



Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 01:29 pm GMT

PDB ID : 6SPG
EMDB ID : EMD-10285
Title : Pseudomonas aeruginosa 70s ribosome from a clinical isolate
Authors : Halfon, Y.; Jimenez-Fernande, A.; La Ros, R.; Espinos, R.; Krogh Johansen, H.; Matzov, D.; Eyal, Z.; Bashan, A.; Zimmerman, E.; Belousoff, M.; Molin, S.; Yonath, A.
Deposited on : 2019-09-01
Resolution : 3.34 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

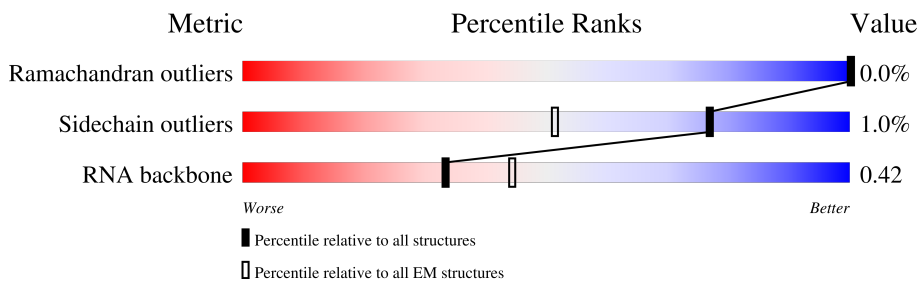
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.34 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	a	1526	
2	b	239	
3	c	205	
4	d	205	
5	e	156	
6	f	105	
7	g	154	
8	h	129	

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Mol	Chain	Length	Quality of chain
9	i	126	60% 98%
10	j	96	68% 96%
11	k	115	21% 100%
12	l	121	18% 98%
13	m	110	68% 96%
14	n	98	44% 100%
15	o	86	15% 100%
16	p	78	10% 100%
17	q	76	16% 96%
18	r	71	34% 97%
19	s	80	72% 99%
20	t	85	7% 99%
21	u	63	63% 97%
22	A	2888	6% 67% 30%
23	B	117	6% 74% 24%
24	C	271	7% 100%
25	D	207	10% 98%
26	E	199	35% 99%
27	F	174	21% 99%
28	G	173	94% 100%
29	H	78	99% 100%
30	I	140	5% 99%
31	J	141	22% 99%
32	K	120	10% 99%
33	L	143	99%

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Mol	Chain	Length	Quality of chain
34	M	135	10% 100%
35	N	118	• 100%
36	O	115	15% 100%
37	P	113	17% 100%
38	Q	117	• 100%
39	R	102	9% 98%
40	S	109	8% 100%
41	T	92	10% 100%
42	U	103	18% 99%
43	V	188	28% 99%
44	W	76	7% 97%
45	X	77	12% 97%
46	Y	60	10% 100%
47	Z	57	9% 100%
48	1	31	65% 100%
49	2	53	9% 100%
50	3	50	28% 100%
51	4	44	5% 98%
52	5	63	• 100%
53	6	38	5% 100%

2 Entry composition [i](#)

There are 54 unique types of molecules in this entry. The entry contains 141963 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1526	32744	14606	6011	10602	1525	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	72	A	G	conflict	GB 1353913695

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	234	1822	1145	329	338	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	205	1627	1028	307	287	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	205	1603	991	311	296	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	156	1145	720	209	210	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	105	Total	C	N	O	S	0	0
			853	531	158	159	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	154	Total	C	N	O	S	0	0
			1190	747	227	211	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			982	618	173	185	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	126	Total	C	N	O	S	0	0
			994	616	198	179	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	96	Total	C	N	O	S	0	0
			765	479	143	142	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	115	Total	C	N	O	S	0	0
			838	517	163	156	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	121	Total	C	N	O	S	0	0
			949	582	196	167	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	110	859	524	174	157	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	n	98	778	479	163	133	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	o	86	686	425	134	126	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	p	78	610	381	121	108	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	q	76	619	387	120	110	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	r	71	556	355	103	97	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	9	ARG	LYS	conflict	UNP A0A2V3DLV3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	80	Total	C	N	O	S	0	0
			635	405	121	106	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			655	404	135	114	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	62	Total	C	N	O	S	0	0
			519	320	112	86	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	28	ALA	VAL	conflict	UNP A0A069QC99

- Molecule 22 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A	2883	Total	C	N	O	P	0	0
			61859	27600	11347	20030	2882		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	361	A	G	conflict	REF 470469287
A	2872	G	U	conflict	REF 470469287

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	117	Total	C	N	O	P	0	0
			2495	1114	448	816	117		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C	271	Total	C	N	O	S	0	0
			2048	1258	422	362	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	D	207	Total	C	N	O	S	0	0
			1549	960	297	287	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	E	199	Total	C	N	O	S	0	0
			1509	948	281	278	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	174	Total	C	N	O	S	0	0
			1288	811	228	246	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	7	LEU	ILE	conflict	UNP A0A072ZMU2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	173	Total	C	N	O	S	0	0
			1294	815	238	239	2		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	H	78	Total	C	N	O	0	0
			577	363	104	110		

- Molecule 30 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	I	140	1026	642	183	198	3	0	0

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	J	141	1122	713	205	201	3	0	0

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	K	120	922	576	178	162	6	0	0

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	L	143	1055	648	213	192	2	0	0

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	M	135	1069	679	209	178	3	0	0

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	N	118	945	590	190	160	5	0	0

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	O	115	881	544	174	161	2	0	0

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	P	113	891	563	168	159	1	0	0

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Q	117	936	592	196	148		0	0

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	R	102	801	509	154	136	2	0	0

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	S	109	825	510	160	152	3	0	0

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	T	92	701	449	124	128		0	0

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	U	103	801	503	152	144	2	0	0

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	V	188	1397	888	254	253	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	6	VAL	LEU	conflict	UNP A0A072ZBM5
V	71	VAL	ALA	conflict	UNP A0A072ZBM5

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	W	76	574	365	110	99	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	40	LEU	GLN	conflict	UNP A0A071LFT4

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	X	77	626	389	134	101	2	0	0

- Molecule 46 is a protein called Ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Y	60	468	286	96	85	1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Z	57	445	277	87	79	2	0	0

- Molecule 48 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	1	31	232	144	40	45	3	0	0

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	2	53	Total	C	N	O	S	0	0
			423	254	90	78	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	3	50	Total	C	N	O	0	0
			418	267	77	74		

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	44	Total	C	N	O	S	1	0
			376	228	91	55	2		

- Molecule 52 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	5	63	Total	C	N	O	S	0	0
			506	314	108	81	3		

- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	6	38	Total	C	N	O	S	0	0
			303	184	69	46	4		

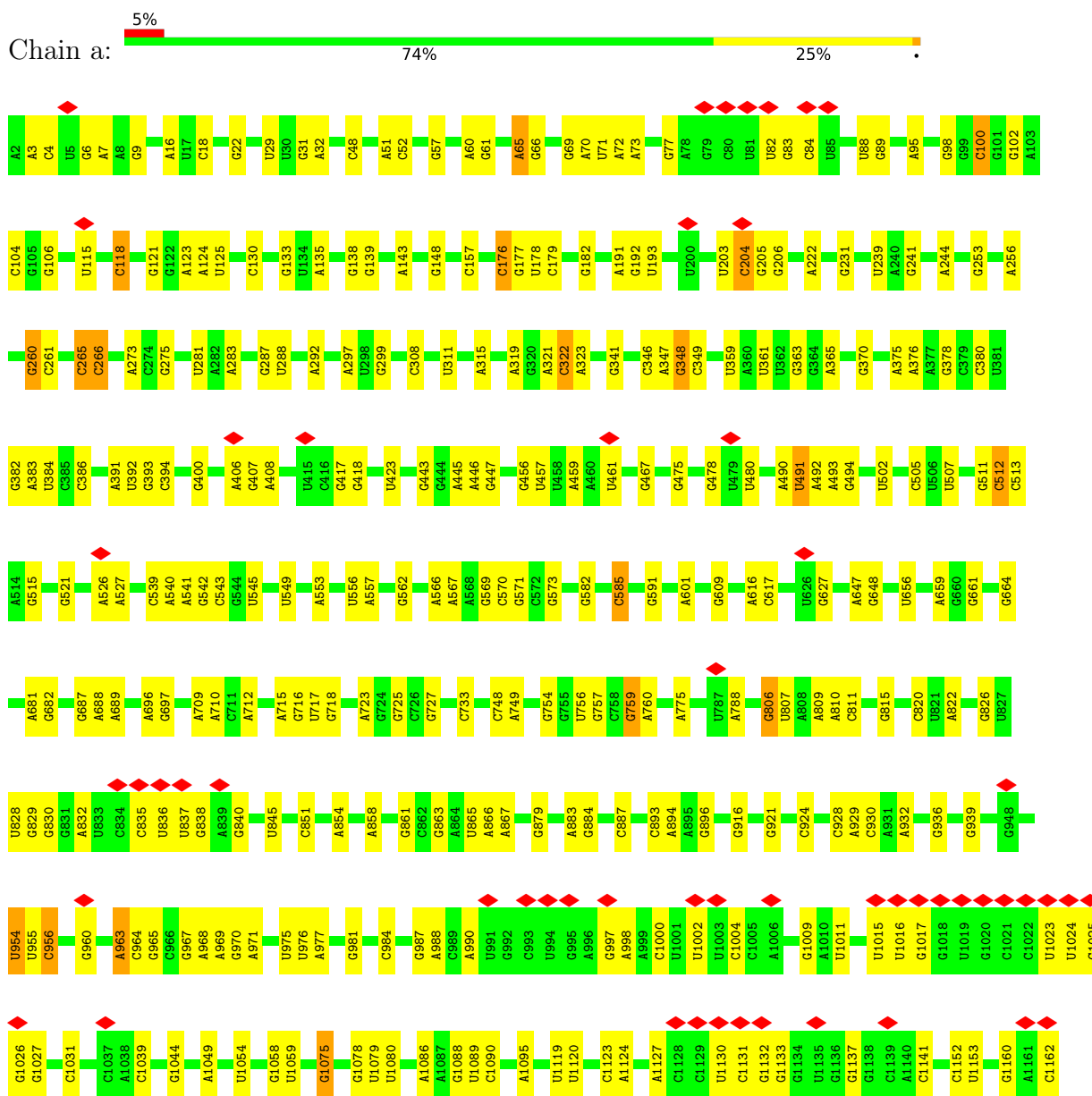
- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

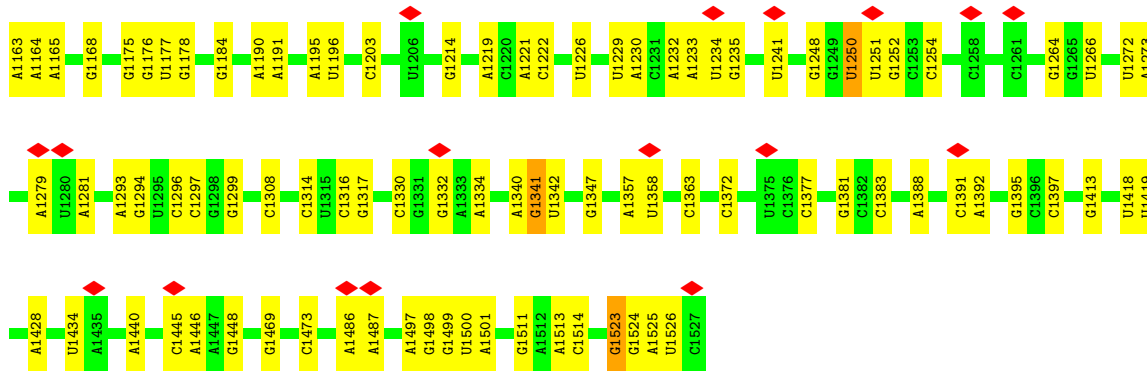
Mol	Chain	Residues	Atoms		AltConf
54	a	17	Total	Mg	0
			17	17	
54	A	152	Total	Mg	0
			152	152	
54	B	1	Total	Mg	0
			1	1	
54	D	1	Total	Mg	0
			1	1	
54	P	1	Total	Mg	0
			1	1	

3 Residue-property plots

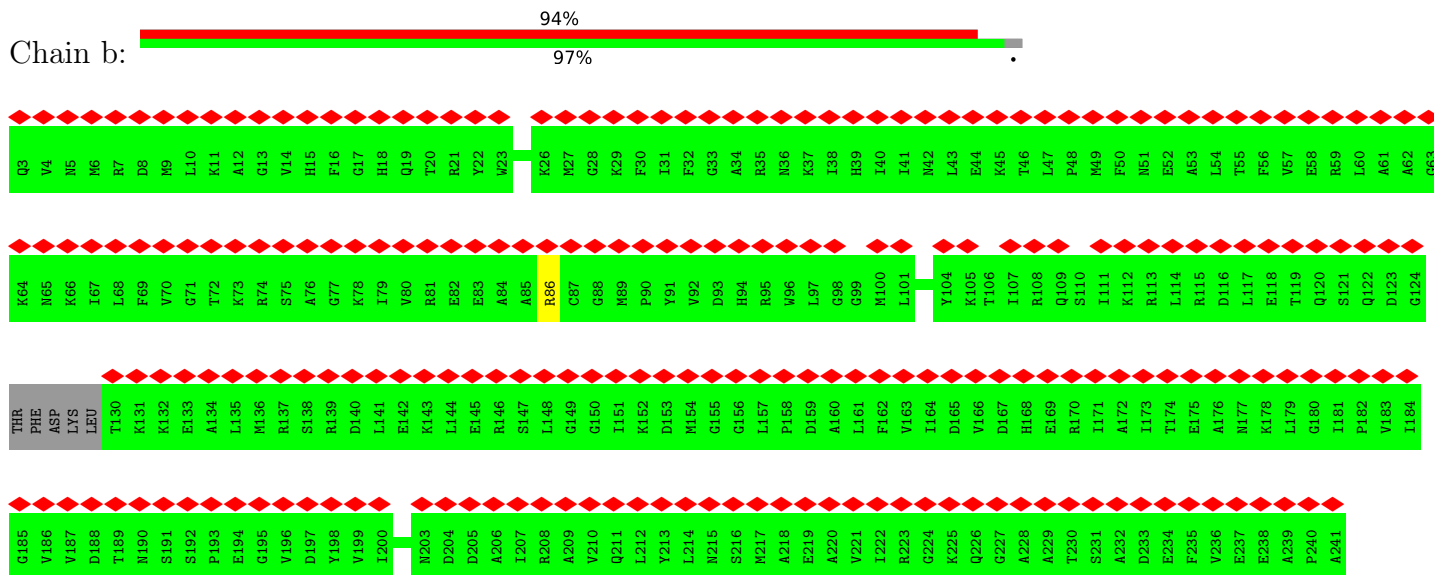
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S ribosomal RNA

