-5.20	118.26	121.90
50	1	374	A	P-O3'-C3'	5.19	125.93	119.70
50	1	1901	A	C4-N9-C1'	5.19	135.65	126.30
50	1	3344	A	C4-C5-N7	5.19	113.30	110.70
50	1	1906	G	N9-C4-C5	-5.19	103.32	105.40
31	4	58	G	P-O3'-C3'	5.19	125.93	119.70
50	1	2951	G	N7-C8-N9	5.19	115.69	113.10
50	1	2928	C	C6-N1-C2	-5.19	118.23	120.30
50	1	3349	C	C5-C6-N1	5.19	123.59	121.00
50	1	421	G	C4-N9-C1'	5.18	133.24	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	2194	G	C4-N9-C1'	5.18	133.24	126.50
50	1	3278	C	C6-N1-C2	-5.18	118.23	120.30
50	1	167	U	N3-C2-O2	-5.18	118.58	122.20
29	3	26	C	C2-N1-C1'	5.18	124.49	118.80
50	1	995	U	N1-C2-O2	5.18	126.42	122.80
50	1	817	A	N1-C6-N6	-5.17	115.50	118.60
50	1	2830	G	C8-N9-C1'	-5.17	120.27	127.00
50	1	2046	U	N1-C1'-C2'	5.17	120.72	114.00
50	1	1608	C	C2-N1-C1'	5.17	124.49	118.80
50	1	2403	G	P-O3'-C3'	5.17	125.90	119.70
50	1	3048	A	C2-N3-C4	5.17	113.18	110.60
50	1	2478	C	C6-N1-C2	-5.17	118.23	120.30
50	1	2726	C	C6-N1-C1'	-5.17	114.60	120.80
50	1	2951	G	N3-C4-N9	5.17	129.10	126.00
50	1	3222	U	N1-C2-O2	5.17	126.42	122.80
50	1	3287	U	N3-C2-O2	-5.16	118.59	122.20
50	1	374	A	OP1-P-O3'	5.16	116.54	105.20
50	1	968	G	C8-N9-C1'	-5.15	120.30	127.00
50	1	1125	U	C5-C6-N1	5.15	125.28	122.70
50	1	1185	C	C5-C6-N1	5.15	123.58	121.00
50	1	90	C	C2-N1-C1'	5.15	124.47	118.80
50	1	382	U	C5-C6-N1	5.15	125.27	122.70
50	1	632	G	N3-C4-N9	5.14	129.09	126.00
50	1	685	G	O5'-P-OP1	-5.14	101.07	105.70
50	1	982	C	C5-C6-N1	5.14	123.57	121.00
50	1	995	U	O5'-P-OP2	-5.14	101.07	105.70
50	1	877	C	N3-C2-O2	-5.14	118.30	121.90
50	1	2873	U	C2-N1-C1'	5.14	123.87	117.70
50	1	1076	C	C2-N1-C1'	5.13	124.45	118.80
50	1	2730	G	N3-C4-C5	-5.13	126.03	128.60
50	1	3066	U	C6-N1-C2	-5.13	117.92	121.00
31	4	119	C	C5-C6-N1	5.13	123.56	121.00
50	1	982	C	C6-N1-C2	-5.13	118.25	120.30
50	1	2553	U	N1-C2-O2	5.13	126.39	122.80
50	1	2262	A	P-O3'-C3'	5.13	125.85	119.70
50	1	2617	U	C2-N1-C1'	5.12	123.85	117.70
50	1	819	U	C5-C6-N1	5.12	125.26	122.70
50	1	2479	C	C6-N1-C2	-5.12	118.25	120.30
50	1	1308	A	C2-N3-C4	5.11	113.16	110.60
50	1	915	A	N3-C4-N9	5.11	131.49	127.40
50	1	1590	G	N3-C4-C5	-5.11	126.05	128.60
50	1	2816	G	O4'-C1'-N9	5.11	112.29	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	101	G	C4-N9-C1'	5.11	133.14	126.50
50	1	379	C	C5-C6-N1	5.11	123.55	121.00
50	1	2948	C	C5-C6-N1	5.11	123.55	121.00
50	1	2335	G	O4'-C1'-N9	-5.10	104.12	108.20
50	1	3218	A	P-O3'-C3'	5.10	125.82	119.70
50	1	1181	U	P-O3'-C3'	5.10	125.82	119.70
50	1	1856	C	C6-N1-C2	-5.10	118.26	120.30
50	1	3111	U	C2-N1-C1'	5.10	123.82	117.70
50	1	964	G	N3-C4-N9	5.09	129.06	126.00
50	1	2980	U	N3-C2-O2	-5.09	118.64	122.20
50	1	2101	C	P-O3'-C3'	5.09	125.81	119.70
50	1	661	G	O4'-C1'-N9	5.09	112.27	108.20
50	1	2984	C	C6-N1-C1'	-5.08	114.70	120.80
29	3	73	C	C5-C6-N1	5.08	123.54	121.00
50	1	2866	U	P-O3'-C3'	5.08	125.80	119.70
50	1	2533	G	N3-C4-N9	5.07	129.04	126.00
50	1	1902	G	C5-C6-O6	-5.07	125.56	128.60
50	1	2629	U	C2-N1-C1'	5.07	123.78	117.70
50	1	3362	A	N7-C8-N9	5.07	116.33	113.80
50	1	1482	A	C2-N3-C4	5.06	113.13	110.60
50	1	2476	C	N1-C2-O2	5.06	121.94	118.90
50	1	1869	C	C6-N1-C2	-5.06	118.28	120.30
50	1	543	C	C6-N1-C2	-5.06	118.28	120.30
50	1	2656	A	P-O3'-C3'	5.06	125.77	119.70
50	1	1488	G	N1-C6-O6	-5.06	116.87	119.90
50	1	2727	A	OP1-P-O3'	5.06	116.32	105.20
50	1	2951	G	N1-C6-O6	5.06	122.93	119.90
50	1	315	C	N1-C2-O2	5.05	121.93	118.90
50	1	3145	C	N1-C2-O2	5.05	121.93	118.90
29	3	73	C	N1-C2-O2	5.05	121.93	118.90
50	1	652	G	C8-N9-C4	-5.05	104.38	106.40
50	1	431	U	C5-C6-N1	5.04	125.22	122.70
50	1	2333	C	C5-C6-N1	5.04	123.52	121.00
50	1	2254	U	N3-C2-O2	-5.04	118.67	122.20
50	1	2402	A	O4'-C1'-N9	5.04	112.23	108.20
50	1	2137	U	C2-N1-C1'	5.04	123.75	117.70
50	1	1551	C	C2-N1-C1'	5.04	124.34	118.80
50	1	915	A	C4-C5-N7	5.04	113.22	110.70
29	3	28	C	C5-C6-N1	5.03	123.52	121.00
50	1	1391	C	OP2-P-O3'	5.03	116.27	105.20
50	1	2928	C	N3-C2-O2	-5.03	118.38	121.90
50	1	1585	C	C5-C6-N1	5.03	123.52	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	2868	U	N3-C2-O2	-5.03	118.68	122.20
50	1	1556	C	C2-N1-C1'	5.03	124.33	118.80
50	1	2322	C	C6-N1-C2	-5.03	118.29	120.30
50	1	2281	A	C5-C6-N6	-5.03	119.68	123.70
50	1	541	U	C5-C6-N1	5.02	125.21	122.70
50	1	36	C	C6-N1-C2	-5.02	118.29	120.30
50	1	2128	C	C6-N1-C2	-5.02	118.29	120.30
50	1	2546	C	C2-N1-C1'	5.02	124.32	118.80
50	1	671	U	C5-C6-N1	5.02	125.21	122.70
50	1	1432	C	P-O3'-C3'	5.02	125.72	119.70
50	1	1227	C	N3-C2-O2	-5.02	118.39	121.90
50	1	2082	U	N1-C2-O2	5.02	126.31	122.80
50	1	2053	C	N3-C2-O2	-5.01	118.39	121.90
50	1	3303	G	OP1-P-O3'	5.01	116.22	105.20
50	1	2509	U	O4'-C1'-N1	5.01	112.21	108.20
50	1	939	U	C5-C6-N1	5.01	125.20	122.70
50	1	2254	U	N1-C2-O2	5.01	126.31	122.80
50	1	283	G	C8-N9-C1'	-5.00	120.50	127.00
50	1	1530	U	C5-C6-N1	5.00	125.20	122.70
50	1	2836	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	7	21	LYS	Peptide
1	A	289	VAL	Peptide
42	F	385	LYS	Peptide
44	G	130	ALA	Peptide
44	G	291	ASN	Peptide
44	G	318	LEU	Peptide
44	G	338	LYS	Peptide
46	H	259	LYS	Peptide
5	J	157	ASN	Peptide
5	J	232	ARG	Peptide
7	K	156	ASP	Peptide
7	K	38	GLN	Peptide
7	K	76	ALA	Peptide
11	M	172	LEU	Peptide
13	N	165	SER	Peptide
13	N	47	ALA	Peptide
13	N	61	PRO	Peptide

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Mol	Chain	Res	Type	Group
23	U	12	ARG	Peptide
3	X	8	GLU	Peptide
35	b	102	GLU	Peptide
37	c	46	ASP	Peptide
39	d	19	ASN	Peptide
6	j	90	ARG	Peptide
6	j	91	ALA	Peptide
12	m	32	ASN	Peptide
21	s	170	TRP	Peptide
21	s	171	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/519 (84%)	411 (94%)	27 (6%)	0	100	100
2	R	300/433 (69%)	286 (95%)	14 (5%)	0	100	100
3	X	222/224 (99%)	206 (93%)	16 (7%)	0	100	100
4	i	110/112 (98%)	104 (94%)	6 (6%)	0	100	100
5	J	220/222 (99%)	205 (93%)	13 (6%)	2 (1%)	17	57
6	j	117/119 (98%)	110 (94%)	4 (3%)	3 (3%)	5	35
7	K	231/233 (99%)	211 (91%)	19 (8%)	1 (0%)	34	71
8	k	97/99 (98%)	87 (90%)	10 (10%)	0	100	100
9	7	189/191 (99%)	176 (93%)	13 (7%)	0	100	100
10	l	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
11	M	167/169 (99%)	148 (89%)	19 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	m	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
13	N	191/193 (99%)	171 (90%)	16 (8%)	4 (2%)	7	40
14	n	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
15	O	134/136 (98%)	119 (89%)	15 (11%)	0	100	100
16	o	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
17	p	201/203 (99%)	179 (89%)	19 (10%)	3 (2%)	10	47
18	Q	195/197 (99%)	187 (96%)	8 (4%)	0	100	100
19	5	181/183 (99%)	164 (91%)	17 (9%)	0	100	100
20	S	183/185 (99%)	169 (92%)	14 (8%)	0	100	100
21	s	218/220 (99%)	187 (86%)	26 (12%)	5 (2%)	6	38
22	T	150/152 (99%)	142 (95%)	7 (5%)	1 (1%)	22	61
23	U	170/172 (99%)	156 (92%)	13 (8%)	1 (1%)	25	64
24	V	157/159 (99%)	144 (92%)	13 (8%)	0	100	100
25	W	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
26	P	144/155 (93%)	122 (85%)	22 (15%)	0	100	100
27	r	117/197 (59%)	110 (94%)	7 (6%)	0	100	100
28	x	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
30	Y	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
32	Z	119/121 (98%)	109 (92%)	10 (8%)	0	100	100
33	a	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
35	b	133/135 (98%)	117 (88%)	15 (11%)	1 (1%)	19	59
36	C	103/105 (98%)	92 (89%)	11 (11%)	0	100	100
37	c	146/148 (99%)	129 (88%)	14 (10%)	3 (2%)	7	40
38	D	89/91 (98%)	81 (91%)	8 (9%)	0	100	100
39	d	56/58 (97%)	49 (88%)	6 (11%)	1 (2%)	8	43
40	E	250/252 (99%)	223 (89%)	27 (11%)	0	100	100
41	e	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
42	F	384/386 (100%)	349 (91%)	34 (9%)	1 (0%)	41	75
43	f	107/109 (98%)	97 (91%)	10 (9%)	0	100	100
44	G	359/361 (99%)	324 (90%)	34 (10%)	1 (0%)	41	75
45	g	125/127 (98%)	119 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	H	294/296 (99%)	271 (92%)	23 (8%)	0	100	100
47	h	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
48	I	152/175 (87%)	143 (94%)	9 (6%)	0	100	100
49	L	202/204 (99%)	165 (82%)	37 (18%)	0	100	100
All	All	7524/7934 (95%)	6877 (91%)	620 (8%)	27 (0%)	38	71

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	s	104	CYS
21	s	106	GLY
37	c	47	LYS
44	G	339	LEU
5	J	158	LYS
6	j	85	THR
21	s	107	ALA
21	s	109	ARG
22	T	131	ALA
6	j	90	ARG
13	N	62	THR
13	N	166	ALA
23	U	13	ARG
35	b	102	GLU
37	c	78	LEU
5	J	233	GLU
7	K	157	VAL
17	p	146	ALA
21	s	108	ASP
37	c	40	HIS
6	j	91	ALA
13	N	48	PRO
13	N	61	PRO
17	p	74	PRO
42	F	188	ILE
17	p	75	VAL
39	d	21	ILE



### 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	
1	A	386/456 (85%)	383 (99%)	3 (1%)	81	91
2	R	288/349 (82%)	284 (99%)	4 (1%)	67	85
3	X	177/192 (92%)	177 (100%)	0	100	100
4	i	95/95 (100%)	94 (99%)	1 (1%)	73	88
5	J	186/186 (100%)	185 (100%)	1 (0%)	88	95
6	j	104/104 (100%)	104 (100%)	0	100	100
7	K	187/191 (98%)	187 (100%)	0	100	100
8	k	81/81 (100%)	81 (100%)	0	100	100
9	7	171/171 (100%)	169 (99%)	2 (1%)	71	87
10	l	70/70 (100%)	70 (100%)	0	100	100
11	M	147/147 (100%)	146 (99%)	1 (1%)	84	93
12	m	68/68 (100%)	67 (98%)	1 (2%)	65	84
13	N	154/154 (100%)	154 (100%)	0	100	100
14	n	45/45 (100%)	45 (100%)	0	100	100
15	O	107/107 (100%)	107 (100%)	0	100	100
16	o	47/47 (100%)	47 (100%)	0	100	100
17	p	175/175 (100%)	174 (99%)	1 (1%)	86	94
18	Q	160/160 (100%)	160 (100%)	0	100	100
19	5	140/145 (97%)	138 (99%)	2 (1%)	67	85
20	S	150/150 (100%)	150 (100%)	0	100	100
21	s	184/186 (99%)	182 (99%)	2 (1%)	73	88
22	T	126/126 (100%)	124 (98%)	2 (2%)	62	83
23	U	156/156 (100%)	155 (99%)	1 (1%)	86	94
24	V	136/136 (100%)	136 (100%)	0	100	100
25	W	87/87 (100%)	87 (100%)	0	100	100
27	r	105/166 (63%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	x	104/104 (100%)	103 (99%)	1 (1%)	76	88
30	Y	54/54 (100%)	54 (100%)	0	100	100
32	Z	104/105 (99%)	104 (100%)	0	100	100
33	a	109/109 (100%)	109 (100%)	0	100	100
35	b	115/115 (100%)	115 (100%)	0	100	100
36	C	90/90 (100%)	90 (100%)	0	100	100
37	c	118/118 (100%)	117 (99%)	1 (1%)	81	91
38	D	71/71 (100%)	71 (100%)	0	100	100
39	d	46/46 (100%)	46 (100%)	0	100	100
40	E	193/194 (100%)	192 (100%)	1 (0%)	88	95
41	e	81/81 (100%)	81 (100%)	0	100	100
42	F	319/322 (99%)	318 (100%)	1 (0%)	92	97
43	f	92/96 (96%)	92 (100%)	0	100	100
44	G	288/288 (100%)	288 (100%)	0	100	100
45	g	109/109 (100%)	109 (100%)	0	100	100
46	H	244/244 (100%)	244 (100%)	0	100	100
47	h	90/90 (100%)	90 (100%)	0	100	100
48	I	134/152 (88%)	132 (98%)	2 (2%)	65	84
49	L	185/185 (100%)	181 (98%)	4 (2%)	52	77
All	All	6278/6523 (96%)	6247 (100%)	31 (0%)	89	95

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

Mol	Chain	Res	Type
1	A	359	ILE
1	A	387	ARG
1	A	535	ASN
2	R	102	ARG
2	R	212	ASN
2	R	214	ARG
2	R	285	TYR
4	i	51	LEU
5	J	110	ARG
9	7	23	ARG
9	7	68	LEU

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Mol	Chain	Res	Type
11	M	84	LEU
12	m	39	ARG
17	p	193	ARG
19	5	24	VAL
19	5	120	ASN
21	s	103	SER
21	s	138	ARG
22	T	99	LEU
22	T	104	ARG
23	U	100	VAL
28	x	93	LEU
37	c	56	VAL
40	E	101	VAL
42	F	104	THR
48	I	31	ARG
48	I	166	LYS
49	L	14	LYS
49	L	57	ASN
49	L	108	ASN
49	L	130	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	ASN
1	A	352	GLN
1	A	413	HIS
1	A	457	HIS
1	A	465	GLN
1	A	535	ASN
1	A	562	ASN
1	A	580	GLN
2	R	212	ASN
2	R	283	HIS
3	X	11	ASN
3	X	106	ASN
4	i	52	GLN
5	J	172	ASN
5	J	225	GLN
6	j	59	ASN
7	K	240	ASN
9	7	77	ASN

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Mol	Chain	Res	Type
9	7	125	ASN
11	M	109	HIS
13	N	19	GLN
16	o	90	ASN
17	p	37	HIS
17	p	95	GLN
17	p	181	ASN
19	5	34	GLN
19	5	54	HIS
19	5	97	ASN
20	S	73	GLN
21	s	208	ASN
22	T	92	GLN
23	U	122	HIS
23	U	142	GLN
28	x	98	ASN
28	x	132	ASN
35	b	57	HIS
36	C	22	GLN
36	C	82	GLN
37	c	64	GLN
39	d	12	GLN
40	E	79	ASN
40	E	209	HIS
42	F	3	HIS
43	f	57	GLN
43	f	87	ASN
44	G	5	GLN
44	G	92	ASN
44	G	114	ASN
46	H	63	GLN
47	h	42	GLN
49	L	57	ASN
49	L	108	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	3	120/121 (99%)	29 (24%)	1 (0%)
31	4	157/158 (99%)	47 (29%)	4 (2%)
34	B	75/76 (98%)	16 (21%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	1	3312/3316 (99%)	966 (29%)	155 (4%)
All	All	3664/3671 (99%)	1058 (28%)	160 (4%)