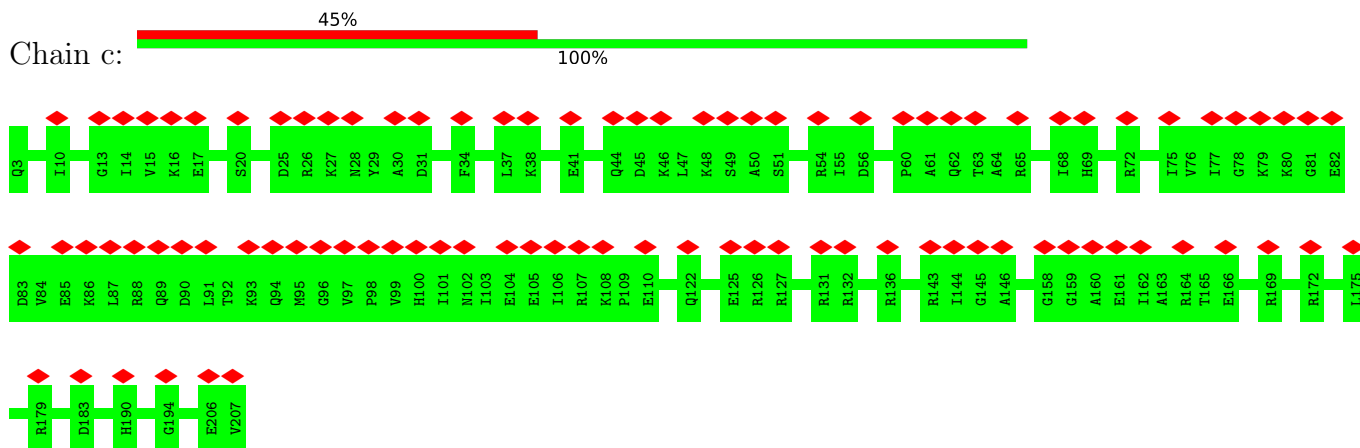




• Molecule 2: 30S ribosomal protein S2

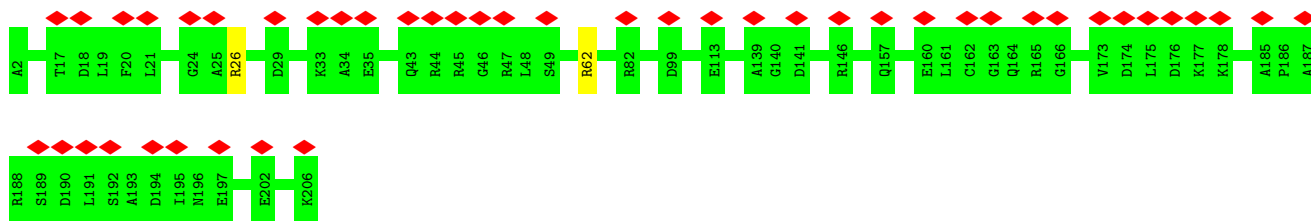


• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

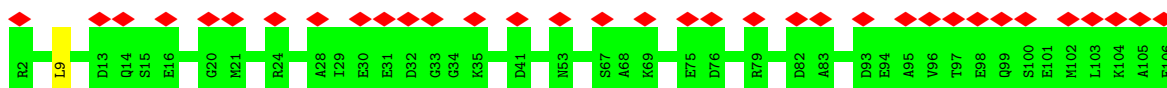




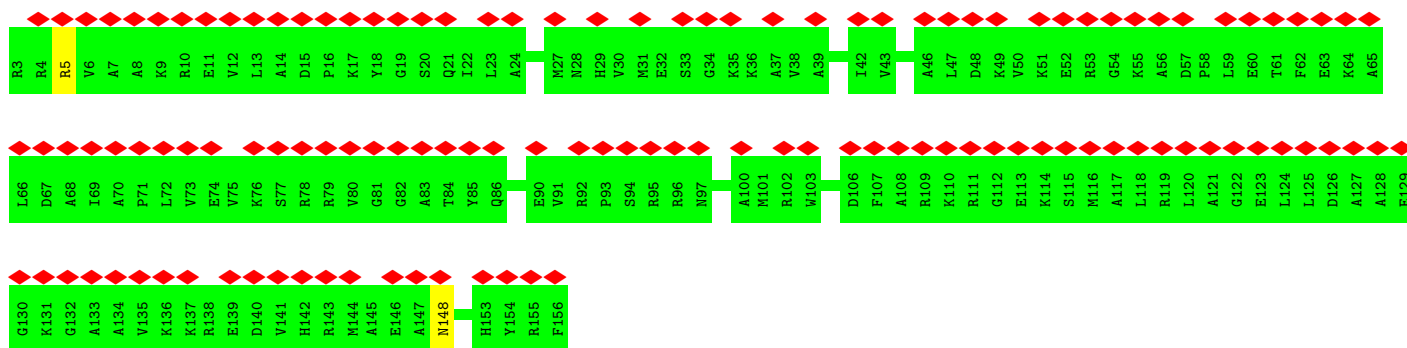
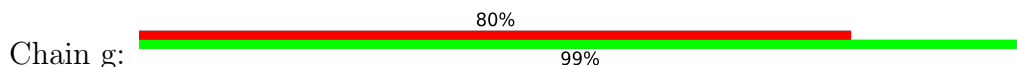
- Molecule 5: 30S ribosomal protein S5



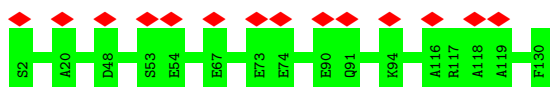
- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7

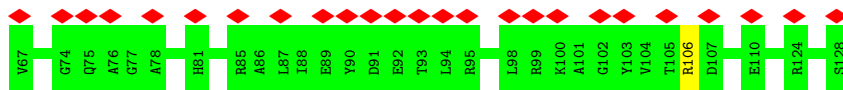
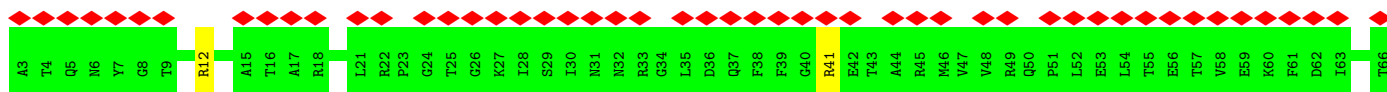


- Molecule 8: 30S ribosomal protein S8

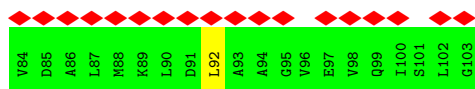
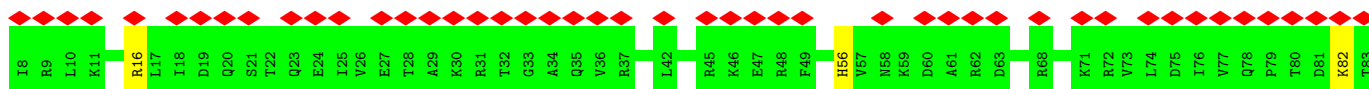
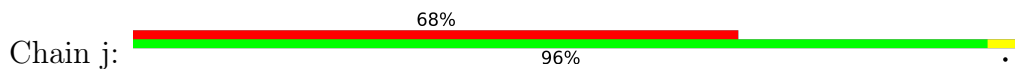


- Molecule 9: 30S ribosomal protein S9

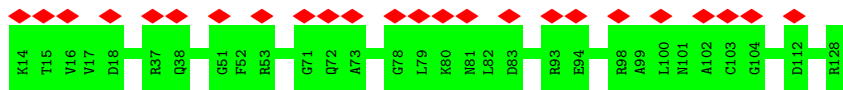




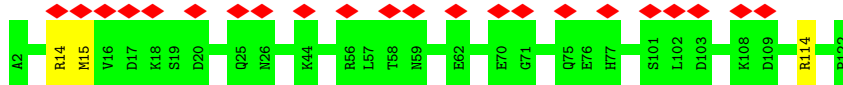
- Molecule 10: 30S ribosomal protein S10



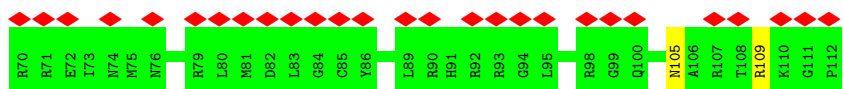
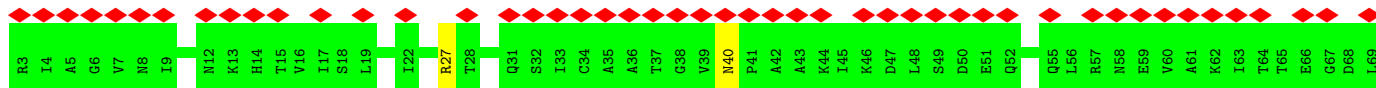
- Molecule 11: 30S ribosomal protein S11



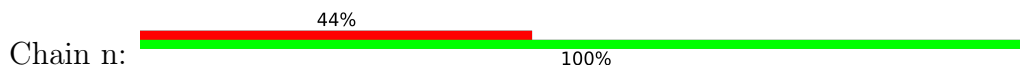
- Molecule 12: 30S ribosomal protein S12

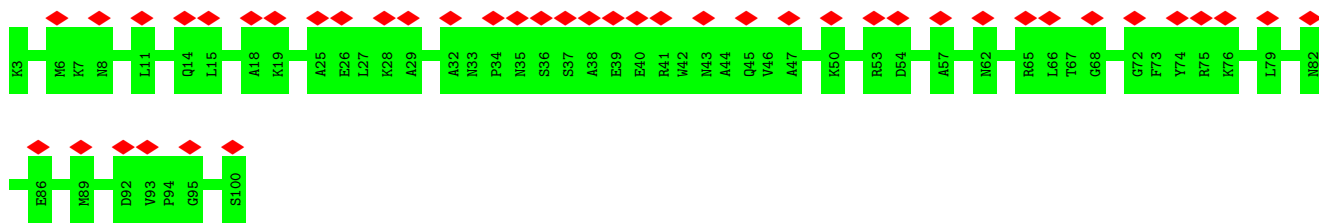


- Molecule 13: 30S ribosomal protein S13

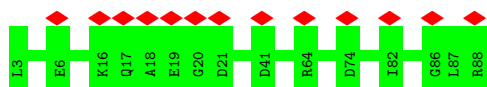


- Molecule 14: 30S ribosomal protein S14

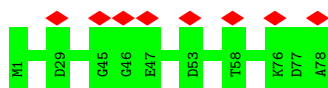




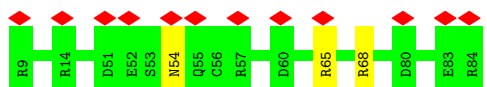
- Molecule 15: 30S ribosomal protein S15



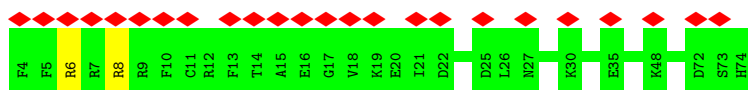
- Molecule 16: 30S ribosomal protein S16



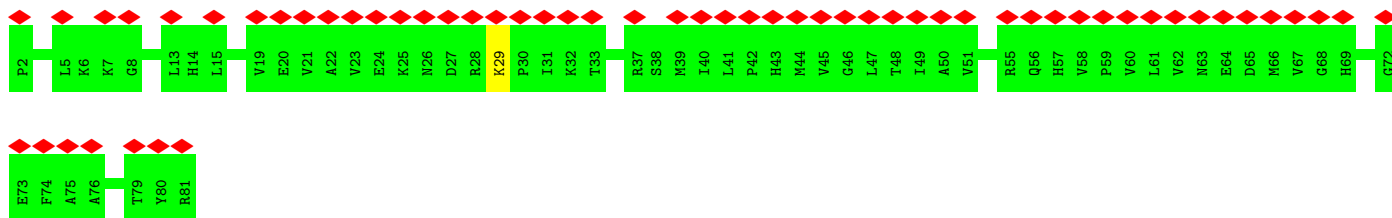
- Molecule 17: 30S ribosomal protein S17



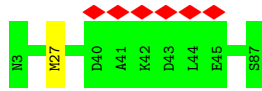
- Molecule 18: 30S ribosomal protein S18



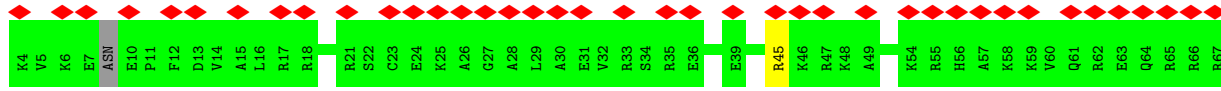
- Molecule 19: 30S ribosomal protein S19



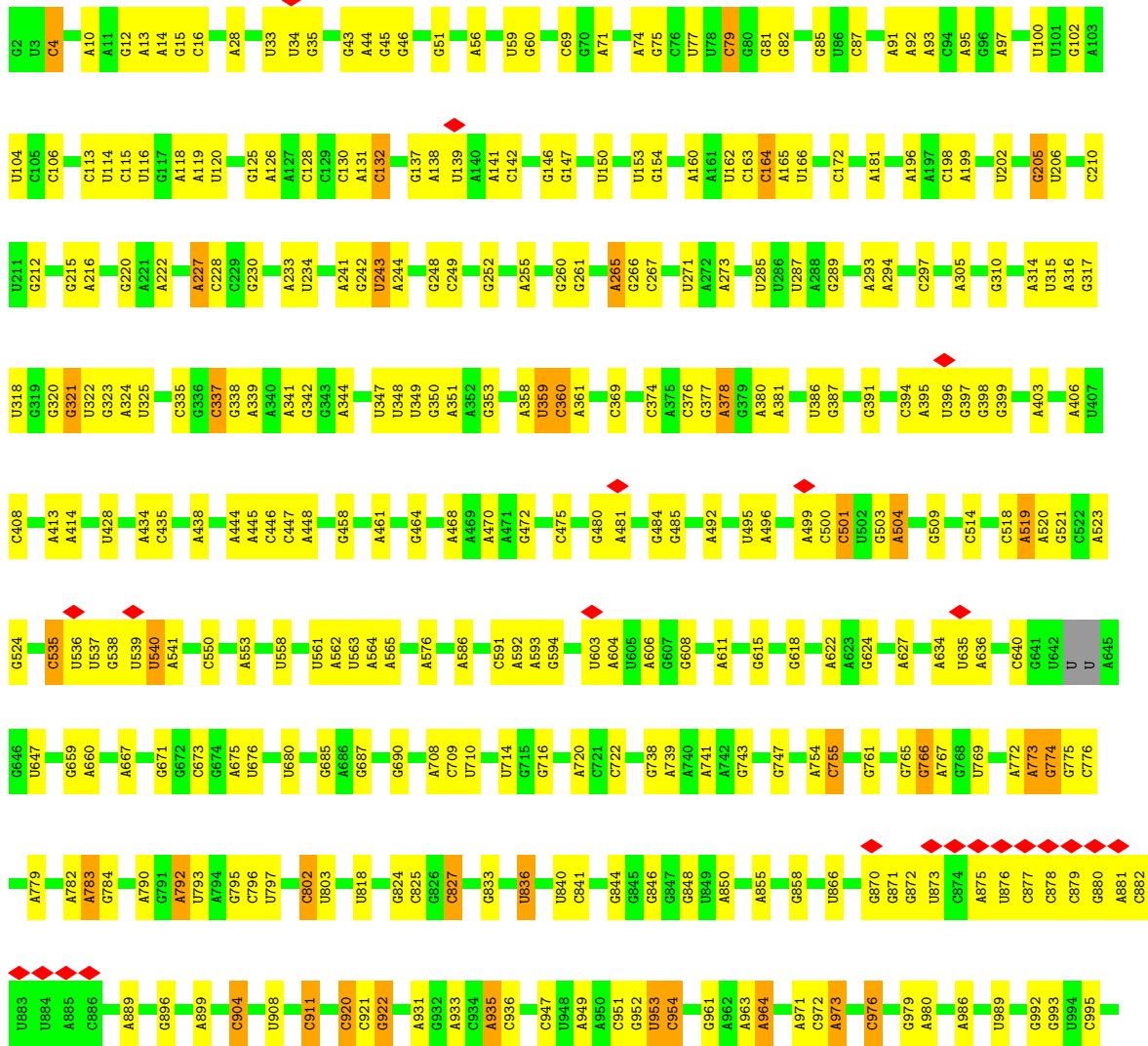
- Molecule 20: 30S ribosomal protein S20

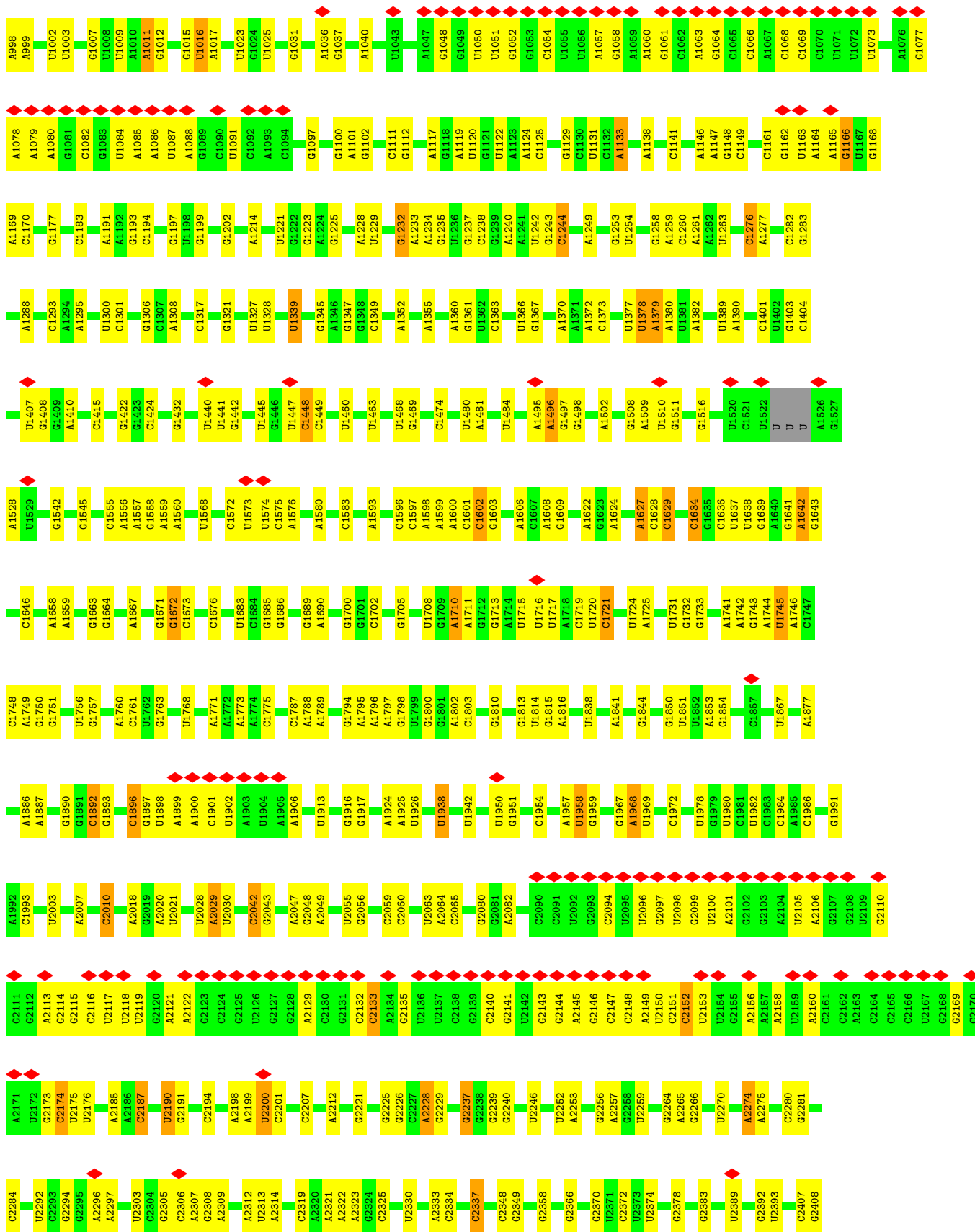


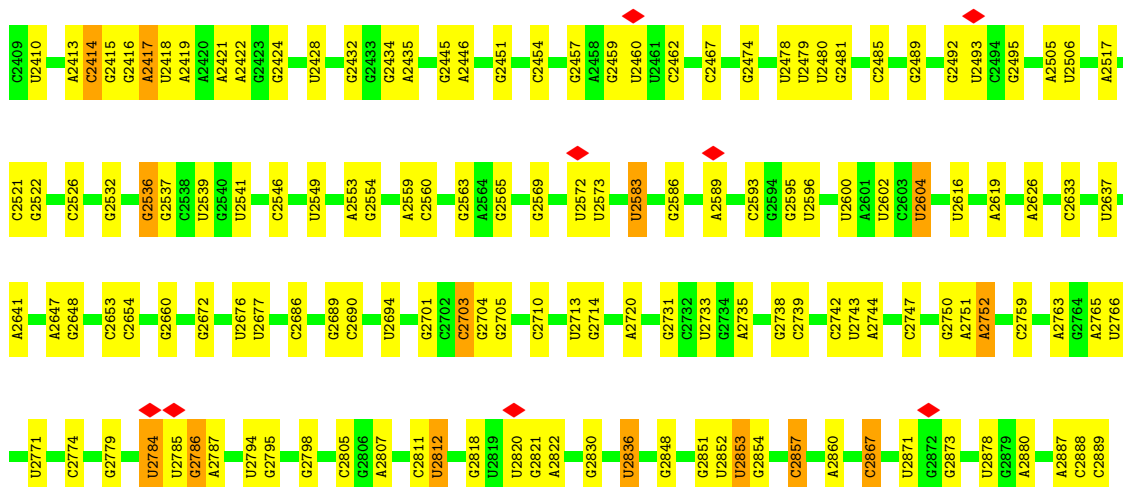
- Molecule 21: 30S ribosomal protein S21



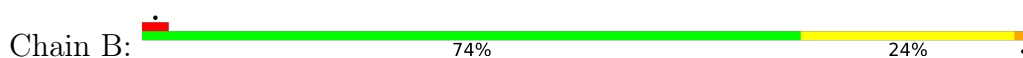
- Molecule 22: 23S ribosomal RNA



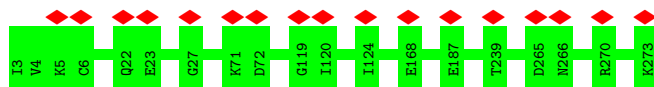




- Molecule 23: 5S ribosomal RNA



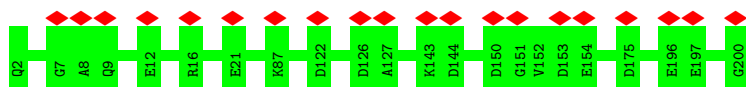
- Molecule 24: 50S ribosomal protein L2



- Molecule 25: 50S ribosomal protein L3

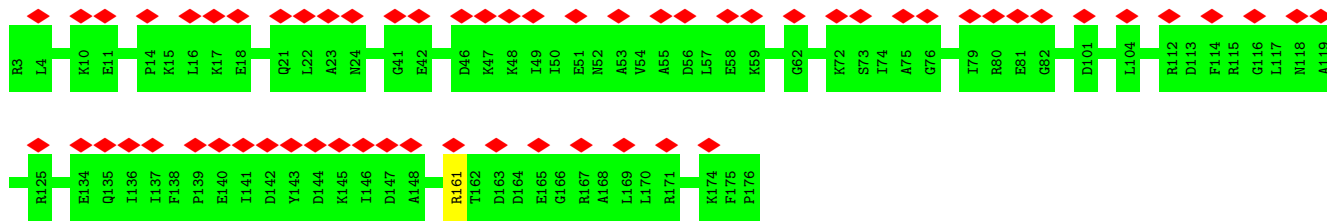


- Molecule 26: 50S ribosomal protein L4

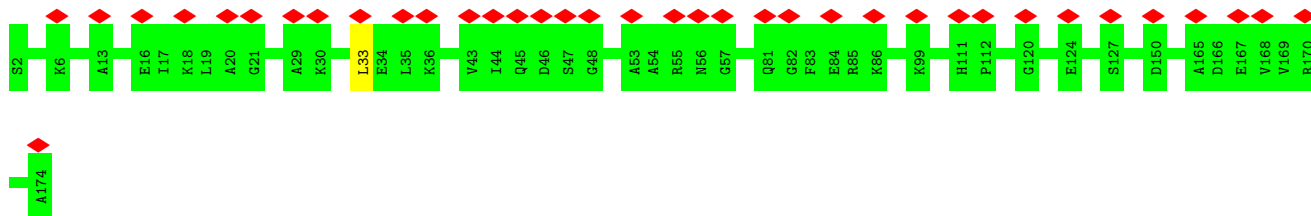


- Molecule 27: 50S ribosomal protein L5

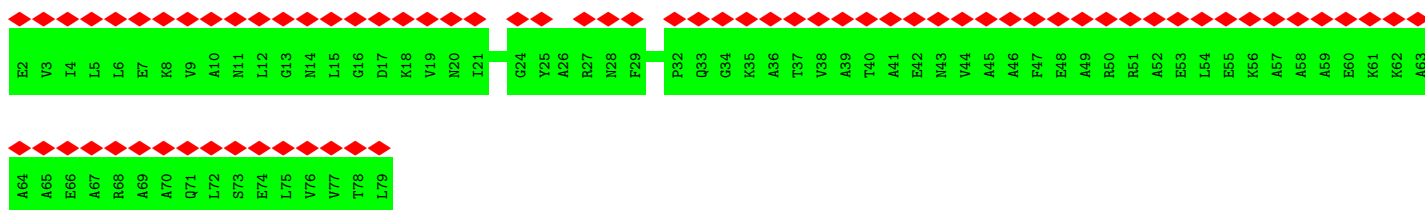




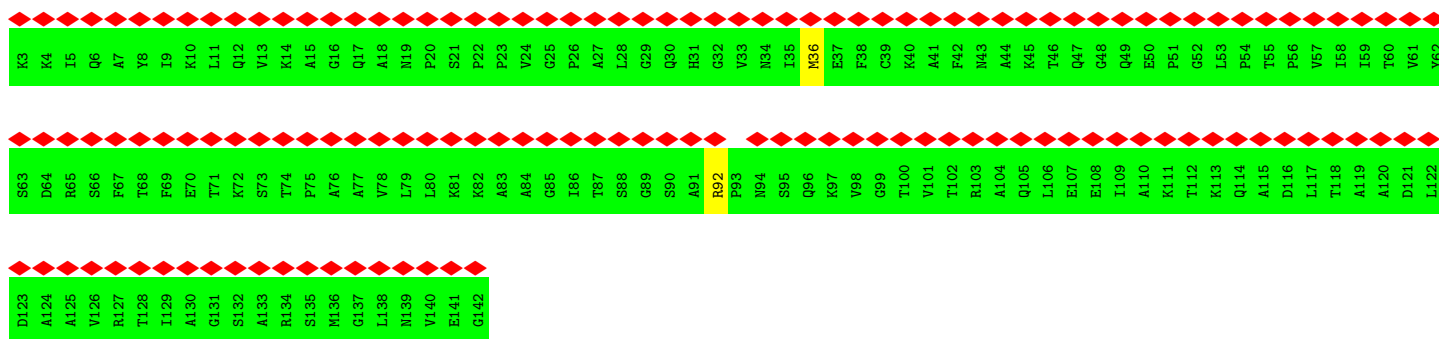
• Molecule 28: 50S ribosomal protein L6



• Molecule 29: 50S ribosomal protein L9

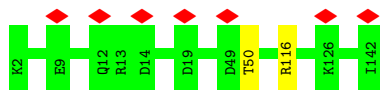


• Molecule 30: 50S ribosomal protein L11



• Molecule 31: 50S ribosomal protein L13

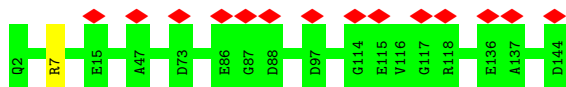




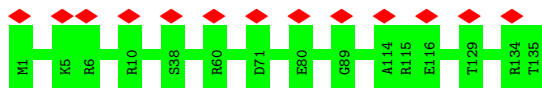
- Molecule 32: 50S ribosomal protein L14



- Molecule 33: 50S ribosomal protein L15



- Molecule 34: 50S ribosomal protein L16



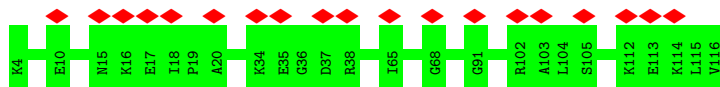
- Molecule 35: 50S ribosomal protein L17



- Molecule 36: 50S ribosomal protein L18

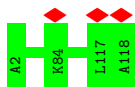


- Molecule 37: 50S ribosomal protein L19



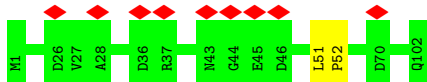
- Molecule 38: 50S ribosomal protein L20

Chain Q:  100%



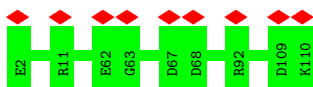
- Molecule 39: 50S ribosomal protein L21

Chain R:  9%  98%



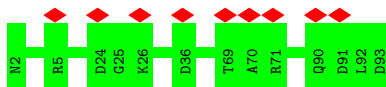
- Molecule 40: 50S ribosomal protein L22

Chain S:  8%  100%



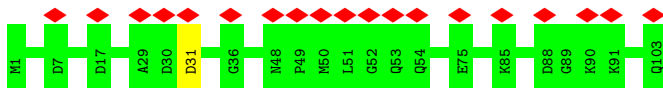
- Molecule 41: 50S ribosomal protein L23

Chain T:  10%  100%



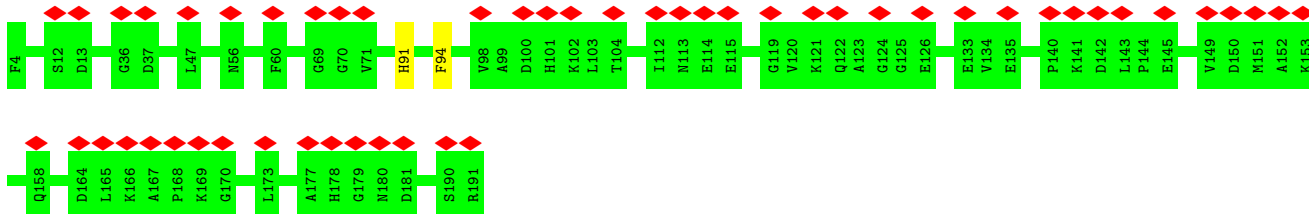
- Molecule 42: 50S ribosomal protein L24

Chain U:  18%  99%



- Molecule 43: 50S ribosomal protein L25

Chain V:  28%  99%

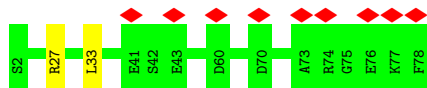


- Molecule 44: 50S ribosomal protein L27

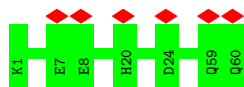
Chain W:  7%  97%



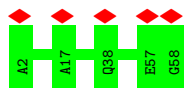
- Molecule 45: 50S ribosomal protein L28



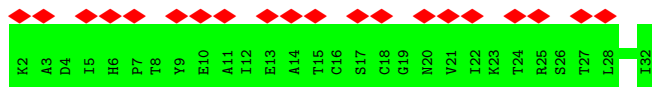
- Molecule 46: Ribosomal protein uL29



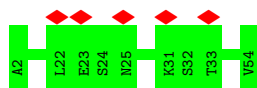
- Molecule 47: 50S ribosomal protein L30



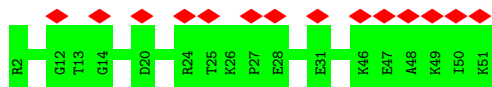
- Molecule 48: 50S ribosomal protein L31



- Molecule 49: 50S ribosomal protein L32

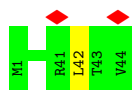


- Molecule 50: 50S ribosomal protein L33



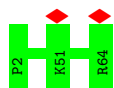
- Molecule 51: 50S ribosomal protein L34

Chain 4:  5% 98%



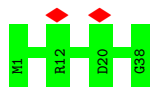
- Molecule 52: 50S ribosomal protein L35