All (1058) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	3	7	G
29	3	11	A
29	3	13	A
29	3	14	U
29	3	26	C
29	3	41	G
29	3	42	A
29	3	45	A
29	3	48	U
29	3	49	G
29	3	53	U
29	3	55	A
29	3	62	U
29	3	64	A
29	3	65	G
29	3	71	G
29	3	74	C
29	3	77	G
29	3	78	U
29	3	79	A
29	3	86	U
29	3	91	G
29	3	93	C
29	3	95	A
29	3	99	G
29	3	102	A
29	3	104	A
29	3	112	G
29	3	121	U
31	4	2	A
31	4	5	U
31	4	15	G
31	4	16	G
31	4	17	A
31	4	22	U
31	4	23	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	4	24	G
31	4	33	A
31	4	34	U
31	4	35	C
31	4	38	U
31	4	39	G
31	4	42	G
31	4	49	G
31	4	51	G
31	4	59	A
31	4	60	U
31	4	63	G
31	4	72	A
31	4	80	A
31	4	81	U
31	4	82	U
31	4	83	C
31	4	85	G
31	4	86	U
31	4	87	G
31	4	90	U
31	4	95	G
31	4	96	A
31	4	99	C
31	4	102	U
31	4	104	A
31	4	106	C
31	4	112	U
31	4	113	U
31	4	116	G
31	4	125	U
31	4	126	A
31	4	129	C
31	4	131	A
31	4	132	G
31	4	148	G
31	4	151	C
31	4	152	G
31	4	155	A
31	4	157	U
34	B	10	G
34	B	16	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	B	18	G
34	B	19	G
34	B	28	U
34	B	37	A
34	B	47	U
34	B	48	C
34	B	49	U
34	B	56	C
34	B	58	A
34	B	59	U
34	B	73	G
34	B	74	C
34	B	75	C
34	B	76	A
50	1	14	U
50	1	15	C
50	1	19	U
50	1	26	A
50	1	30	G
50	1	40	A
50	1	44	U
50	1	48	A
50	1	49	A
50	1	57	A
50	1	59	G
50	1	60	A
50	1	65	A
50	1	66	A
50	1	67	A
50	1	74	G
50	1	77	A
50	1	85	A
50	1	86	G
50	1	87	U
50	1	92	G
50	1	94	G
50	1	99	A
50	1	109	A
50	1	110	G
50	1	111	C
50	1	116	A
50	1	117	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	118	U
50	1	119	U
50	1	121	A
50	1	122	A
50	1	123	A
50	1	124	U
50	1	134	U
50	1	135	C
50	1	136	G
50	1	142	C
50	1	146	U
50	1	147	U
50	1	148	G
50	1	155	G
50	1	156	G
50	1	157	A
50	1	166	C
50	1	169	U
50	1	182	U
50	1	187	A
50	1	188	U
50	1	189	G
50	1	190	U
50	1	191	U
50	1	192	C
50	1	200	C
50	1	206	G
50	1	210	U
50	1	211	A
50	1	212	G
50	1	213	A
50	1	218	G
50	1	219	A
50	1	220	G
50	1	221	A
50	1	222	A
50	1	231	G
50	1	234	G
50	1	240	U
50	1	241	G
50	1	242	C
50	1	251	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	252	U
50	1	254	A
50	1	263	C
50	1	268	A
50	1	269	G
50	1	270	U
50	1	281	G
50	1	283	G
50	1	286	U
50	1	295	A
50	1	297	G
50	1	298	U
50	1	304	G
50	1	305	U
50	1	306	A
50	1	316	U
50	1	323	A
50	1	329	U
50	1	330	G
50	1	339	C
50	1	340	C
50	1	342	A
50	1	344	A
50	1	349	A
50	1	350	C
50	1	351	A
50	1	353	G
50	1	354	U
50	1	375	A
50	1	376	G
50	1	385	A
50	1	395	A
50	1	397	A
50	1	398	A
50	1	399	A
50	1	401	U
50	1	402	A
50	1	403	C
50	1	404	G
50	1	405	U
50	1	406	G
50	1	421	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	422	A
50	1	439	C
50	1	495	G
50	1	517	G
50	1	518	G
50	1	520	U
50	1	521	A
50	1	523	A
50	1	535	G
50	1	536	U
50	1	546	C
50	1	547	G
50	1	548	G
50	1	550	A
50	1	552	G
50	1	555	U
50	1	556	U
50	1	558	U
50	1	559	A
50	1	569	A
50	1	578	A
50	1	579	G
50	1	581	U
50	1	589	A
50	1	590	G
50	1	591	G
50	1	592	A
50	1	597	G
50	1	600	G
50	1	604	G
50	1	609	G
50	1	610	G
50	1	611	A
50	1	619	A
50	1	620	U
50	1	621	A
50	1	622	A
50	1	623	U
50	1	637	C
50	1	641	C
50	1	645	A
50	1	646	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	648	C
50	1	649	A
50	1	660	A
50	1	661	G
50	1	662	U
50	1	667	C
50	1	671	U
50	1	677	A
50	1	678	G
50	1	681	U
50	1	682	U
50	1	683	U
50	1	684	G
50	1	690	A
50	1	691	A
50	1	692	A
50	1	705	A
50	1	708	G
50	1	712	G
50	1	716	A
50	1	719	U
50	1	720	A
50	1	750	G
50	1	758	C
50	1	759	U
50	1	760	G
50	1	764	U
50	1	765	C
50	1	766	U
50	1	767	U
50	1	768	C
50	1	770	G
50	1	776	U
50	1	777	U
50	1	781	G
50	1	784	A
50	1	786	A
50	1	799	G
50	1	801	A
50	1	806	A
50	1	808	A
50	1	815	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	817	A
50	1	826	G
50	1	830	A
50	1	837	A
50	1	849	C
50	1	851	C
50	1	858	A
50	1	859	G
50	1	860	G
50	1	861	C
50	1	867	G
50	1	871	U
50	1	872	U
50	1	874	U
50	1	879	U
50	1	881	C
50	1	884	A
50	1	885	U
50	1	888	A
50	1	890	C
50	1	894	G
50	1	895	A
50	1	906	A
50	1	907	G
50	1	914	A
50	1	915	A
50	1	916	G
50	1	917	A
50	1	921	A
50	1	923	C
50	1	925	A
50	1	932	U
50	1	933	A
50	1	934	G
50	1	937	G
50	1	939	U
50	1	944	C
50	1	953	G
50	1	959	C
50	1	960	U
50	1	962	A
50	1	963	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	980	A
50	1	981	U
50	1	982	C
50	1	995	U
50	1	1001	G
50	1	1002	A
50	1	1006	A
50	1	1008	U
50	1	1015	U
50	1	1016	C
50	1	1017	C
50	1	1018	G
50	1	1021	G
50	1	1025	A
50	1	1026	A
50	1	1029	G
50	1	1032	C
50	1	1036	A
50	1	1037	C
50	1	1038	C
50	1	1041	U
50	1	1045	C
50	1	1047	A
50	1	1049	C
50	1	1054	A
50	1	1063	G
50	1	1065	A
50	1	1066	G
50	1	1075	A
50	1	1076	C
50	1	1080	A
50	1	1081	U
50	1	1082	U
50	1	1083	G
50	1	1093	A
50	1	1094	U
50	1	1095	U
50	1	1096	U
50	1	1097	G
50	1	1098	A
50	1	1103	A
50	1	1104	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	1117	G
50	1	1128	U
50	1	1131	G
50	1	1132	C
50	1	1135	A
50	1	1138	U
50	1	1142	G
50	1	1143	A
50	1	1144	U
50	1	1145	G
50	1	1150	A
50	1	1151	U
50	1	1152	G
50	1	1153	A
50	1	1155	C
50	1	1156	C
50	1	1159	A
50	1	1177	G
50	1	1178	G
50	1	1180	A
50	1	1181	U
50	1	1182	A
50	1	1191	U
50	1	1192	C
50	1	1193	A
50	1	1196	C
50	1	1199	C
50	1	1200	A
50	1	1201	C
50	1	1202	A
50	1	1209	G
50	1	1212	A
50	1	1219	C
50	1	1220	U
50	1	1221	A
50	1	1222	G
50	1	1223	A
50	1	1232	C
50	1	1235	U
50	1	1236	G
50	1	1237	G
50	1	1239	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	1241	U
50	1	1242	G
50	1	1244	A
50	1	1245	A
50	1	1246	G
50	1	1254	C
50	1	1258	U
50	1	1259	A
50	1	1262	G
50	1	1263	A
50	1	1264	G
50	1	1282	G
50	1	1285	G
50	1	1287	A
50	1	1292	C
50	1	1294	A
50	1	1300	G
50	1	1301	A
50	1	1303	A
50	1	1306	G
50	1	1307	G
50	1	1308	A
50	1	1313	G
50	1	1315	U
50	1	1316	C
50	1	1322	U
50	1	1323	G
50	1	1325	U
50	1	1329	U
50	1	1330	A
50	1	1331	U
50	1	1332	A
50	1	1345	G
50	1	1349	G
50	1	1351	U
50	1	1352	A
50	1	1353	U
50	1	1355	A
50	1	1356	U
50	1	1357	G
50	1	1366	A
50	1	1380	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	1386	A
50	1	1387	G
50	1	1390	A
50	1	1391	C
50	1	1392	G
50	1	1399	A
50	1	1400	G
50	1	1418	A
50	1	1419	A
50	1	1432	C
50	1	1433	A
50	1	1434	G
50	1	1435	A
50	1	1436	U
50	1	1437	C
50	1	1443	G
50	1	1446	A
50	1	1447	G
50	1	1448	U
50	1	1450	G
50	1	1451	C
50	1	1455	U
50	1	1456	A
50	1	1467	A
50	1	1468	A
50	1	1470	U
50	1	1477	A
50	1	1481	A
50	1	1482	A
50	1	1483	G
50	1	1484	U
50	1	1485	G
50	1	1486	G
50	1	1487	G
50	1	1496	C
50	1	1502	C
50	1	1503	A
50	1	1508	C
50	1	1511	U
50	1	1512	U
50	1	1515	A
50	1	1523	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	1528	G
50	1	1531	C
50	1	1535	A
50	1	1536	G
50	1	1542	G
50	1	1549	U
50	1	1554	U
50	1	1555	U
50	1	1556	C
50	1	1557	A
50	1	1558	A
50	1	1559	A
50	1	1560	G
50	1	1561	G
50	1	1563	C
50	1	1565	G
50	1	1567	U
50	1	1568	U
50	1	1569	U
50	1	1570	U
50	1	1571	A
50	1	1572	U
50	1	1573	G
50	1	1575	A
50	1	1578	C
50	1	1579	C
50	1	1580	A
50	1	1581	C
50	1	1582	C
50	1	1583	A
50	1	1588	A
50	1	1589	A
50	1	1590	G
50	1	1593	A
50	1	1595	U
50	1	1603	A
50	1	1604	G
50	1	1605	A
50	1	1613	A
50	1	1620	U
50	1	1623	G
50	1	1629	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	1630	U
50	1	1631	C