Chain 5:  5% 100%



- Molecule 53: 50S ribosomal protein L36

Chain 6:  5% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	128795	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 ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.474	Depositor
Minimum map value	-0.214	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.0731	Depositor
Map size (\AA)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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: MG

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	0.86	0/36667	1.01	109/57202 (0.2%)
2	b	0.30	0/1850	0.53	0/2486
3	c	0.36	0/1656	0.58	0/2232
4	d	0.40	0/1622	0.55	0/2171
5	e	0.44	0/1159	0.63	0/1559
6	f	0.38	0/867	0.53	0/1167
7	g	0.29	0/1207	0.52	0/1616
8	h	0.42	0/993	0.54	0/1332
9	i	0.37	0/1006	0.57	0/1347
10	j	0.35	0/775	0.58	1/1046 (0.1%)
11	k	0.36	0/854	0.51	0/1159
12	l	0.43	0/963	0.60	0/1292
13	m	0.29	0/867	0.54	0/1165
14	n	0.35	0/788	0.53	0/1048
15	o	0.37	0/693	0.50	0/926
16	p	0.47	0/621	0.57	0/837
17	q	0.44	0/627	0.59	0/844
18	r	0.40	0/566	0.55	0/763
19	s	0.30	0/649	0.54	0/874
20	t	0.35	0/662	0.50	0/881
21	u	0.35	0/524	0.48	0/689
22	A	0.94	3/69275 (0.0%)	1.12	357/108063 (0.3%)
23	B	0.69	0/2789	1.02	7/4345 (0.2%)
24	C	0.39	0/2084	0.58	0/2800
25	D	0.44	0/1572	0.61	0/2118
26	E	0.37	0/1529	0.59	0/2060
27	F	0.30	0/1304	0.58	0/1766
28	G	0.33	0/1311	0.56	0/1767
29	H	0.27	0/580	0.45	0/781
30	I	0.29	0/1041	0.57	0/1408
31	J	0.42	0/1148	0.54	0/1549
32	K	0.38	0/931	0.64	1/1247 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	L	0.36	0/1067	0.62	0/1422
34	M	0.41	0/1089	0.55	0/1456
35	N	0.38	0/960	0.60	0/1282
36	O	0.33	0/888	0.55	0/1183
37	P	0.40	0/900	0.56	0/1203
38	Q	0.45	0/946	0.57	0/1257
39	R	0.36	0/814	0.60	0/1091
40	S	0.35	0/829	0.54	0/1104
41	T	0.39	0/710	0.60	0/953
42	U	0.35	0/809	0.65	1/1079 (0.1%)
43	V	0.35	0/1420	0.61	0/1927
44	W	0.40	0/582	0.68	0/773
45	X	0.36	0/637	0.60	1/849 (0.1%)
46	Y	0.32	0/471	0.55	0/630
47	Z	0.36	0/449	0.60	0/602
48	1	0.28	0/235	0.54	0/318
49	2	0.38	0/429	0.59	0/572
50	3	0.35	0/425	0.62	0/566
51	4	0.41	0/379	0.61	0/496
52	5	0.36	0/511	0.65	0/668
53	6	0.38	0/304	0.55	0/399
All	All	0.79	3/154034 (0.0%)	0.97	477/230370 (0.2%)

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
10	j	0	1
25	D	0	1
39	R	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1011	A	N9-C4	-6.33	1.34	1.37
22	A	1133	A	N9-C4	-5.72	1.34	1.37
22	A	519	A	N9-C4	-5.59	1.34	1.37