50	1	1638	A
50	1	1644	C
50	1	1645	U
50	1	1646	G
50	1	1656	A
50	1	1657	C
50	1	1662	G
50	1	1683	A
50	1	1688	U
50	1	1696	A
50	1	1713	G
50	1	1715	A
50	1	1717	U
50	1	1719	G
50	1	1722	U
50	1	1724	U
50	1	1730	G
50	1	1741	A
50	1	1742	U
50	1	1749	A
50	1	1750	A
50	1	1752	A
50	1	1756	C
50	1	1760	A
50	1	1762	C
50	1	1763	U
50	1	1765	U
50	1	1766	G
50	1	1769	G
50	1	1770	G
50	1	1771	C
50	1	1773	C
50	1	1775	G
50	1	1780	G
50	1	1785	U
50	1	1788	C
50	1	1794	G
50	1	1796	G
50	1	1797	A
50	1	1813	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	1814	A
50	1	1815	U
50	1	1816	A
50	1	1817	G
50	1	1818	U
50	1	1819	U
50	1	1820	U
50	1	1821	U
50	1	1822	C
50	1	1835	A
50	1	1839	A
50	1	1840	U
50	1	1841	A
50	1	1843	C
50	1	1846	C
50	1	1847	A
50	1	1848	G
50	1	1849	C
50	1	1850	A
50	1	1851	G
50	1	1854	C
50	1	1855	U
50	1	1866	C
50	1	1867	A
50	1	1869	C
50	1	1876	U
50	1	1878	G
50	1	1879	A
50	1	1880	U
50	1	1881	A
50	1	1886	A
50	1	1887	A
50	1	1889	G
50	1	1892	G
50	1	1893	A
50	1	1901	A
50	1	1906	G
50	1	1909	A
50	1	1926	C
50	1	1927	G
50	1	1930	A
50	1	1931	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	1932	A
50	1	1935	G
50	1	1939	G
50	1	1948	G
50	1	1953	G
50	1	1954	G
50	1	1955	U
50	1	1959	G
50	1	1960	A
50	1	1961	G
50	1	1962	A
50	1	1963	G
50	1	1964	C
50	1	1972	A
50	1	1973	G
50	1	1979	G
50	1	1981	G
50	1	1986	U
50	1	1994	G
50	1	1999	C
50	1	2001	U
50	1	2002	G
50	1	2004	U
50	1	2005	G
50	1	2006	G
50	1	2010	U
50	1	2013	C
50	1	2017	G
50	1	2020	A
50	1	2022	G
50	1	2024	G
50	1	2026	A
50	1	2032	U
50	1	2033	G
50	1	2034	C
50	1	2035	G
50	1	2038	C
50	1	2039	C
50	1	2044	U
50	1	2045	G
50	1	2046	U
50	1	2047	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	2048	G
50	1	2049	A
50	1	2050	C
50	1	2053	C
50	1	2055	U
50	1	2056	U
50	1	2058	G
50	1	2059	U
50	1	2081	U
50	1	2082	U
50	1	2085	U
50	1	2087	C
50	1	2101	C
50	1	2102	U
50	1	2107	A
50	1	2111	G
50	1	2112	U
50	1	2113	A
50	1	2114	C
50	1	2121	G
50	1	2122	G
50	1	2131	A
50	1	2134	G
50	1	2138	A
50	1	2139	A
50	1	2140	U
50	1	2142	A
50	1	2144	A
50	1	2145	A
50	1	2158	A
50	1	2159	U
50	1	2160	G
50	1	2169	G
50	1	2170	U
50	1	2175	U
50	1	2176	U
50	1	2178	A
50	1	2179	C
50	1	2184	U
50	1	2187	G
50	1	2188	A
50	1	2205	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	2206	G
50	1	2209	U
50	1	2210	G
50	1	2211	U
50	1	2218	G
50	1	2228	A
50	1	2243	A
50	1	2244	A
50	1	2248	C
50	1	2249	G
50	1	2250	G
50	1	2253	G
50	1	2254	U
50	1	2256	A
50	1	2257	C
50	1	2258	U
50	1	2261	G
50	1	2262	A
50	1	2263	C
50	1	2268	U
50	1	2270	A
50	1	2272	G
50	1	2273	G
50	1	2274	U
50	1	2279	A
50	1	2281	A
50	1	2282	U
50	1	2283	G
50	1	2284	C
50	1	2285	C
50	1	2288	G
50	1	2298	U
50	1	2299	A
50	1	2306	C
50	1	2307	G
50	1	2308	C
50	1	2309	A
50	1	2313	A
50	1	2314	U
50	1	2315	G
50	1	2319	U
50	1	2334	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	2336	U
50	1	2339	C
50	1	2340	U
50	1	2363	A
50	1	2365	C
50	1	2372	A
50	1	2373	A
50	1	2374	C
50	1	2375	G
50	1	2377	G
50	1	2385	G
50	1	2386	A
50	1	2388	U
50	1	2393	G
50	1	2394	G
50	1	2397	A
50	1	2402	A
50	1	2403	G
50	1	2404	A
50	1	2411	U
50	1	2412	G
50	1	2418	G
50	1	2419	A
50	1	2424	A
50	1	2434	U
50	1	2435	G
50	1	2440	G
50	1	2441	A
50	1	2444	C
50	1	2447	A
50	1	2448	G
50	1	2453	U
50	1	2454	G
50	1	2459	A
50	1	2462	A
50	1	2469	G
50	1	2471	U
50	1	2482	U
50	1	2486	A
50	1	2487	U
50	1	2488	A
50	1	2496	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	2500	A
50	1	2504	U
50	1	2505	U
50	1	2506	U
50	1	2507	C
50	1	2509	U
50	1	2510	U
50	1	2513	U
50	1	2514	U
50	1	2515	A
50	1	2522	G
50	1	2523	A
50	1	2531	C
50	1	2532	U
50	1	2533	G
50	1	2534	G
50	1	2537	U
50	1	2538	U
50	1	2539	C
50	1	2540	A
50	1	2541	U
50	1	2542	U
50	1	2543	U
50	1	2547	A
50	1	2549	G
50	1	2552	C
50	1	2554	A
50	1	2561	A
50	1	2569	A
50	1	2570	U
50	1	2571	U
50	1	2572	C
50	1	2573	G
50	1	2585	G
50	1	2593	A
50	1	2594	C
50	1	2595	A
50	1	2606	G
50	1	2607	G
50	1	2613	U
50	1	2614	G
50	1	2617	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	2618	G
50	1	2619	G
50	1	2626	A
50	1	2628	A
50	1	2629	U
50	1	2635	A
50	1	2636	A
50	1	2642	A
50	1	2644	C
50	1	2652	U
50	1	2655	U
50	1	2657	A
50	1	2666	C
50	1	2674	A
50	1	2676	A
50	1	2678	A
50	1	2681	U
50	1	2688	U
50	1	2689	A
50	1	2691	A
50	1	2694	A
50	1	2703	A
50	1	2704	A
50	1	2707	C
50	1	2713	U
50	1	2716	U
50	1	2720	G
50	1	2728	G
50	1	2729	U
50	1	2737	C
50	1	2742	C
50	1	2752	U
50	1	2753	G
50	1	2754	G
50	1	2755	C
50	1	2762	A
50	1	2773	C
50	1	2777	G
50	1	2778	G
50	1	2797	C
50	1	2798	C
50	1	2799	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	2800	G
50	1	2801	A
50	1	2802	A
50	1	2804	A
50	1	2805	G
50	1	2808	A
50	1	2810	C
50	1	2814	G
50	1	2816	G
50	1	2817	A
50	1	2827	U
50	1	2829	U
50	1	2830	G
50	1	2842	U
50	1	2845	A
50	1	2849	C
50	1	2856	G
50	1	2860	U
50	1	2861	U
50	1	2866	U
50	1	2867	C
50	1	2871	G
50	1	2872	A
50	1	2873	U
50	1	2874	G
50	1	2875	U
50	1	2876	C
50	1	2887	A
50	1	2888	U
50	1	2889	C
50	1	2904	U
50	1	2912	G
50	1	2919	A
50	1	2920	U
50	1	2922	G
50	1	2923	U
50	1	2935	U
50	1	2936	A
50	1	2941	A
50	1	2942	C
50	1	2946	A
50	1	2947	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	2950	G
50	1	2951	G
50	1	2954	U
50	1	2965	U
50	1	2971	A
50	1	2972	G
50	1	2977	G
50	1	2978	U
50	1	2979	U
50	1	2983	C
50	1	2992	U
50	1	2996	U
50	1	2997	G
50	1	3011	A
50	1	3012	A
50	1	3021	A
50	1	3022	G
50	1	3023	U
50	1	3026	G
50	1	3047	U
50	1	3056	U
50	1	3058	U
50	1	3059	G
50	1	3078	U
50	1	3079	U
50	1	3080	G
50	1	3086	A
50	1	3088	G
50	1	3092	C
50	1	3098	G
50	1	3109	G
50	1	3111	U
50	1	3113	A
50	1	3115	C
50	1	3117	C
50	1	3118	C
50	1	3119	U
50	1	3122	A
50	1	3130	A
50	1	3131	U
50	1	3139	A
50	1	3142	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	3143	C
50	1	3144	G
50	1	3151	U
50	1	3153	U
50	1	3154	C
50	1	3155	U
50	1	3156	U
50	1	3157	U
50	1	3158	G
50	1	3170	A
50	1	3172	A
50	1	3173	G
50	1	3174	A
50	1	3176	G
50	1	3179	U
50	1	3180	A
50	1	3181	C
50	1	3185	U
50	1	3186	A
50	1	3187	A
50	1	3194	C
50	1	3196	U
50	1	3197	G
50	1	3198	U
50	1	3205	G
50	1	3206	C
50	1	3207	U
50	1	3208	G
50	1	3209	A
50	1	3210	A
50	1	3217	C
50	1	3218	A
50	1	3219	G
50	1	3220	G
50	1	3222	U
50	1	3227	A
50	1	3228	C
50	1	3237	U
50	1	3243	A
50	1	3244	A
50	1	3245	A
50	1	3246	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	3247	G
50	1	3253	G
50	1	3259	U
50	1	3260	G
50	1	3263	G
50	1	3268	A
50	1	3269	U
50	1	3270	U
50	1	3271	G
50	1	3272	C
50	1	3273	A
50	1	3274	A
50	1	3275	U
50	1	3276	G
50	1	3277	U
50	1	3278	C
50	1	3279	A
50	1	3286	G
50	1	3287	U
50	1	3288	G
50	1	3289	G
50	1	3290	G
50	1	3292	A
50	1	3293	U
50	1	3294	A
50	1	3295	A
50	1	3296	A
50	1	3305	A
50	1	3307	A
50	1	3313	U
50	1	3316	A
50	1	3317	U
50	1	3318	G
50	1	3319	U
50	1	3335	A
50	1	3340	G
50	1	3341	U
50	1	3345	G
50	1	3351	U
50	1	3352	U
50	1	3353	G
50	1	3354	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	3355	U
50	1	3357	U
50	1	3358	U
50	1	3362	A
50	1	3363	U
50	1	3368	U
50	1	3369	G
50	1	3370	A
50	1	3375	A
50	1	3378	C
50	1	3382	U
50	1	3383	G
50	1	3386	G
50	1	3390	G

All (160) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
29	3	77	G
31	4	22	U
31	4	38	U
31	4	48	A
31	4	58	G
50	1	14	U
50	1	43	A
50	1	73	C
50	1	86	G
50	1	116	A
50	1	122	A
50	1	147	U
50	1	155	G
50	1	156	G
50	1	189	G
50	1	211	A
50	1	218	G
50	1	219	A
50	1	239	G
50	1	268	A
50	1	269	G
50	1	282	G
50	1	285	A
50	1	341	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	353	G
50	1	374	A
50	1	375	A
50	1	400	G
50	1	494	G
50	1	547	G
50	1	558	U
50	1	621	A
50	1	645	A
50	1	648	C
50	1	661	G
50	1	677	A
50	1	715	A
50	1	764	U
50	1	767	U
50	1	870	G
50	1	884	A
50	1	896	A
50	1	906	A
50	1	914	A
50	1	916	G
50	1	923	C
50	1	924	G
50	1	933	A
50	1	962	A
50	1	979	U
50	1	994	G
50	1	1064	A
50	1	1065	A
50	1	1075	A
50	1	1103	A
50	1	1144	U
50	1	1177	G
50	1	1192	C
50	1	1196	C
50	1	1199	C
50	1	1241	U
50	1	1307	G
50	1	1329	U
50	1	1348	U
50	1	1352	A
50	1	1365	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	1391	C
50	1	1417	G
50	1	1418	A
50	1	1432	C
50	1	1433	A
50	1	1434	G
50	1	1455	U
50	1	1482	A
50	1	1483	G
50	1	1553	U
50	1	1554	U
50	1	1557	A
50	1	1568	U
50	1	1580	A
50	1	1589	A
50	1	1695	U
50	1	1716	U
50	1	1740	U
50	1	1815	U
50	1	1816	A
50	1	1840	U
50	1	1849	C
50	1	1850	A
50	1	1900	A
50	1	1913	A
50	1	1931	U
50	1	1938	U
50	1	1953	G
50	1	1959	G
50	1	1971	C
50	1	2047	A
50	1	2086	A
50	1	2101	C
50	1	2111	G
50	1	2112	U
50	1	2139	A
50	1	2144	A
50	1	2158	A
50	1	2175	U
50	1	2177	G
50	1	2178	A
50	1	2187	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	1	2208	A
50	1	2262	A
50	1	2267	C
50	1	2271	A
50	1	2273	G
50	1	2313	A
50	1	2372	A
50	1	2385	G
50	1	2393	G
50	1	2402	A
50	1	2403	G
50	1	2447	A
50	1	2468	A
50	1	2487	U
50	1	2509	U
50	1	2513	U
50	1	2537	U
50	1	2541	U
50	1	2593	A
50	1	2635	A
50	1	2656	A
50	1	2715	A
50	1	2727	A
50	1	2728	G
50	1	2761	G
50	1	2772	C
50	1	2797	C
50	1	2803	A
50	1	2816	G
50	1	2866	U
50	1	2911	A
50	1	2941	A
50	1	2950	G
50	1	2983	C
50	1	3021	A
50	1	3022	G
50	1	3078	U
50	1	3121	U
50	1	3152	U
50	1	3156	U
50	1	3172	A
50	1	3175	U