All (477) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	359	U	N3-C2-O2	-10.61	114.77	122.20
22	A	359	U	N1-C2-O2	10.16	129.91	122.80
22	A	359	U	C2-N1-C1'	10.01	129.72	117.70
22	A	1448	C	C6-N1-C2	-9.89	116.34	120.30
1	a	104	C	C2-N1-C1'	9.72	129.49	118.80
22	A	113	C	N1-C2-O2	9.64	124.68	118.90
22	A	1407	U	N3-C2-O2	-9.61	115.48	122.20
22	A	1300	U	C2-N1-C1'	9.47	129.07	117.70
22	A	113	C	C2-N1-C1'	9.46	129.21	118.80
22	A	1300	U	N1-C2-O2	9.45	129.41	122.80
22	A	1300	U	N3-C2-O2	-9.42	115.60	122.20
22	A	2742	C	C2-N1-C1'	9.27	128.99	118.80
22	A	1448	C	C5-C6-N1	9.26	125.63	121.00
22	A	1407	U	N1-C2-O2	9.24	129.27	122.80
22	A	2742	C	N1-C2-O2	9.08	124.35	118.90
22	A	1379	A	O5'-P-OP1	-8.90	97.69	105.70
1	a	975	U	N1-C2-O2	8.89	129.02	122.80
1	a	806	G	N3-C4-N9	8.75	131.25	126.00
1	a	975	U	N3-C2-O2	-8.73	116.09	122.20
1	a	203	U	C2-N1-C1'	8.70	128.14	117.70
22	A	2003	U	C2-N1-C1'	8.57	127.98	117.70
1	a	203	U	N1-C2-O2	8.52	128.76	122.80
22	A	2021	U	N3-C2-O2	-8.49	116.26	122.20
1	a	203	U	N3-C2-O2	-8.46	116.28	122.20
22	A	2812	U	C2-N1-C1'	8.39	127.77	117.70
22	A	2259	U	N3-C2-O2	-8.35	116.36	122.20
22	A	2742	C	N3-C2-O2	-8.35	116.06	121.90
1	a	806	G	N3-C4-C5	-8.27	124.47	128.60
22	A	518	C	C2-N1-C1'	8.26	127.89	118.80
22	A	113	C	N3-C2-O2	-8.22	116.14	121.90
22	A	2851	G	N3-C4-C5	-8.21	124.49	128.60
22	A	2021	U	N1-C2-O2	8.21	128.54	122.80
22	A	2583	U	N3-C2-O2	-8.15	116.50	122.20
22	A	1009	U	C2-N1-C1'	8.14	127.47	117.70
22	A	1009	U	N3-C2-O2	-8.09	116.54	122.20
22	A	1054	C	C5-C6-N1	8.08	125.04	121.00
22	A	1407	U	C2-N1-C1'	8.01	127.31	117.70
22	A	1980	U	C2-N1-C1'	7.91	127.19	117.70
22	A	2851	G	N3-C4-N9	7.84	130.70	126.00
22	A	1339	U	N3-C2-O2	-7.80	116.74	122.20
1	a	104	C	C6-N1-C2	-7.75	117.20	120.30
22	A	2583	U	N1-C2-O2	7.66	128.16	122.80
22	A	802	C	C6-N1-C2	-7.59	117.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	2417	A	C2-N3-C4	7.53	114.36	110.60
22	A	1980	U	N1-C2-O2	7.50	128.05	122.80
22	A	1980	U	N3-C2-O2	-7.46	116.97	122.20
22	A	1054	C	C5-C4-N4	-7.46	114.98	120.20
22	A	1761	C	C6-N1-C2	-7.42	117.33	120.30
22	A	535	C	O4'-C1'-N1	7.40	114.12	108.20
22	A	1378	U	OP1-P-O3'	7.38	121.43	105.20
22	A	922	G	C4-N9-C1'	7.37	136.08	126.50
22	A	2407	C	N1-C2-O2	7.36	123.32	118.90
22	A	518	C	N3-C2-O2	-7.32	116.78	121.90
22	A	1958	U	N3-C2-O2	-7.31	117.08	122.20
22	A	2812	U	N1-C2-O2	7.30	127.91	122.80
22	A	1634	C	N1-C2-O2	7.29	123.28	118.90
1	a	266	C	C5-C6-N1	7.23	124.61	121.00
22	A	265	A	O4'-C1'-N9	7.22	113.98	108.20
22	A	1363	C	C6-N1-C2	-7.22	117.41	120.30
22	A	2549	U	N3-C2-O2	-7.21	117.16	122.20
22	A	113	C	C6-N1-C1'	-7.18	112.18	120.80
22	A	1327	U	C2-N1-C1'	7.18	126.32	117.70
22	A	2786	G	C5-C6-O6	-7.18	124.29	128.60
1	a	975	U	C2-N1-C1'	7.15	126.28	117.70
22	A	518	C	N1-C2-O2	7.12	123.17	118.90
22	A	818	U	C2-N1-C1'	7.11	126.23	117.70
22	A	818	U	N1-C2-O2	7.10	127.77	122.80
1	a	104	C	N3-C2-O2	-7.09	116.94	121.90
22	A	836	U	N3-C2-O2	-7.09	117.24	122.20
22	A	2021	U	C2-N1-C1'	7.09	126.20	117.70
1	a	130	C	N3-C2-O2	-7.06	116.95	121.90
1	a	130	C	N1-C2-O2	7.01	123.11	118.90
1	a	266	C	C6-N1-C2	-6.94	117.52	120.30
22	A	1892	C	N1-C2-O2	6.94	123.07	118.90
22	A	2703	C	C6-N1-C2	-6.93	117.53	120.30
22	A	2812	U	N3-C2-O2	-6.92	117.35	122.20
22	A	1339	U	N1-C2-O2	6.91	127.64	122.80
22	A	1009	U	N1-C2-O2	6.91	127.64	122.80
22	A	2549	U	N1-C2-O2	6.91	127.64	122.80
22	A	2003	U	N3-C2-O2	-6.90	117.37	122.20
22	A	2187	C	C6-N1-C2	-6.90	117.54	120.30
22	A	2003	U	N1-C2-O2	6.88	127.62	122.80
1	a	963	A	P-O3'-C3'	6.88	127.96	119.70
22	A	722	C	N1-C2-O2	6.83	123.00	118.90
22	A	2784	U	P-O3'-C3'	6.83	127.90	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1814	U	N3-C2-O2	-6.80	117.44	122.20
22	A	836	U	C2-N1-C1'	6.77	125.82	117.70
1	a	806	G	C2-N3-C4	6.75	115.28	111.90
22	A	2836	U	N3-C2-O2	-6.74	117.48	122.20
1	a	130	C	C6-N1-C2	-6.73	117.61	120.30
22	A	989	U	N3-C2-O2	-6.73	117.49	122.20
22	A	2259	U	N1-C2-O2	6.73	127.51	122.80
22	A	659	G	C4-N9-C1'	6.70	135.21	126.50
22	A	920	C	P-O3'-C3'	6.70	127.73	119.70
22	A	518	C	C6-N1-C2	-6.67	117.63	120.30
22	A	2445	G	O4'-C1'-N9	6.67	113.53	108.20
1	a	987	G	C4-N9-C1'	6.66	135.16	126.50
22	A	836	U	N1-C2-O2	6.64	127.45	122.80
1	a	104	C	N1-C2-O2	6.64	122.89	118.90
22	A	2853	U	P-O3'-C3'	6.63	127.66	119.70
22	A	2867	C	C6-N1-C2	-6.63	117.65	120.30
1	a	1195	A	P-O3'-C3'	6.56	127.58	119.70
1	a	759	G	C6-C5-N7	-6.52	126.49	130.40
1	a	1250	U	N3-C2-O2	-6.50	117.65	122.20
1	a	176	C	N1-C2-O2	6.49	122.79	118.90
22	A	989	U	N1-C2-O2	6.49	127.34	122.80
22	A	2546	C	C6-N1-C2	-6.49	117.71	120.30
22	A	2152	C	N1-C2-O2	6.47	122.78	118.90
22	A	2274	A	P-O3'-C3'	6.46	127.46	119.70
1	a	319	A	C2-N3-C4	6.46	113.83	110.60
1	a	963	A	OP1-P-O3'	6.46	119.40	105.20
22	A	1892	C	C2-N1-C1'	6.45	125.90	118.80
22	A	1596	C	N3-C2-O2	-6.44	117.39	121.90
22	A	2060	C	N1-C2-O2	6.44	122.77	118.90
42	U	31	ASP	CB-CG-OD1	6.41	124.07	118.30
22	A	591	C	C6-N1-C2	-6.40	117.74	120.30
22	A	1073	U	N3-C2-O2	-6.39	117.73	122.20
22	A	1166	G	C4-N9-C1'	6.38	134.79	126.50
22	A	503	G	C4-N9-C1'	-6.38	118.21	126.50
22	A	774	G	P-O3'-C3'	6.37	127.34	119.70
22	A	1349	C	C6-N1-C2	-6.37	117.75	120.30
1	a	1341	G	P-O3'-C3'	6.36	127.34	119.70
22	A	2742	C	C6-N1-C1'	-6.34	113.19	120.80
1	a	383	A	N1-C6-N6	6.33	122.40	118.60
1	a	1308	C	N1-C2-O2	6.32	122.69	118.90
22	A	1745	U	N1-C2-O2	6.31	127.22	122.80
22	A	2252	U	C2-N1-C1'	6.31	125.27	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	227	A	P-O3'-C3'	6.30	127.26	119.70
22	A	922	G	N3-C4-N9	6.30	129.78	126.00
22	A	922	G	C8-N9-C1'	-6.29	118.82	127.00
22	A	2888	C	N1-C2-O2	6.29	122.67	118.90
22	A	1054	C	N3-C4-N4	6.28	122.40	118.00
22	A	640	C	C6-N1-C2	-6.27	117.79	120.30
22	A	2003	U	C6-N1-C1'	-6.26	112.43	121.20
22	A	1161	C	N1-C2-O2	6.25	122.65	118.90
23	B	42	C	N1-C2-O2	6.25	122.65	118.90
1	a	104	C	C6-N1-C1'	-6.24	113.31	120.80
22	A	1622	A	N7-C8-N9	6.24	116.92	113.80
22	A	369	C	C6-N1-C2	-6.24	117.80	120.30
22	A	1958	U	N1-C2-O2	6.24	127.17	122.80
22	A	359	U	C6-N1-C1'	-6.23	112.48	121.20
22	A	1166	G	N3-C4-C5	-6.23	125.49	128.60
22	A	2742	C	C6-N1-C2	-6.22	117.81	120.30
22	A	1282	C	C6-N1-C2	-6.22	117.81	120.30
22	A	1896	C	N1-C2-O2	6.21	122.63	118.90
22	A	1596	C	C2-N1-C1'	6.21	125.63	118.80
22	A	2065	C	C6-N1-C2	-6.21	117.82	120.30
22	A	132	C	N1-C2-O2	6.20	122.62	118.90
22	A	1721	C	C5-C6-N1	6.20	124.10	121.00
22	A	2836	U	N1-C2-O2	6.20	127.14	122.80
1	a	984	C	N1-C2-O2	6.20	122.62	118.90
22	A	321	G	O4'-C1'-N9	6.19	113.15	108.20
22	A	16	C	N1-C2-O2	6.18	122.61	118.90
22	A	1282	C	N1-C2-O2	6.18	122.61	118.90
22	A	2759	C	C6-N1-C2	-6.18	117.83	120.30
22	A	1054	C	C6-N1-C2	-6.17	117.83	120.30
1	a	585	C	N1-C2-O2	6.16	122.60	118.90
22	A	802	C	C5-C6-N1	6.16	124.08	121.00
22	A	2654	C	C6-N1-C2	-6.16	117.84	120.30
22	A	2786	G	N1-C6-O6	6.15	123.59	119.90
22	A	106	C	C6-N1-C2	-6.14	117.84	120.30
22	A	1634	C	N3-C2-O2	-6.14	117.60	121.90
1	a	759	G	C8-N9-C4	-6.11	103.96	106.40
22	A	773	A	C8-N9-C4	-6.11	103.36	105.80
22	A	2445	G	C4-N9-C1'	6.10	134.43	126.50
22	A	1814	U	N1-C2-O2	6.09	127.06	122.80
22	A	1938	U	C2-N1-C1'	6.09	125.00	117.70
22	A	2252	U	N3-C2-O2	-6.09	117.94	122.20
22	A	1972	C	C6-N1-C2	-6.08	117.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	2200	U	P-O3'-C3'	6.08	127.00	119.70
22	A	2187	C	C5-C6-N1	6.08	124.04	121.00
22	A	755	C	N1-C2-O2	6.08	122.55	118.90
22	A	818	U	N3-C2-O2	-6.07	117.95	122.20
22	A	2337	C	N1-C2-O2	6.06	122.54	118.90
22	A	2710	C	C6-N1-C2	-6.06	117.88	120.30
22	A	1131	U	N3-C2-O2	-6.06	117.96	122.20
22	A	1596	C	N1-C2-O2	6.05	122.53	118.90
1	a	4	C	C6-N1-C2	-6.05	117.88	120.30
22	A	2374	U	N3-C2-O2	-6.04	117.97	122.20
22	A	911	C	C5-C6-N1	6.04	124.02	121.00
22	A	971	A	N7-C8-N9	6.04	116.82	113.80
1	a	319	A	N3-C4-C5	-6.01	122.59	126.80
22	A	126	A	C5-N7-C8	-6.01	100.89	103.90
22	A	503	G	C8-N9-C1'	6.01	134.81	127.00
22	A	1011	A	N3-C4-N9	-6.00	122.60	127.40
22	A	2414	C	C5-C6-N1	6.00	124.00	121.00
23	B	42	C	N3-C2-O2	-6.00	117.70	121.90
1	a	370	G	O4'-C1'-N9	5.98	112.98	108.20
22	A	1627	A	P-O3'-C3'	5.98	126.88	119.70
22	A	2653	C	C2-N1-C1'	5.98	125.37	118.80
22	A	872	G	N3-C4-C5	-5.97	125.62	128.60
22	A	1166	G	N3-C4-N9	5.96	129.58	126.00
1	a	1250	U	C2-N1-C1'	5.95	124.84	117.70
22	A	1244	C	C6-N1-C2	-5.95	117.92	120.30
1	a	893	C	P-O3'-C3'	5.93	126.82	119.70
1	a	987	G	N3-C4-N9	5.93	129.56	126.00
22	A	1378	U	P-O3'-C3'	5.93	126.82	119.70
22	A	2060	C	N3-C2-O2	-5.93	117.75	121.90
1	a	759	G	N3-C4-C5	-5.93	125.64	128.60
22	A	872	G	N3-C4-N9	5.92	129.56	126.00
23	B	42	C	C2-N1-C1'	5.91	125.30	118.80
22	A	1301	C	C5-C6-N1	5.91	123.95	121.00
22	A	922	G	N3-C4-C5	-5.90	125.65	128.60
22	A	1761	C	C5-C6-N1	5.90	123.95	121.00
22	A	1300	U	C6-N1-C1'	-5.89	112.96	121.20
22	A	2812	U	C6-N1-C1'	-5.89	112.96	121.20
1	a	954	U	P-O3'-C3'	5.88	126.76	119.70
22	A	802	C	N1-C2-O2	5.87	122.42	118.90
22	A	1016	U	P-O3'-C3'	5.87	126.75	119.70
22	A	1575	C	N1-C2-O2	5.87	122.42	118.90
22	A	1745	U	N3-C2-O2	-5.86	118.10	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	540	U	P-O3'-C3'	5.86	126.73	119.70
22	A	1671	G	N7-C8-N9	5.86	116.03	113.10
22	A	210	C	N1-C2-O2	5.84	122.40	118.90
22	A	2042	C	C2-N1-C1'	5.84	125.22	118.80
22	A	1968	A	N7-C8-N9	5.83	116.72	113.80
1	a	851	C	N1-C2-O2	5.83	122.40	118.90
22	A	1161	C	C2-N1-C1'	5.83	125.22	118.80
1	a	370	G	C8-N9-C4	-5.83	104.07	106.40
22	A	659	G	C8-N9-C1'	-5.83	119.43	127.00
1	a	748	C	C2-N1-C1'	5.82	125.21	118.80
22	A	722	C	N3-C2-O2	-5.81	117.83	121.90
1	a	65	A	C2-N3-C4	5.81	113.51	110.60
1	a	976	U	N3-C2-O2	-5.81	118.13	122.20
1	a	987	G	C8-N9-C1'	-5.81	119.44	127.00
22	A	2851	G	C4-N9-C1'	5.81	134.06	126.50
22	A	973	A	O4'-C1'-N9	5.81	112.85	108.20
1	a	617	C	C6-N1-C2	-5.81	117.98	120.30
22	A	1073	U	N1-C2-O2	5.81	126.86	122.80
22	A	2407	C	N3-C2-O2	-5.81	117.84	121.90
22	A	2374	U	C2-N1-C1'	5.80	124.67	117.70
22	A	1254	U	N3-C2-O2	-5.80	118.14	122.20
22	A	16	C	N3-C2-O2	-5.79	117.85	121.90
1	a	265	C	OP1-P-O3'	5.78	117.90	105.20
1	a	347	A	O4'-C1'-N9	5.77	112.82	108.20
22	A	2257	A	O4'-C1'-N9	5.77	112.82	108.20
22	A	2851	G	C2-N3-C4	5.77	114.79	111.90
1	a	806	G	C5-C6-N1	5.77	114.38	111.50
1	a	1250	U	N1-C2-O2	5.76	126.83	122.80
22	A	973	A	N7-C8-N9	5.76	116.68	113.80
22	A	503	G	O4'-C1'-N9	5.76	112.81	108.20
22	A	783	A	P-O3'-C3'	5.76	126.61	119.70
1	a	924	C	C6-N1-C2	-5.75	118.00	120.30
22	A	776	C	N1-C2-O2	5.75	122.35	118.90
22	A	935	A	O4'-C1'-N9	5.74	112.79	108.20
22	A	792	A	P-O3'-C3'	5.74	126.59	119.70
22	A	2526	C	N1-C2-O2	5.74	122.34	118.90
22	A	2532	G	N3-C4-C5	-5.74	125.73	128.60
22	A	1646	C	C5-C6-N1	5.73	123.87	121.00
22	A	2042	C	N1-C2-O2	5.73	122.34	118.90
22	A	2445	G	N7-C8-N9	5.73	115.97	113.10
22	A	1183	C	C6-N1-C2	-5.73	118.01	120.30
22	A	1775	C	C6-N1-C2	-5.71	118.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	100	C	C6-N1-C2	-5.70	118.02	120.30
22	A	2653	C	N3-C2-O2	-5.68	117.92	121.90
22	A	1448	C	P-O3'-C3'	5.68	126.52	119.70
1	a	319	A	C4-N9-C1'	5.68	136.52	126.30
22	A	1602	C	C6-N1-C2	-5.68	118.03	120.30
22	A	1601	C	N1-C2-O2	5.67	122.31	118.90
22	A	2653	C	C6-N1-C2	-5.67	118.03	120.30
22	A	773	A	C5-N7-C8	-5.67	101.07	103.90
22	A	2252	U	N1-C2-O2	5.66	126.77	122.80
22	A	1761	C	N3-C2-O2	-5.66	117.94	121.90
22	A	773	A	N7-C8-N9	5.66	116.63	113.80
22	A	971	A	O4'-C1'-N9	5.65	112.72	108.20
22	A	1282	C	N3-C2-O2	-5.65	117.94	121.90
22	A	769	U	C5-C6-N1	5.65	125.52	122.70
1	a	322	C	P-O3'-C3'	5.64	126.47	119.70
22	A	1232	G	P-O3'-C3'	5.64	126.47	119.70
22	A	1131	U	N1-C2-O2	5.64	126.75	122.80
22	A	1301	C	C6-N1-C2	-5.63	118.05	120.30
22	A	79	C	N1-C2-O2	5.63	122.28	118.90
22	A	797	U	N3-C2-O2	-5.62	118.26	122.20
22	A	995	C	N1-C2-O2	5.62	122.28	118.90
22	A	164	C	N1-C2-O2	5.62	122.27	118.90
22	A	2042	C	N3-C2-O2	-5.62	117.97	121.90
22	A	4	C	C5-C6-N1	5.61	123.81	121.00
1	a	512	C	P-O3'-C3'	5.61	126.43	119.70
22	A	1761	C	C2-N1-C1'	5.60	124.96	118.80
1	a	319	A	N3-C4-N9	5.60	131.88	127.40
22	A	1672	G	P-O3'-C3'	5.59	126.41	119.70
1	a	976	U	P-O3'-C3'	5.59	126.41	119.70
1	a	837	U	C2-N1-C1'	5.59	124.41	117.70
1	a	349	C	C6-N1-C2	-5.59	118.07	120.30
22	A	954	C	C6-N1-C2	-5.58	118.07	120.30
22	A	2174	C	C5-C6-N1	5.58	123.79	121.00
1	a	1233	A	P-O3'-C3'	5.57	126.39	119.70
22	A	1407	U	C6-N1-C2	-5.57	117.66	121.00
22	A	2857	C	C6-N1-C2	-5.57	118.07	120.30
22	A	2786	G	C6-C5-N7	-5.56	127.06	130.40
22	A	911	C	C6-N1-C2	-5.55	118.08	120.30
22	A	1232	G	C8-N9-C4	-5.55	104.18	106.40
22	A	126	A	O4'-C1'-N9	5.55	112.64	108.20
22	A	1676	C	N1-C2-O2	5.55	122.23	118.90
1	a	1377	C	N1-C2-O2	5.54	122.22	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1708	U	N3-C2-O2	-5.54	118.33	122.20
22	A	2096	U	N1-C2-O2	5.53	126.67	122.80
22	A	2786	G	N3-C4-N9	5.53	129.32	126.00
22	A	2460	U	N3-C2-O2	-5.53	118.33	122.20
22	A	514	C	C6-N1-C2	-5.52	118.09	120.30
1	a	18	C	C6-N1-C2	-5.51	118.09	120.30
1	a	1024	U	C2-N1-C1'	5.50	124.30	117.70
22	A	2888	C	N3-C2-O2	-5.50	118.05	121.90
1	a	348	G	C4-N9-C1'	5.49	133.64	126.50
1	a	956	C	C6-N1-C2	-5.48	118.11	120.30
1	a	204	C	C2-N1-C1'	5.48	124.83	118.80
22	A	202	U	C2-N1-C1'	5.48	124.28	117.70
22	A	1659	A	C4-N9-C1'	5.48	136.16	126.30
22	A	904	C	C6-N1-C2	-5.47	118.11	120.30
22	A	116	U	N3-C2-O2	-5.46	118.38	122.20
22	A	1913	U	C2-N1-C1'	5.46	124.25	117.70
22	A	2546	C	C5-C6-N1	5.46	123.73	121.00
22	A	1463	U	N3-C2-O2	-5.46	118.38	122.20
1	a	617	C	C5-C6-N1	5.45	123.73	121.00
1	a	311	U	N3-C2-O2	-5.45	118.39	122.20
1	a	829	G	O4'-C1'-N9	5.45	112.56	108.20
1	a	359	U	C2-N1-C1'	5.45	124.23	117.70
22	A	16	C	C6-N1-C2	-5.44	118.12	120.30
1	a	203	U	C6-N1-C1'	-5.44	113.58	121.20
22	A	933	A	O4'-C1'-N9	5.43	112.55	108.20
22	A	2259	U	C2-N1-C1'	5.43	124.22	117.70
22	A	2759	C	C5-C6-N1	5.43	123.72	121.00
22	A	1468	U	C2-N1-C1'	5.43	124.21	117.70
22	A	504	A	O5'-P-OP2	-5.43	100.81	105.70
22	A	1629	C	N3-C2-O2	-5.43	118.10	121.90
1	a	467	G	O4'-C1'-N9	5.42	112.54	108.20
22	A	360	C	P-O3'-C3'	5.42	126.21	119.70
22	A	1448	C	N1-C2-O2	5.41	122.15	118.90
1	a	265	C	P-O3'-C3'	5.41	126.19	119.70
22	A	1232	G	N7-C8-N9	5.41	115.80	113.10
22	A	243	U	P-O3'-C3'	5.39	126.17	119.70
22	A	872	G	C4-N9-C1'	5.39	133.51	126.50
22	A	1642	A	P-O3'-C3'	5.39	126.17	119.70
22	A	2337	C	N3-C2-O2	-5.39	118.13	121.90
1	a	1308	C	N3-C2-O2	-5.38	118.13	121.90
22	A	2747	C	N1-C2-O2	5.38	122.13	118.90
22	A	1339	U	C2-N1-C1'	5.37	124.15	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	66	A	P-O3'-C3'	5.37	126.15	119.70
1	a	1316	C	C2-N1-C1'	5.37	124.70	118.80
22	A	1708	U	N1-C2-O2	5.37	126.56	122.80
22	A	1892	C	N3-C2-O2	-5.37	118.14	121.90
22	A	518	C	C6-N1-C1'	-5.36	114.36	120.80
22	A	130	C	C6-N1-C2	-5.36	118.16	120.30
22	A	359	U	C6-N1-C2	-5.36	117.78	121.00
22	A	1300	U	C5-C6-N1	5.36	125.38	122.70
22	A	1601	C	N3-C2-O2	-5.36	118.15	121.90
22	A	1232	G	C4-C5-N7	5.36	112.94	110.80
22	A	2686	C	C5-C6-N1	5.36	123.68	121.00
22	A	1710	A	C8-N9-C4	-5.36	103.66	105.80
22	A	2100	U	C2-N1-C1'	5.36	124.13	117.70
22	A	1671	G	C5-N7-C8	-5.35	101.62	104.30
22	A	1111	C	N1-C2-O2	5.35	122.11	118.90
22	A	1407	U	C5-C6-N1	5.35	125.38	122.70
22	A	818	U	C6-N1-C1'	-5.35	113.71	121.20
22	A	1496	A	P-O3'-C3'	5.35	126.11	119.70
1	a	585	C	C6-N1-C2	-5.34	118.16	120.30
22	A	2604	U	N3-C2-O2	-5.34	118.46	122.20
1	a	176	C	C2-N1-C1'	5.34	124.67	118.80
22	A	369	C	C5-C6-N1	5.34	123.67	121.00
1	a	102	G	C4-C5-N7	5.33	112.93	110.80
22	A	2096	U	C5-C6-N1	5.33	125.36	122.70
22	A	995	C	N3-C2-O2	-5.33	118.17	121.90
22	A	1629	C	N1-C2-O2	5.32	122.09	118.90
1	a	1024	U	N1-C2-O2	5.31	126.52	122.80
1	a	1266	U	N1-C2-O2	5.31	126.52	122.80
1	a	1357	A	C4-N9-C1'	5.31	135.86	126.30
22	A	1194	C	N1-C2-O2	5.31	122.09	118.90
22	A	766	G	N1-C6-O6	-5.31	116.72	119.90
1	a	661	G	C4-N9-C1'	5.31	133.40	126.50
22	A	2853	U	OP2-P-O3'	5.31	116.87	105.20
22	A	2774	C	C6-N1-C2	-5.30	118.18	120.30
22	A	1968	A	C8-N9-C4	-5.30	103.68	105.80
22	A	1254	U	N1-C2-O2	5.30	126.51	122.80
22	A	1166	G	C8-N9-C1'	-5.29	120.12	127.00
22	A	1463	U	N1-C2-O2	5.29	126.50	122.80
22	A	2419	A	O4'-C1'-N9	5.28	112.42	108.20
22	A	79	C	N3-C2-O2	-5.28	118.21	121.90
1	a	1523	G	C4-N9-C1'	5.27	133.36	126.50
45	X	33	LEU	CA-CB-CG	5.27	127.43	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	2445	G	C6-C5-N7	-5.27	127.24	130.40
1	a	930	C	N1-C2-O2	5.27	122.06	118.90
22	A	1011	A	C8-N9-C4	-5.27	103.69	105.80
22	A	882	C	C5-C6-N1	5.27	123.63	121.00
1	a	260	G	P-O3'-C3'	5.25	126.00	119.70
22	A	205	G	O4'-C1'-N9	5.25	112.40	108.20
22	A	953	U	C6-N1-C2	-5.25	117.85	121.00
22	A	2583	U	C2-N1-C1'	5.25	124.00	117.70
1	a	987	G	N3-C4-C5	-5.24	125.98	128.60
1	a	1075	G	C4-C5-N7	5.24	112.90	110.80
22	A	2786	G	C4-C5-N7	5.24	112.90	110.80
22	A	1775	C	C5-C6-N1	5.24	123.62	121.00
22	A	2417	A	N3-C4-C5	-5.24	123.13	126.80
1	a	102	G	C4-N9-C1'	5.24	133.31	126.50
22	A	2888	C	C6-N1-C2	-5.24	118.20	120.30
22	A	973	A	C5-N7-C8	-5.24	101.28	103.90
1	a	319	A	N7-C8-N9	5.23	116.42	113.80
22	A	69	C	N1-C2-O2	5.23	122.04	118.90
22	A	2228	A	P-O3'-C3'	5.23	125.98	119.70
22	A	501	C	N1-C2-O2	5.23	122.04	118.90
1	a	104	C	O4'-C1'-N1	5.23	112.38	108.20
22	A	825	C	C6-N1-C2	-5.21	118.22	120.30
22	A	475	C	C5-C6-N1	5.21	123.61	121.00
22	A	2325	C	C6-N1-C2	-5.21	118.22	120.30
1	a	759	G	N3-C4-N9	5.21	129.13	126.00
1	a	491	U	P-O3'-C3'	5.21	125.95	119.70
22	A	1622	A	C5-N7-C8	-5.20	101.30	103.90
22	A	2028	U	N1-C2-O2	5.20	126.44	122.80
1	a	100	C	N1-C2-O2	5.20	122.02	118.90
22	A	2029	A	P-O3'-C3'	5.19	125.93	119.70
22	A	2280	C	N1-C2-O2	5.19	122.02	118.90
22	A	2703	C	C5-C6-N1	5.19	123.59	121.00
22	A	2010	C	C6-N1-C2	-5.18	118.23	120.30
22	A	470	A	OP1-P-O3'	5.18	116.59	105.20
1	a	585	C	C5-C6-N1	5.17	123.58	121.00
22	A	2541	U	C2-N1-C1'	5.16	123.89	117.70
22	A	2174	C	C6-N1-C2	-5.15	118.24	120.30
22	A	1972	C	C5-C6-N1	5.15	123.57	121.00
22	A	12	G	O4'-C1'-N9	5.14	112.31	108.20
22	A	1293	C	C6-N1-C2	-5.13	118.25	120.30
1	a	311	U	N1-C2-O2	5.12	126.39	122.80
22	A	337	C	N1-C2-O2	5.12	121.97	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	2536	G	P-O3'-C3'	5.12	125.85	119.70
1	a	130	C	C2-N1-C1'	5.12	124.43	118.80
22	A	1282	C	C5-C6-N1	5.12	123.56	121.00
1	a	806	G	C4-N9-C1'	5.12	133.16	126.50
22	A	1131	U	C2-N1-C1'	5.12	123.84	117.70
22	A	2237	G	N7-C8-N9	5.12	115.66	113.10
22	A	1676	C	N3-C2-O2	-5.12	118.32	121.90
1	a	806	G	C8-N9-C1'	-5.11	120.35	127.00
22	A	1986	C	C6-N1-C2	-5.11	118.26	120.30
22	A	79	C	C6-N1-C2	-5.11	118.26	120.30
22	A	2654	C	C5-C6-N1	5.11	123.55	121.00
22	A	2485	C	N1-C2-O2	5.11	121.96	118.90
23	B	88	C	C2-N1-C1'	5.11	124.42	118.80
1	a	118	C	C5-C6-N1	5.10	123.55	121.00
22	A	1646	C	C6-N1-C2	-5.09	118.26	120.30
22	A	1009	U	O4'-C1'-N1	5.09	112.28	108.20
23	B	68	C	N1-C2-O2	5.09	121.96	118.90
1	a	104	C	C5-C6-N1	5.09	123.55	121.00
1	a	851	C	N3-C2-O2	-5.09	118.34	121.90
22	A	964	A	N7-C8-N9	5.09	116.34	113.80
22	A	802	C	N3-C2-O2	-5.09	118.34	121.90
22	A	2460	U	N1-C2-O2	5.08	126.36	122.80
22	A	776	C	N3-C2-O2	-5.08	118.34	121.90
22	A	1166	G	C2-N3-C4	5.08	114.44	111.90
22	A	1761	C	N1-C2-O2	5.08	121.95	118.90
22	A	126	A	N7-C8-N9	5.08	116.34	113.80
22	A	2133	C	C2-N1-C1'	5.07	124.38	118.80
10	j	92	LEU	CA-CB-CG	5.07	126.95	115.30
22	A	1622	A	O4'-C1'-N9	5.07	112.25	108.20
23	B	37	C	N1-C2-O2	5.06	121.94	118.90
22	A	1913	U	N1-C2-O2	5.06	126.34	122.80
22	A	1009	U	C6-N1-C1'	-5.06	114.12	121.20
22	A	2190	U	C2-N1-C1'	5.05	123.76	117.70
32	K	9	ASP	CB-CG-OD1	5.05	122.85	118.30
22	A	2237	G	C4-C5-N7	5.05	112.82	110.80
22	A	2752	A	O4'-C1'-N9	5.04	112.23	108.20
22	A	2059	C	C6-N1-C2	-5.04	118.28	120.30
22	A	1896	C	C2-N1-C1'	5.04	124.34	118.80
22	A	1401	C	N1-C2-O2	5.04	121.92	118.90
22	A	1300	U	C6-N1-C2	-5.04	117.98	121.00
22	A	976	C	N1-C2-O2	5.02	121.91	118.90
1	a	956	C	C5-C6-N1	5.02	123.51	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1980	U	C5-C6-N1	5.02	125.21	122.70
22	A	2532	G	C8-N9-C4	-5.02	104.39	106.40
1	a	984	C	N3-C2-O2	-5.02	118.39	121.90
22	A	2274	A	OP1-P-O3'	5.02	116.25	105.20
1	a	319	A	C8-N9-C4	-5.02	103.79	105.80
22	A	378	A	O4'-C1'-N9	5.01	112.21	108.20
22	A	198	C	C6-N1-C2	-5.01	118.30	120.30
22	A	1276	C	N1-C2-O2	5.01	121.91	118.90
1	a	828	U	N3-C2-O2	-5.01	118.69	122.20
22	A	741	A	O4'-C1'-N9	5.00	112.20	108.20
22	A	827	C	C6-N1-C2	-5.00	118.30	120.30
22	A	1671	G	C4-N9-C1'	5.00	133.00	126.50
1	a	102	G	C6-C5-N7	-5.00	127.40	130.40
1	a	1363	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	D	151	THR	Peptide
39	R	51	LEU	Peptide
10	j	56	HIS	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
2	b	230/239 (96%)	211 (92%)	19 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	203/205 (99%)	180 (89%)	23 (11%)	0	100	100
4	d	203/205 (99%)	185 (91%)	18 (9%)	0	100	100
5	e	154/156 (99%)	133 (86%)	21 (14%)	0	100	100
6	f	103/105 (98%)	92 (89%)	11 (11%)	0	100	100
7	g	152/154 (99%)	141 (93%)	11 (7%)	0	100	100
8	h	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
9	i	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
10	j	94/96 (98%)	85 (90%)	9 (10%)	0	100	100
11	k	113/115 (98%)	103 (91%)	10 (9%)	0	100	100
12	l	119/121 (98%)	100 (84%)	19 (16%)	0	100	100
13	m	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
14	n	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
15	o	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
16	p	76/78 (97%)	70 (92%)	6 (8%)	0	100	100
17	q	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
18	r	69/71 (97%)	65 (94%)	4 (6%)	0	100	100
19	s	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
20	t	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
21	u	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
24	C	269/271 (99%)	241 (90%)	28 (10%)	0	100	100
25	D	205/207 (99%)	179 (87%)	25 (12%)	1 (0%)	29	63
26	E	197/199 (99%)	188 (95%)	9 (5%)	0	100	100
27	F	172/174 (99%)	154 (90%)	18 (10%)	0	100	100
28	G	171/173 (99%)	157 (92%)	14 (8%)	0	100	100
29	H	76/78 (97%)	74 (97%)	2 (3%)	0	100	100
30	I	138/140 (99%)	118 (86%)	20 (14%)	0	100	100
31	J	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
32	K	118/120 (98%)	108 (92%)	10 (8%)	0	100	100
33	L	141/143 (99%)	128 (91%)	13 (9%)	0	100	100
34	M	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
35	N	116/118 (98%)	102 (88%)	14 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	O	113/115 (98%)	104 (92%)	9 (8%)	0	100	100
37	P	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
38	Q	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
39	R	100/102 (98%)	89 (89%)	10 (10%)	1 (1%)	15	49
40	S	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
41	T	90/92 (98%)	80 (89%)	10 (11%)	0	100	100
42	U	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
43	V	186/188 (99%)	169 (91%)	17 (9%)	0	100	100
44	W	74/76 (97%)	55 (74%)	19 (26%)	0	100	100
45	X	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
46	Y	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
47	Z	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
48	1	29/31 (94%)	24 (83%)	5 (17%)	0	100	100
49	2	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
50	3	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
51	4	43/44 (98%)	38 (88%)	5 (12%)	0	100	100
52	5	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
53	6	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
All	All	5676/5785 (98%)	5184 (91%)	490 (9%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	R	52	PRO
25	D	152	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	191/197 (97%)	190 (100%)	1 (0%)	88	93
3	c	165/171 (96%)	165 (100%)	0	100	100
4	d	166/173 (96%)	164 (99%)	2 (1%)	71	84
5	e	114/115 (99%)	111 (97%)	3 (3%)	46	73
6	f	88/90 (98%)	87 (99%)	1 (1%)	73	86
7	g	116/120 (97%)	114 (98%)	2 (2%)	60	80
8	h	108/108 (100%)	108 (100%)	0	100	100
9	i	102/102 (100%)	99 (97%)	3 (3%)	42	71
10	j	85/85 (100%)	83 (98%)	2 (2%)	49	75
11	k	84/87 (97%)	84 (100%)	0	100	100
12	l	105/105 (100%)	102 (97%)	3 (3%)	42	71
13	m	92/92 (100%)	88 (96%)	4 (4%)	29	62
14	n	78/80 (98%)	78 (100%)	0	100	100
15	o	73/73 (100%)	73 (100%)	0	100	100
16	p	61/63 (97%)	61 (100%)	0	100	100
17	q	70/70 (100%)	67 (96%)	3 (4%)	29	62
18	r	54/61 (88%)	52 (96%)	2 (4%)	34	64
19	s	69/71 (97%)	68 (99%)	1 (1%)	67	83
20	t	67/68 (98%)	66 (98%)	1 (2%)	65	82
21	u	51/52 (98%)	50 (98%)	1 (2%)	55	78
24	C	206/212 (97%)	206 (100%)	0	100	100
25	D	157/159 (99%)	155 (99%)	2 (1%)	69	83
26	E	155/157 (99%)	155 (100%)	0	100	100
27	F	124/149 (83%)	123 (99%)	1 (1%)	81	90
28	G	133/137 (97%)	132 (99%)	1 (1%)	81	90
29	H	55/55 (100%)	55 (100%)	0	100	100
30	I	108/108 (100%)	106 (98%)	2 (2%)	57	79
31	J	118/118 (100%)	116 (98%)	2 (2%)	60	80
32	K	100/100 (100%)	100 (100%)	0	100	100
33	L	104/105 (99%)	103 (99%)	1 (1%)	76	87
34	M	108/108 (100%)	108 (100%)	0	100	100
35	N	97/97 (100%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	O	86/86 (100%)	86 (100%)	0	100	100
37	P	94/95 (99%)	94 (100%)	0	100	100
38	Q	87/87 (100%)	87 (100%)	0	100	100
39	R	82/86 (95%)	82 (100%)	0	100	100
40	S	86/86 (100%)	86 (100%)	0	100	100
41	T	73/77 (95%)	73 (100%)	0	100	100
42	U	88/88 (100%)	88 (100%)	0	100	100
43	V	144/153 (94%)	142 (99%)	2 (1%)	67	83
44	W	56/56 (100%)	54 (96%)	2 (4%)	35	65
45	X	65/66 (98%)	64 (98%)	1 (2%)	65	82
46	Y	51/53 (96%)	51 (100%)	0	100	100
47	Z	48/48 (100%)	48 (100%)	0	100	100
48	1	27/27 (100%)	27 (100%)	0	100	100
49	2	46/46 (100%)	46 (100%)	0	100	100
50	3	46/46 (100%)	46 (100%)	0	100	100
51	4	38/37 (103%)	37 (97%)	1 (3%)	46	73
52	5	54/54 (100%)	54 (100%)	0	100	100
53	6	33/34 (97%)	33 (100%)	0	100	100
All	All	4608/4713 (98%)	4564 (99%)	44 (1%)	77	87