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Mol	Chain	Res	Type
50	1	3179	U
50	1	3186	A
50	1	3208	G
50	1	3216	G
50	1	3218	A
50	1	3219	G
50	1	3246	G
50	1	3259	U
50	1	3269	U
50	1	3334	U

#### 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 1 ligands modelled in this entry, 1 is 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
2	R	5
50	1	4
42	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	35:SER	C	74:CYS	N	41.41
1	1	2087:C	O3'	2093:A	P	28.40
1	R	529:GLY	C	535:UNK	N	19.42
1	R	105:ARG	C	113:UNK	N	18.44
1	R	123:UNK	C	156:UNK	N	13.45
1	1	440:A	O3'	494:G	P	13.22
1	1	2059:U	O3'	2080:C	P	11.99
1	R	80:SER	C	90:HIS	N	8.91
1	1	1984:C	O3'	1985:G	P	6.66
1	F	237:LYS	C	238:LEU	N	1.13

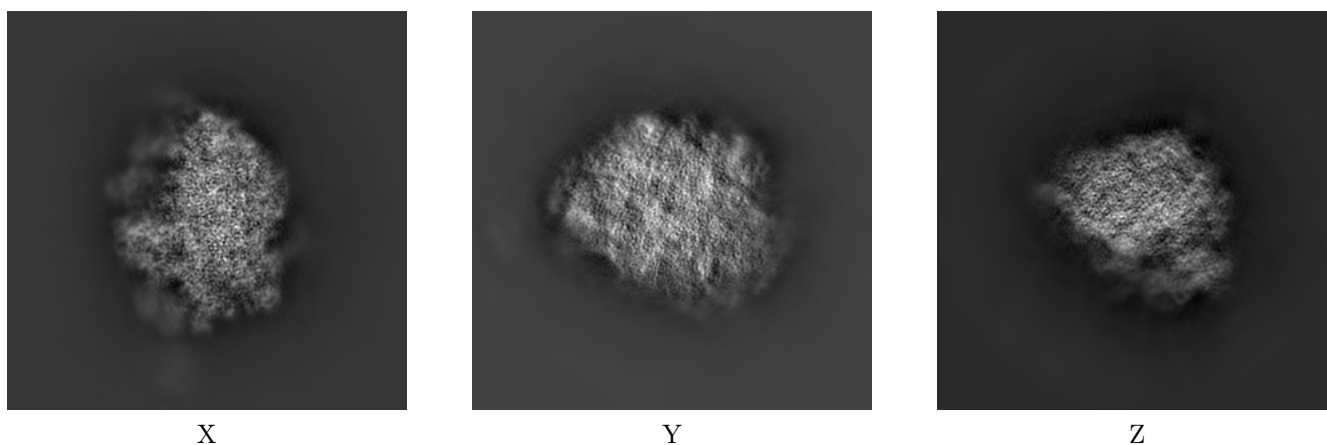
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4751. 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](#)

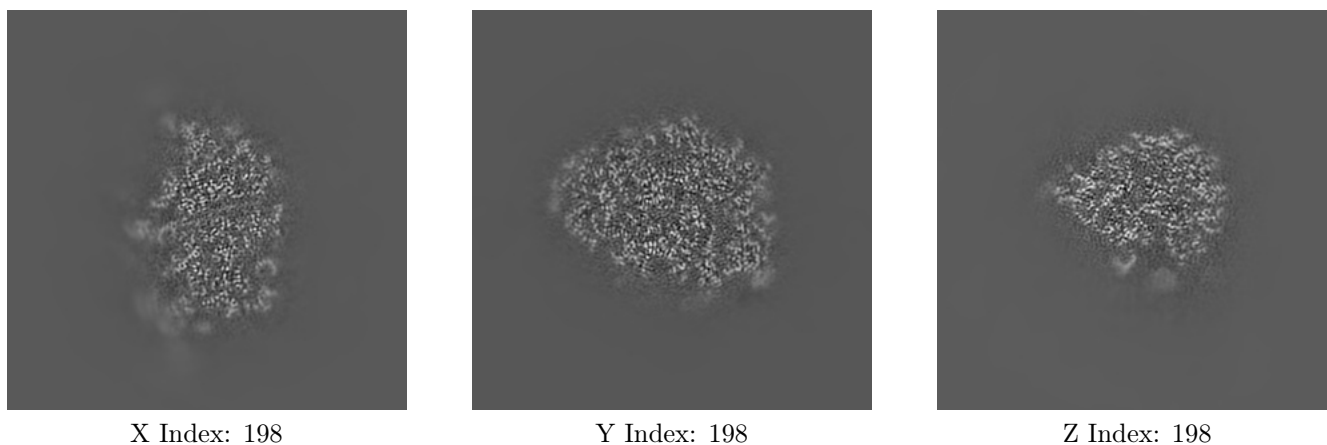
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

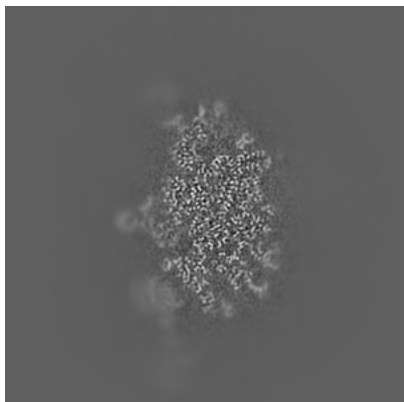
#### 6.2.1 Primary map



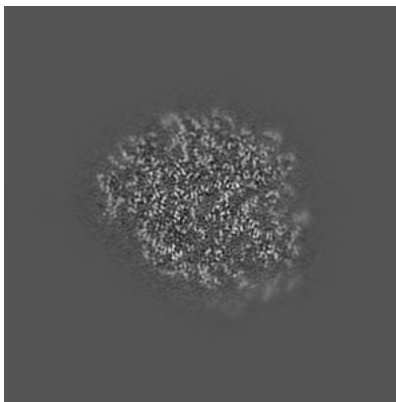
The images above show central slices of the map in three orthogonal directions.

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

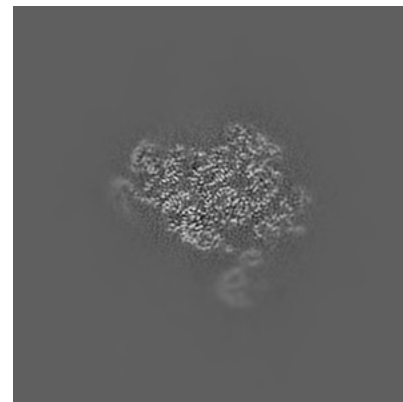
### 6.3.1 Primary map



X Index: 183



Y Index: 209

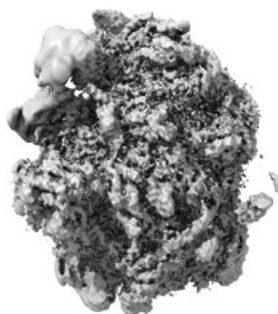


Z Index: 214

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

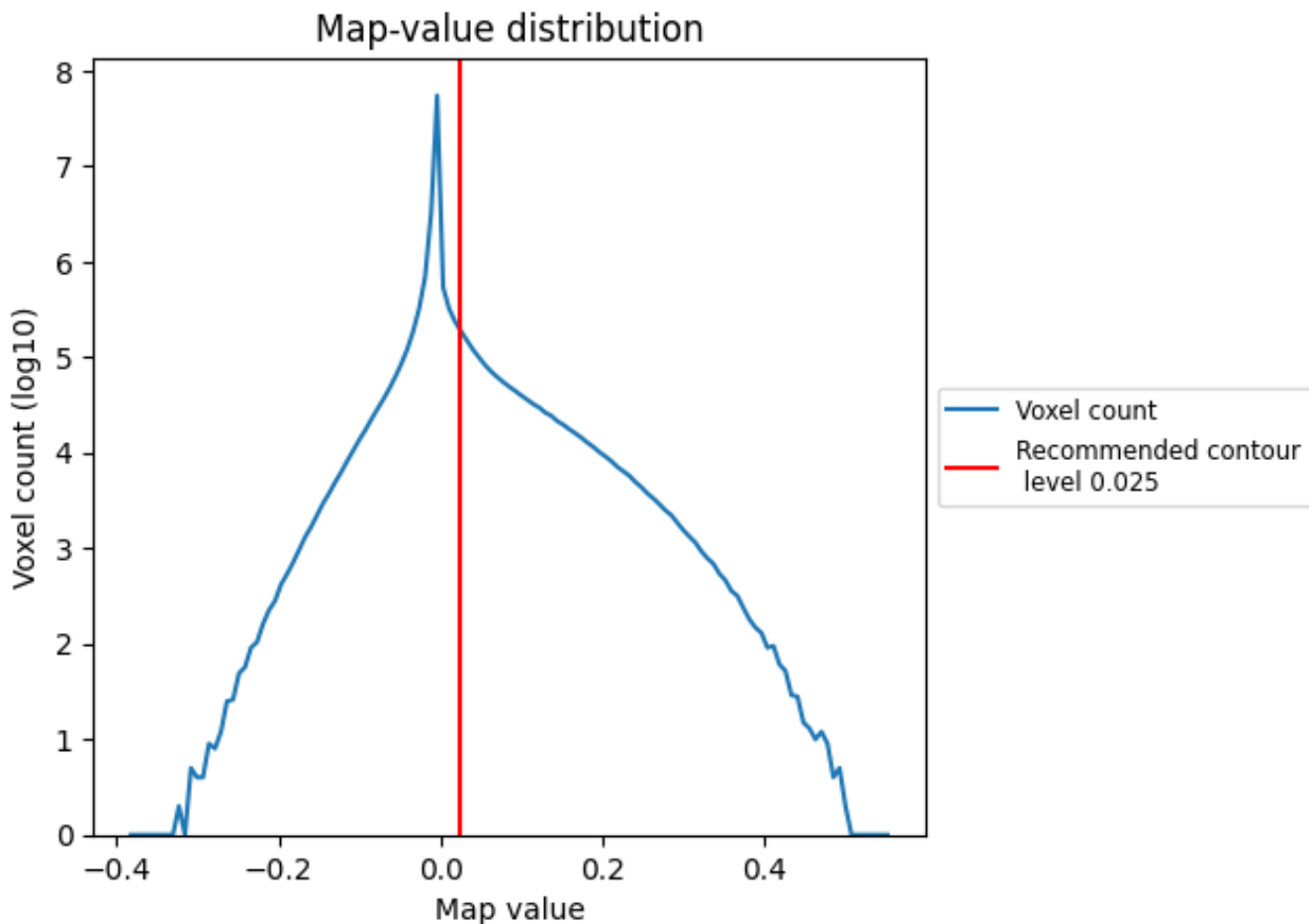
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