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	86	ARG
4	d	26	ARG
4	d	62	ARG
5	e	27	LYS
5	e	133	ASN
5	e	158	ARG
6	f	9	LEU
7	g	5	ARG
7	g	148	ASN
9	i	12	ARG
9	i	41	ARG
9	i	106	ARG
10	j	16	ARG

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Mol	Chain	Res	Type
10	j	82	LYS
12	l	14	ARG
12	l	15	MET
12	l	114	ARG
13	m	27	ARG
13	m	40	ASN
13	m	105	ASN
13	m	109	ARG
17	q	54	ASN
17	q	65	ARG
17	q	68	ARG
18	r	6	ARG
18	r	8	ARG
19	s	29	LYS
20	t	27	MET
21	u	45	ARG
25	D	34	ARG
25	D	154	ARG
27	F	161	ARG
28	G	33	LEU
30	I	36	MET
30	I	92	ARG
31	J	50	THR
31	J	116	ARG
33	L	7	ARG
43	V	91	HIS
43	V	94	PHE
44	W	40	LEU
44	W	41	ARG
45	X	27	ARG
51	4	42	LEU

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

Mol	Chain	Res	Type
2	b	24	ASN
3	c	6	HIS
4	d	100	ASN
5	e	123	ASN
5	e	133	ASN
6	f	14	GLN
6	f	81	ASN

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Mol	Chain	Res	Type
11	k	22	HIS
11	k	81	ASN
12	l	72	HIS
13	m	40	ASN
13	m	58	ASN
13	m	91	HIS
13	m	105	ASN
14	n	8	ASN
14	n	45	GLN
15	o	13	ASN
17	q	34	HIS
17	q	54	ASN
19	s	26	ASN
19	s	52	HIS
19	s	53	ASN
20	t	68	HIS
24	C	90	HIS
25	D	33	ASN
26	E	6	ASN
26	E	40	GLN
26	E	61	GLN
26	E	91	HIS
27	F	52	ASN
28	G	23	GLN
28	G	60	GLN
30	I	17	GLN
30	I	19	ASN
31	J	77	HIS
32	K	91	GLN
35	N	22	GLN
37	P	7	GLN
38	Q	44	GLN
39	R	83	HIS
41	T	90	GLN
42	U	44	HIS
43	V	83	HIS
43	V	110	HIS
43	V	178	HIS
44	W	35	ASN
46	Y	20	HIS
51	4	26	ASN

5.3.3 RNA 

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1525/1526 (99%)	365 (23%)	0
22	A	2880/2888 (99%)	824 (28%)	46 (1%)
23	B	116/117 (99%)	25 (21%)	4 (3%)
All	All	4521/4531 (99%)	1214 (26%)	50 (1%)

All (1214) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	3	A
1	a	6	G
1	a	7	A
1	a	9	G
1	a	16	A
1	a	22	G
1	a	29	U
1	a	31	G
1	a	32	A
1	a	48	C
1	a	51	A
1	a	52	C
1	a	57	G
1	a	60	A
1	a	61	G
1	a	65	A
1	a	66	G
1	a	69	G
1	a	70	A
1	a	71	U
1	a	72	A
1	a	73	A
1	a	77	G
1	a	82	U
1	a	83	G
1	a	84	C
1	a	88	U
1	a	89	G
1	a	95	A
1	a	98	G
1	a	100	C
1	a	106	G
1	a	115	U

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Mol	Chain	Res	Type
1	a	118	C
1	a	121	G
1	a	123	A
1	a	124	A
1	a	125	U
1	a	133	G
1	a	135	A
1	a	138	G
1	a	139	G
1	a	143	A
1	a	148	G
1	a	157	C
1	a	176	C
1	a	177	G
1	a	178	U
1	a	179	C
1	a	182	G
1	a	191	A
1	a	192	G
1	a	193	U
1	a	204	C
1	a	205	G
1	a	206	G
1	a	222	A
1	a	231	G
1	a	239	U
1	a	241	G
1	a	244	A
1	a	253	G
1	a	256	A
1	a	260	G
1	a	261	C
1	a	265	C
1	a	266	C
1	a	273	A
1	a	275	G
1	a	281	U
1	a	283	A
1	a	287	G
1	a	288	U
1	a	292	A
1	a	297	A

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Mol	Chain	Res	Type
1	a	299	G
1	a	308	C
1	a	315	A
1	a	321	A
1	a	322	C
1	a	323	A
1	a	341	G
1	a	346	C
1	a	348	G
1	a	361	U
1	a	363	G
1	a	365	A
1	a	375	A
1	a	376	A
1	a	378	G
1	a	380	C
1	a	382	G
1	a	384	U
1	a	386	C
1	a	391	A
1	a	392	U
1	a	393	G
1	a	394	C
1	a	400	G
1	a	406	A
1	a	407	G
1	a	408	A
1	a	417	G
1	a	418	G
1	a	423	U
1	a	443	G
1	a	445	A
1	a	446	A
1	a	447	G
1	a	456	G
1	a	457	U
1	a	459	A
1	a	461	U
1	a	475	G
1	a	478	G
1	a	480	U
1	a	490	A

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Mol	Chain	Res	Type
1	a	491	U
1	a	492	A
1	a	493	A
1	a	494	G
1	a	502	U
1	a	505	C
1	a	507	U
1	a	511	G
1	a	512	C
1	a	513	C
1	a	515	G
1	a	521	G
1	a	526	A
1	a	527	A
1	a	539	C
1	a	540	A
1	a	541	A
1	a	542	G
1	a	543	C
1	a	545	U
1	a	549	U
1	a	553	A
1	a	556	U
1	a	557	A
1	a	562	G
1	a	566	A
1	a	567	A
1	a	569	G
1	a	570	C
1	a	571	G
1	a	573	G
1	a	582	G
1	a	585	C
1	a	591	G
1	a	601	A
1	a	609	G
1	a	616	A
1	a	627	G
1	a	647	A
1	a	648	G
1	a	656	U
1	a	659	A

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Mol	Chain	Res	Type
1	a	664	G
1	a	681	A
1	a	682	G
1	a	687	G
1	a	688	A
1	a	689	A
1	a	696	A
1	a	697	G
1	a	709	A
1	a	710	A
1	a	712	A
1	a	715	A
1	a	716	G
1	a	717	U
1	a	718	G
1	a	723	A
1	a	725	G
1	a	727	G
1	a	733	C
1	a	749	A
1	a	754	G
1	a	756	U
1	a	757	G
1	a	759	G
1	a	760	A
1	a	775	A
1	a	788	A
1	a	806	G
1	a	807	U
1	a	809	A
1	a	810	A
1	a	811	C
1	a	815	G
1	a	820	C
1	a	822	A
1	a	826	G
1	a	830	G
1	a	832	A
1	a	835	C
1	a	836	U
1	a	838	G
1	a	840	G

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Mol	Chain	Res	Type
1	a	845	U
1	a	854	A
1	a	858	A
1	a	861	G
1	a	863	G
1	a	865	U
1	a	866	A
1	a	867	A
1	a	879	G
1	a	883	A
1	a	884	G
1	a	887	C
1	a	894	A
1	a	896	G
1	a	916	G
1	a	921	G
1	a	928	C
1	a	929	A
1	a	932	A
1	a	936	G
1	a	939	G
1	a	954	U
1	a	955	U
1	a	956	C
1	a	960	G
1	a	963	A
1	a	964	C
1	a	965	G
1	a	967	G
1	a	968	A
1	a	969	A
1	a	970	G
1	a	971	A
1	a	977	A
1	a	981	G
1	a	988	A
1	a	990	A
1	a	997	G
1	a	998	A
1	a	1000	C
1	a	1002	U
1	a	1004	C

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Mol	Chain	Res	Type
1	a	1009	G
1	a	1011	U
1	a	1015	U
1	a	1016	U
1	a	1017	G
1	a	1023	U
1	a	1025	C
1	a	1026	G
1	a	1027	G
1	a	1031	C
1	a	1039	C
1	a	1044	G
1	a	1049	A
1	a	1054	U
1	a	1058	G
1	a	1059	U
1	a	1075	G
1	a	1078	G
1	a	1079	U
1	a	1080	U
1	a	1086	A
1	a	1088	G
1	a	1089	U
1	a	1090	C
1	a	1095	A
1	a	1119	U
1	a	1120	U
1	a	1123	C
1	a	1124	A
1	a	1127	A
1	a	1130	U
1	a	1131	C
1	a	1132	G
1	a	1133	G
1	a	1137	G
1	a	1141	C
1	a	1152	C
1	a	1153	U
1	a	1160	G
1	a	1162	C
1	a	1163	A
1	a	1164	A

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Mol	Chain	Res	Type
1	a	1165	A
1	a	1168	G
1	a	1175	G
1	a	1176	G
1	a	1177	U
1	a	1178	G
1	a	1184	G
1	a	1190	A
1	a	1191	A
1	a	1196	U
1	a	1203	C
1	a	1214	G
1	a	1219	A
1	a	1221	A
1	a	1222	C
1	a	1226	U
1	a	1229	U
1	a	1230	A
1	a	1232	A
1	a	1234	U
1	a	1235	G
1	a	1241	U
1	a	1248	G
1	a	1250	U
1	a	1251	U
1	a	1252	G
1	a	1254	C
1	a	1264	G
1	a	1272	U
1	a	1273	A
1	a	1279	A
1	a	1281	A
1	a	1293	A
1	a	1294	G
1	a	1296	C
1	a	1297	C
1	a	1299	G
1	a	1314	C
1	a	1317	G
1	a	1330	C
1	a	1332	G
1	a	1334	A

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Mol	Chain	Res	Type
1	a	1340	A
1	a	1341	G
1	a	1342	U
1	a	1347	G
1	a	1358	U
1	a	1372	C
1	a	1381	G
1	a	1383	C
1	a	1388	A
1	a	1391	C
1	a	1392	A
1	a	1395	G
1	a	1397	C
1	a	1413	G
1	a	1418	U
1	a	1419	U
1	a	1428	A
1	a	1434	U
1	a	1440	A
1	a	1445	C
1	a	1446	A
1	a	1448	G
1	a	1469	G
1	a	1473	C
1	a	1486	A
1	a	1487	A
1	a	1497	A
1	a	1498	G
1	a	1499	G
1	a	1500	U
1	a	1501	A
1	a	1511	G
1	a	1513	A
1	a	1514	C
1	a	1523	G
1	a	1524	G
1	a	1525	A
1	a	1526	U
22	A	4	C
22	A	10	A
22	A	13	A
22	A	14	A

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Mol	Chain	Res	Type
22	A	15	G
22	A	28	A
22	A	33	U
22	A	34	U
22	A	35	G
22	A	43	G
22	A	44	A
22	A	45	G
22	A	46	G
22	A	51	G
22	A	56	A
22	A	59	U
22	A	60	G
22	A	71	A
22	A	74	A
22	A	75	G
22	A	77	U
22	A	79	C
22	A	82	G
22	A	85	G
22	A	91	A
22	A	92	A
22	A	93	A
22	A	95	A
22	A	97	A
22	A	100	U
22	A	102	G
22	A	104	U
22	A	114	U
22	A	115	C
22	A	118	A
22	A	119	A
22	A	120	U
22	A	125	G
22	A	128	C
22	A	131	A
22	A	132	C
22	A	137	G
22	A	138	A
22	A	139	U
22	A	141	A
22	A	142	C

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Mol	Chain	Res	Type
22	A	146	G
22	A	147	G
22	A	150	U
22	A	153	U
22	A	154	G
22	A	160	A
22	A	162	U
22	A	163	C
22	A	164	C
22	A	165	A
22	A	166	U
22	A	172	C
22	A	181	A
22	A	196	A
22	A	199	A
22	A	205	G
22	A	206	U
22	A	212	G
22	A	215	G
22	A	216	A
22	A	220	G
22	A	222	A
22	A	227	A
22	A	228	C
22	A	230	G
22	A	233	A
22	A	234	U
22	A	241	A
22	A	242	G
22	A	244	A
22	A	248	G
22	A	249	C
22	A	252	G
22	A	255	A
22	A	261	G
22	A	265	A
22	A	266	G
22	A	267	C
22	A	271	U
22	A	273	A
22	A	285	U
22	A	287	U

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Mol	Chain	Res	Type
22	A	289	G
22	A	293	A
22	A	294	A
22	A	297	C
22	A	305	A
22	A	310	G
22	A	315	U
22	A	316	A
22	A	317	G
22	A	318	U
22	A	320	G
22	A	321	G
22	A	322	U
22	A	323	G
22	A	324	A
22	A	325	U
22	A	335	C
22	A	337	C
22	A	338	G
22	A	339	A
22	A	341	A
22	A	342	G
22	A	344	A
22	A	347	U
22	A	348	U
22	A	349	U
22	A	350	G
22	A	351	A
22	A	353	G
22	A	358	A
22	A	359	U
22	A	361	A
22	A	374	C
22	A	376	C
22	A	377	G
22	A	378	A
22	A	380	A
22	A	381	A
22	A	386	U
22	A	387	G
22	A	391	G
22	A	394	C

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Mol	Chain	Res	Type
22	A	395	A
22	A	396	U
22	A	397	G
22	A	398	G
22	A	399	G
22	A	403	A
22	A	406	A
22	A	408	C
22	A	413	A
22	A	414	A
22	A	428	U
22	A	435	C
22	A	438	A
22	A	445	A
22	A	446	C
22	A	447	C
22	A	448	A
22	A	458	G
22	A	461	A
22	A	464	G
22	A	468	A
22	A	472	G
22	A	480	G
22	A	481	A
22	A	484	G
22	A	485	G
22	A	492	A
22	A	495	U
22	A	496	A
22	A	499	A
22	A	500	C
22	A	501	C
22	A	504	A
22	A	509	G
22	A	519	A
22	A	520	A
22	A	521	G
22	A	523	A
22	A	524	G
22	A	535	C
22	A	536	U
22	A	537	U

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Mol	Chain	Res	Type
22	A	538	G
22	A	539	U
22	A	540	U
22	A	541	A
22	A	550	C
22	A	553	A
22	A	558	U
22	A	561	U
22	A	562	A
22	A	563	U
22	A	564	A
22	A	565	A
22	A	576	A
22	A	586	A
22	A	592	A
22	A	593	A
22	A	594	G
22	A	603	U
22	A	604	A
22	A	606	A
22	A	608	G
22	A	611	A
22	A	615	G
22	A	618	G
22	A	622	A
22	A	624	G
22	A	627	A
22	A	634	A
22	A	635	U
22	A	636	A
22	A	647	U
22	A	660	A
22	A	667	A
22	A	671	G
22	A	673	C
22	A	675	A
22	A	676	U
22	A	680	U
22	A	685	G
22	A	687	G
22	A	690	G
22	A	708	A

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Mol	Chain	Res	Type
22	A	709	C
22	A	710	U
22	A	714	U
22	A	716	G
22	A	720	A
22	A	738	G
22	A	739	A
22	A	743	G
22	A	747	G
22	A	754	A
22	A	755	C
22	A	761	G
22	A	765	G
22	A	766	G
22	A	767	A
22	A	772	A
22	A	773	A
22	A	774	G
22	A	775	G
22	A	779	A
22	A	782	A
22	A	783	A
22	A	784	G
22	A	790	A
22	A	793	U
22	A	795	G
22	A	796	C
22	A	802	C
22	A	803	U
22	A	824	G
22	A	827	C
22	A	833	G
22	A	836	U
22	A	841	C
22	A	844	G
22	A	846	G
22	A	848	G
22	A	850	A
22	A	855	A
22	A	858	G
22	A	866	U
22	A	870	G

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Mol	Chain	Res	Type
22	A	871	G
22	A	873	U
22	A	875	A
22	A	876	U
22	A	877	C
22	A	878	C
22	A	879	C
22	A	880	G
22	A	881	A
22	A	889	A
22	A	896	G
22	A	899	A
22	A	904	C
22	A	908	U
22	A	911	C
22	A	921	C
22	A	922	G
22	A	931	A
22	A	935	A
22	A	936	C
22	A	947	C
22	A	949	A
22	A	951	C
22	A	952	G
22	A	954	C
22	A	961	G
22	A	964	A
22	A	972	C
22	A	973	A
22	A	976	C
22	A	979	G
22	A	980	A
22	A	986	A
22	A	992	G
22	A	993	G
22	A	998	A
22	A	999	A
22	A	1002	U
22	A	1003	U
22	A	1007	G
22	A	1011	A
22	A	1012	G

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Mol	Chain	Res	Type
22	A	1015	G
22	A	1016	U
22	A	1017	A
22	A	1023	U
22	A	1025	U
22	A	1031	G
22	A	1036	A
22	A	1037	G
22	A	1040	A
22	A	1048	G
22	A	1050	U
22	A	1051	U
22	A	1052	G
22	A	1057	A
22	A	1058	G
22	A	1060	A
22	A	1061	G
22	A	1063	A
22	A	1064	G
22	A	1066	C
22	A	1068	C
22	A	1069	C
22	A	1077	G
22	A	1078	A
22	A	1079	A
22	A	1080	A
22	A	1082	C
22	A	1084	U
22	A	1085	A
22	A	1086	A
22	A	1087	U
22	A	1088	A
22	A	1091	U
22	A	1097	G
22	A	1100	G
22	A	1101	A
22	A	1102	G
22	A	1112	G
22	A	1117	A
22	A	1119	A
22	A	1120	U
22	A	1122	U

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Mol	Chain	Res	Type
22	A	1124	A
22	A	1125	C
22	A	1129	G
22	A	1133	A
22	A	1138	A
22	A	1141	C
22	A	1146	A
22	A	1147	A
22	A	1148	G
22	A	1149	C
22	A	1162	G
22	A	1163	U
22	A	1164	A
22	A	1165	A
22	A	1166	G
22	A	1168	G
22	A	1170	C
22	A	1177	G
22	A	1191	A
22	A	1193	G
22	A	1197	G
22	A	1199	G
22	A	1202	G
22	A	1214	A
22	A	1221	U
22	A	1223	G
22	A	1225	G
22	A	1228	A
22	A	1229	U
22	A	1232	G
22	A	1233	A
22	A	1234	A
22	A	1235	G
22	A	1237	G
22	A	1238	C
22	A	1240	A
22	A	1242	U
22	A	1243	G
22	A	1244	C
22	A	1249	A
22	A	1253	G
22	A	1258	G

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Mol	Chain	Res	Type
22	A	1259	A
22	A	1260	C
22	A	1261	A
22	A	1263	U
22	A	1276	C
22	A	1277	A
22	A	1283	G
22	A	1288	A
22	A	1295	A
22	A	1306	G
22	A	1308	A
22	A	1317	C
22	A	1321	G
22	A	1328	U
22	A	1339	U
22	A	1345	G
22	A	1347	G
22	A	1352	A
22	A	1355	A
22	A	1360	A
22	A	1361	G
22	A	1366	U
22	A	1367	G
22	A	1370	A
22	A	1372	A
22	A	1373	C
22	A	1377	U
22	A	1379	A
22	A	1380	A
22	A	1382	A
22	A	1389	U
22	A	1390	A
22	A	1403	G
22	A	1404	C
22	A	1408	G
22	A	1410	A
22	A	1415	C
22	A	1422	G
22	A	1424	C
22	A	1432	G
22	A	1440	U
22	A	1441	U

Continued on next page...