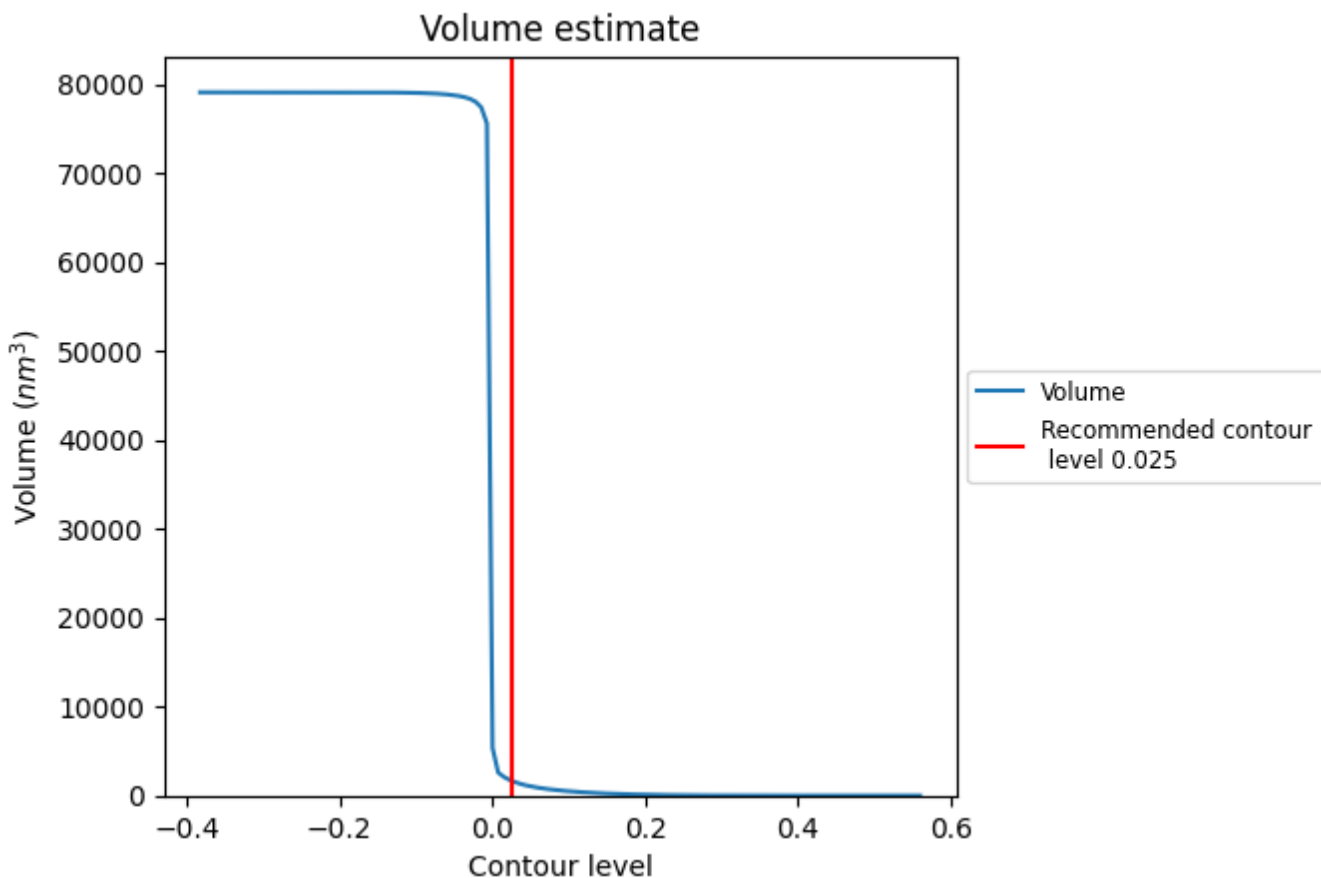
This section contains the results of statistical analysis of the map.

### 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](#)

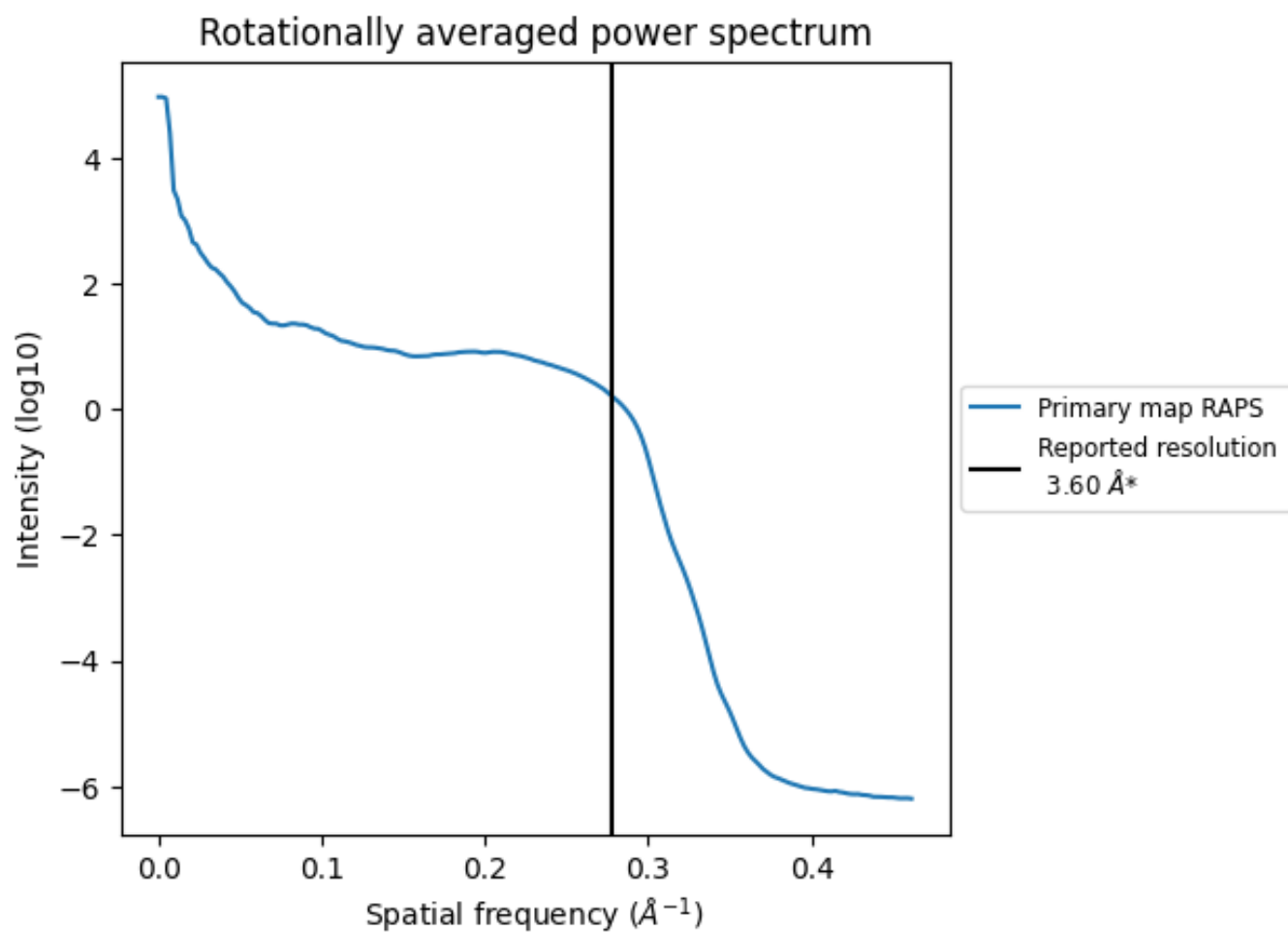


The volume at the recommended contour level is 1693 nm<sup>3</sup>; this corresponds to an approximate mass of 1530 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum



\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

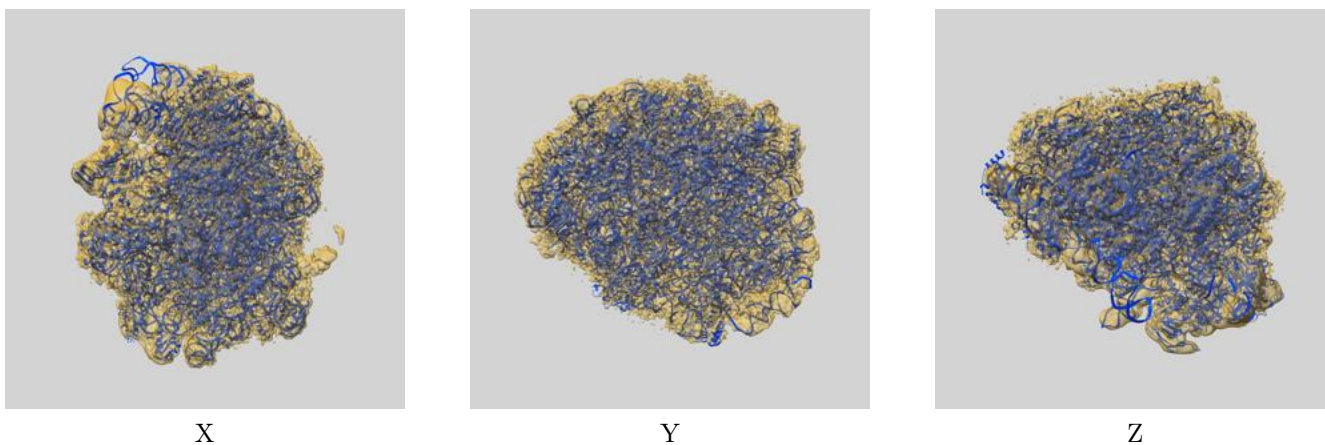
## 8 Fourier-Shell correlation

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

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

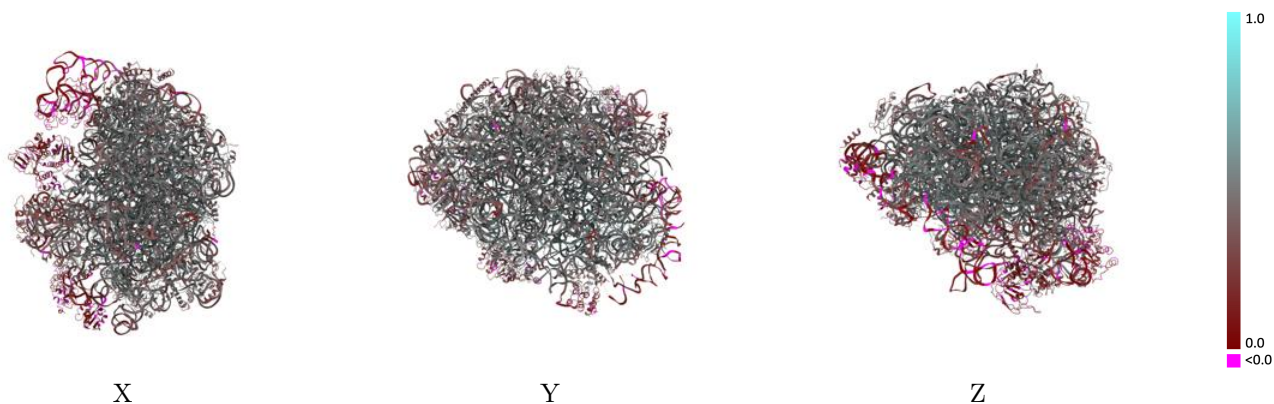
This section contains information regarding the fit between EMDB map EMD-4751 and PDB model 6R84. Per-residue inclusion information can be found in section 3 on page 14.

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



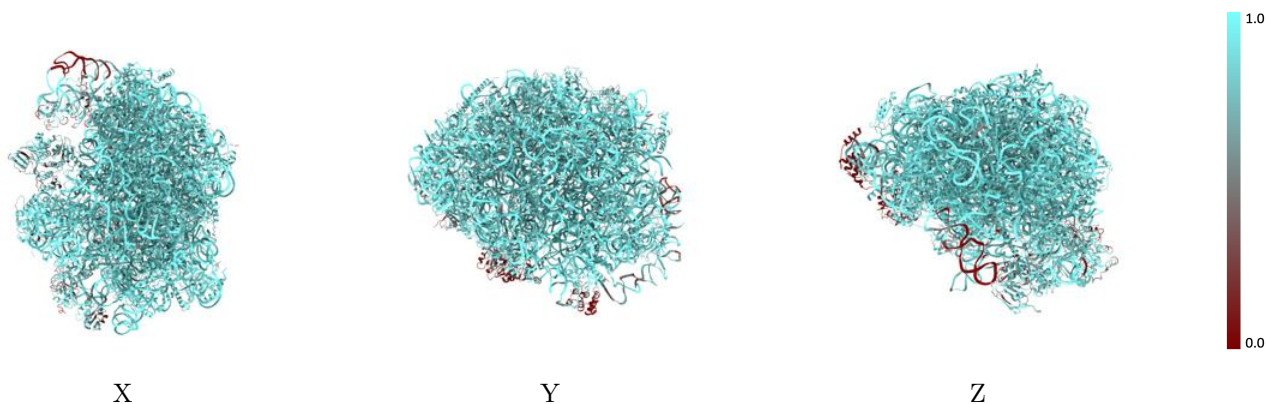
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



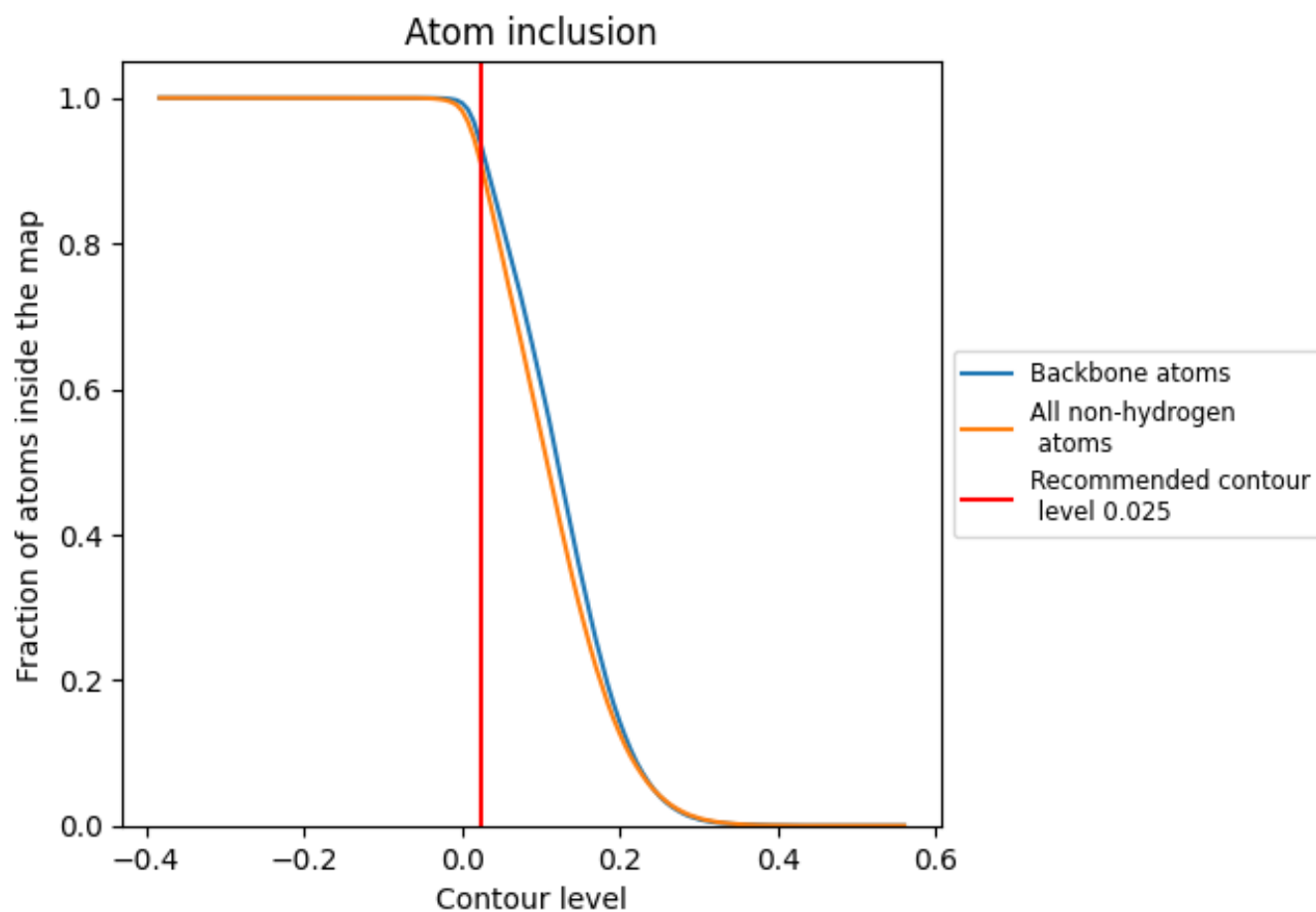
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 91% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9074	 0.4220
1	 0.9512	 0.4380
3	 0.9845	 0.4350
4	 0.9812	 0.4760
5	 0.9186	 0.4750
7	 0.9034	 0.4520
A	 0.7480	 0.1760
B	 0.9242	 0.2640
C	 0.8841	 0.4570
D	 0.9312	 0.4890
E	 0.9223	 0.5030
F	 0.9321	 0.4880
G	 0.9155	 0.4590
H	 0.8754	 0.3560
I	 0.8813	 0.4160
J	 0.9059	 0.4460
K	 0.8950	 0.4130
L	 0.5220	 0.0610
M	 0.8662	 0.3550
N	 0.9139	 0.4410
O	 0.9269	 0.4450
P	 0.4627	 0.1180
Q	 0.9386	 0.4920
R	 0.5591	 0.2560
S	 0.9211	 0.4640
T	 0.9255	 0.4730
U	 0.9144	 0.4760
V	 0.9008	 0.4590
W	 0.9079	 0.4110
X	 0.2340	 0.2510
Y	 0.9336	 0.4640
Z	 0.9204	 0.4840
a	 0.9182	 0.4570
b	 0.9010	 0.4480
c	 0.9299	 0.4670



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Chain	Atom inclusion	Q-score
d	 0.8938	 0.4180
e	 0.9042	 0.4300
f	 0.9118	 0.4770
g	 0.9115	 0.4850
h	 0.9269	 0.4970
i	 0.9201	 0.4920
j	 0.9141	 0.4510
k	 0.8752	 0.4260
l	 0.9557	 0.5230
m	 0.8481	 0.4190
n	 0.9422	 0.5110
o	 0.9330	 0.4730
p	 0.9340	 0.5050
r	 0.7005	 0.0920
s	 0.8793	 0.4360
x	 0.9183	 0.4790