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Mol	Chain	Res	Type
22	A	1442	G
22	A	1445	U
22	A	1447	U
22	A	1448	C
22	A	1449	C
22	A	1460	U
22	A	1469	G
22	A	1474	C
22	A	1480	U
22	A	1481	A
22	A	1484	U
22	A	1495	A
22	A	1496	A
22	A	1497	G
22	A	1498	G
22	A	1502	A
22	A	1508	G
22	A	1509	A
22	A	1510	U
22	A	1511	G
22	A	1516	G
22	A	1528	A
22	A	1542	G
22	A	1545	G
22	A	1555	C
22	A	1556	A
22	A	1557	A
22	A	1558	G
22	A	1559	A
22	A	1560	A
22	A	1568	U
22	A	1572	C
22	A	1573	U
22	A	1574	U
22	A	1576	A
22	A	1580	A
22	A	1583	C
22	A	1593	A
22	A	1597	C
22	A	1598	A
22	A	1599	A
22	A	1600	A

Continued on next page...

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Mol	Chain	Res	Type
22	A	1602	C
22	A	1603	G
22	A	1606	A
22	A	1608	A
22	A	1609	G
22	A	1624	A
22	A	1628	C
22	A	1629	C
22	A	1634	C
22	A	1636	C
22	A	1637	U
22	A	1638	U
22	A	1639	G
22	A	1641	G
22	A	1643	G
22	A	1658	A
22	A	1663	G
22	A	1664	G
22	A	1667	A
22	A	1673	C
22	A	1683	U
22	A	1685	G
22	A	1686	G
22	A	1689	G
22	A	1690	A
22	A	1700	G
22	A	1702	C
22	A	1705	G
22	A	1711	A
22	A	1713	G
22	A	1715	U
22	A	1716	U
22	A	1717	U
22	A	1719	C
22	A	1720	U
22	A	1721	C
22	A	1724	U
22	A	1725	A
22	A	1731	U
22	A	1732	G
22	A	1733	G
22	A	1741	A

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Mol	Chain	Res	Type
22	A	1742	A
22	A	1743	G
22	A	1744	A
22	A	1745	U
22	A	1746	A
22	A	1748	C
22	A	1749	A
22	A	1750	G
22	A	1751	G
22	A	1756	U
22	A	1757	G
22	A	1760	A
22	A	1763	G
22	A	1768	U
22	A	1771	A
22	A	1773	A
22	A	1787	C
22	A	1788	A
22	A	1789	A
22	A	1794	G
22	A	1795	A
22	A	1796	A
22	A	1797	A
22	A	1798	G
22	A	1800	G
22	A	1802	A
22	A	1803	C
22	A	1810	G
22	A	1813	G
22	A	1815	G
22	A	1816	A
22	A	1838	U
22	A	1841	A
22	A	1844	G
22	A	1850	G
22	A	1851	U
22	A	1853	A
22	A	1854	G
22	A	1867	U
22	A	1877	A
22	A	1886	A
22	A	1887	A

Continued on next page...

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Mol	Chain	Res	Type
22	A	1890	G
22	A	1892	C
22	A	1893	G
22	A	1896	C
22	A	1897	G
22	A	1898	U
22	A	1899	A
22	A	1900	A
22	A	1901	C
22	A	1902	U
22	A	1906	A
22	A	1916	G
22	A	1917	G
22	A	1924	A
22	A	1925	A
22	A	1926	U
22	A	1938	U
22	A	1942	U
22	A	1950	U
22	A	1951	G
22	A	1954	C
22	A	1957	A
22	A	1958	U
22	A	1959	G
22	A	1967	G
22	A	1968	A
22	A	1969	U
22	A	1978	U
22	A	1982	U
22	A	1984	C
22	A	1991	G
22	A	1993	C
22	A	2007	A
22	A	2010	C
22	A	2018	A
22	A	2020	A
22	A	2029	A
22	A	2030	U
22	A	2042	C
22	A	2043	G
22	A	2047	A
22	A	2048	G

Continued on next page...

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Mol	Chain	Res	Type
22	A	2049	A
22	A	2055	U
22	A	2056	G
22	A	2063	U
22	A	2064	A
22	A	2080	G
22	A	2082	A
22	A	2094	C
22	A	2097	G
22	A	2098	U
22	A	2099	G
22	A	2101	A
22	A	2105	U
22	A	2106	A
22	A	2110	G
22	A	2113	A
22	A	2114	G
22	A	2115	G
22	A	2116	C
22	A	2117	U
22	A	2118	U
22	A	2119	U
22	A	2121	A
22	A	2122	A
22	A	2129	A
22	A	2132	C
22	A	2133	C
22	A	2135	G
22	A	2140	C
22	A	2141	G
22	A	2143	G
22	A	2144	G
22	A	2145	A
22	A	2146	G
22	A	2147	C
22	A	2148	C
22	A	2149	A
22	A	2150	U
22	A	2151	C
22	A	2152	C
22	A	2153	U
22	A	2156	A

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Mol	Chain	Res	Type
22	A	2158	A
22	A	2160	A
22	A	2169	G
22	A	2173	G
22	A	2174	C
22	A	2175	U
22	A	2176	U
22	A	2185	A
22	A	2187	C
22	A	2190	U
22	A	2191	G
22	A	2194	C
22	A	2198	A
22	A	2199	A
22	A	2200	U
22	A	2201	C
22	A	2207	C
22	A	2212	A
22	A	2221	G
22	A	2225	G
22	A	2226	G
22	A	2229	G
22	A	2237	G
22	A	2239	G
22	A	2240	G
22	A	2246	U
22	A	2253	A
22	A	2256	G
22	A	2264	G
22	A	2265	A
22	A	2266	G
22	A	2270	U
22	A	2274	A
22	A	2275	A
22	A	2281	G
22	A	2284	C
22	A	2292	U
22	A	2294	G
22	A	2296	A
22	A	2297	A
22	A	2303	U
22	A	2305	G

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Mol	Chain	Res	Type
22	A	2306	C
22	A	2307	A
22	A	2308	G
22	A	2309	A
22	A	2312	A
22	A	2313	U
22	A	2314	A
22	A	2319	C
22	A	2321	A
22	A	2322	A
22	A	2323	A
22	A	2330	U
22	A	2333	A
22	A	2334	C
22	A	2337	C
22	A	2348	C
22	A	2349	G
22	A	2358	G
22	A	2366	G
22	A	2370	G
22	A	2372	C
22	A	2378	G
22	A	2383	G
22	A	2389	U
22	A	2392	G
22	A	2393	U
22	A	2408	G
22	A	2410	U
22	A	2413	A
22	A	2414	C
22	A	2415	G
22	A	2416	G
22	A	2417	A
22	A	2418	U
22	A	2421	A
22	A	2422	A
22	A	2424	G
22	A	2428	U
22	A	2432	G
22	A	2434	G
22	A	2435	A
22	A	2446	A

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Mol	Chain	Res	Type
22	A	2451	G
22	A	2454	C
22	A	2457	G
22	A	2459	G
22	A	2462	C
22	A	2467	C
22	A	2474	G
22	A	2478	U
22	A	2479	U
22	A	2480	U
22	A	2481	G
22	A	2489	G
22	A	2492	G
22	A	2493	U
22	A	2495	G
22	A	2505	A
22	A	2506	U
22	A	2517	A
22	A	2521	C
22	A	2522	G
22	A	2537	G
22	A	2539	U
22	A	2553	A
22	A	2554	G
22	A	2559	A
22	A	2560	C
22	A	2563	G
22	A	2565	G
22	A	2569	G
22	A	2572	U
22	A	2573	U
22	A	2583	U
22	A	2586	G
22	A	2589	A
22	A	2593	C
22	A	2595	G
22	A	2596	U
22	A	2600	U
22	A	2602	U
22	A	2604	U
22	A	2616	U
22	A	2619	A

Continued on next page...

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Mol	Chain	Res	Type
22	A	2626	A
22	A	2633	C
22	A	2637	U
22	A	2641	A
22	A	2647	A
22	A	2648	G
22	A	2660	G
22	A	2672	G
22	A	2676	U
22	A	2677	U
22	A	2689	G
22	A	2690	C
22	A	2694	U
22	A	2701	G
22	A	2703	C
22	A	2704	G
22	A	2705	G
22	A	2713	U
22	A	2714	G
22	A	2720	A
22	A	2731	G
22	A	2733	U
22	A	2735	A
22	A	2738	G
22	A	2739	C
22	A	2743	U
22	A	2744	A
22	A	2751	A
22	A	2752	A
22	A	2763	A
22	A	2765	A
22	A	2766	U
22	A	2771	U
22	A	2779	G
22	A	2784	U
22	A	2785	U
22	A	2786	G
22	A	2787	A
22	A	2794	U
22	A	2795	G
22	A	2798	G
22	A	2805	C

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Mol	Chain	Res	Type
22	A	2807	A
22	A	2811	C
22	A	2812	U
22	A	2818	G
22	A	2820	U
22	A	2821	G
22	A	2822	A
22	A	2830	G
22	A	2836	U
22	A	2848	G
22	A	2852	U
22	A	2853	U
22	A	2854	G
22	A	2857	C
22	A	2860	A
22	A	2867	C
22	A	2871	U
22	A	2873	G
22	A	2878	U
22	A	2880	A
22	A	2887	A
22	A	2889	C
23	B	13	A
23	B	16	G
23	B	24	G
23	B	25	A
23	B	33	G
23	B	35	U
23	B	41	C
23	B	51	G
23	B	52	A
23	B	53	A
23	B	54	G
23	B	57	A
23	B	61	G
23	B	67	U
23	B	73	A
23	B	84	G
23	B	85	G
23	B	88	C
23	B	89	U
23	B	90	C

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Mol	Chain	Res	Type
23	B	91	C
23	B	105	G
23	B	109	A
23	B	114	C
23	B	117	G

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	A	81	G
22	A	87	C
22	A	114	U
22	A	227	A
22	A	243	U
22	A	260	G
22	A	314	A
22	A	348	U
22	A	360	C
22	A	434	A
22	A	444	A
22	A	538	G
22	A	540	U
22	A	774	G
22	A	783	A
22	A	792	A
22	A	840	U
22	A	920	C
22	A	953	U
22	A	963	A
22	A	1016	U
22	A	1051	U
22	A	1169	A
22	A	1232	G
22	A	1233	A
22	A	1378	U
22	A	1448	C
22	A	1627	A
22	A	1642	A
22	A	1672	G
22	A	1710	A
22	A	1715	U
22	A	1741	A

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Mol	Chain	Res	Type
22	A	1899	A
22	A	1968	A
22	A	2029	A
22	A	2149	A
22	A	2200	U
22	A	2228	A
22	A	2274	A
22	A	2333	A
22	A	2536	G
22	A	2703	C
22	A	2750	G
22	A	2784	U
22	A	2853	U
23	B	34	A
23	B	51	G
23	B	52	A
23	B	66	A

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 172 ligands modelled in this entry, 172 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

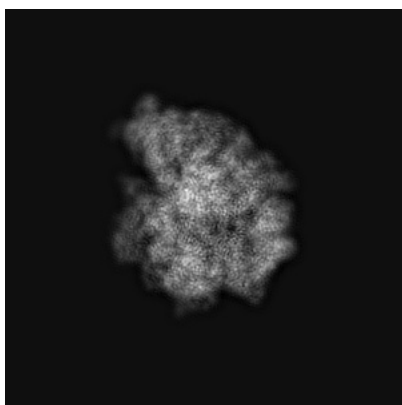
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10285. These allow visual inspection of the internal detail of the map and identification of artifacts.

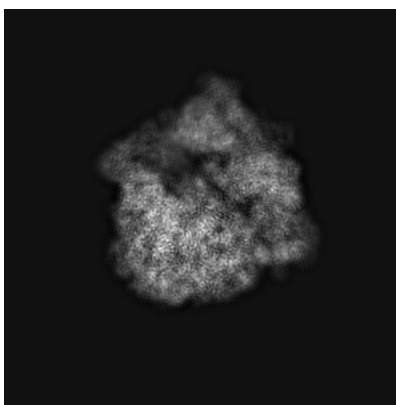
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

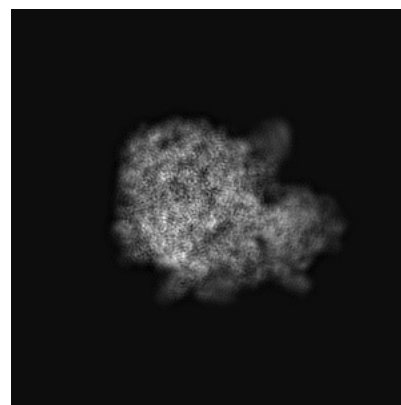
6.1.1 Primary map



X



Y

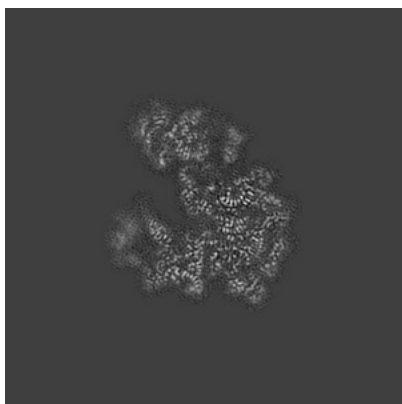


Z

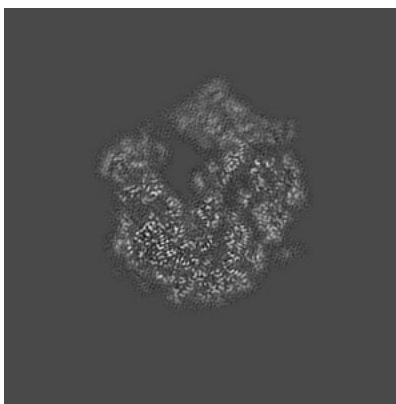
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

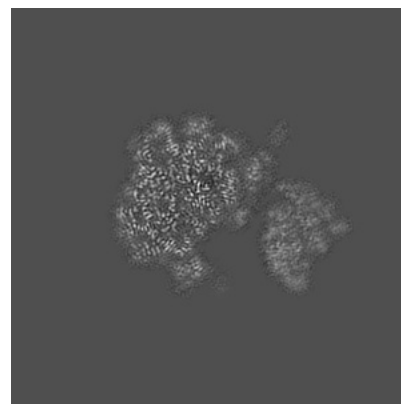
6.2.1 Primary map



X Index: 200



Y Index: 200

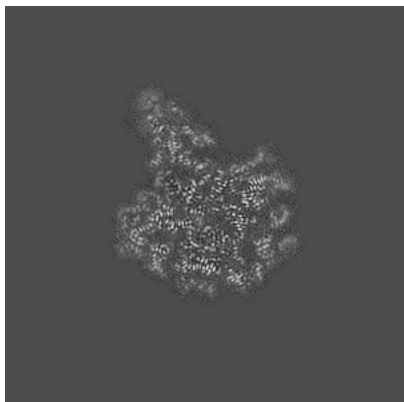


Z Index: 200

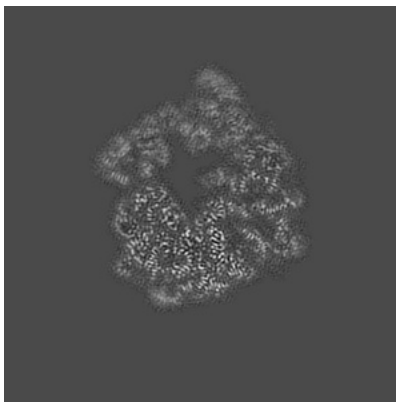
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

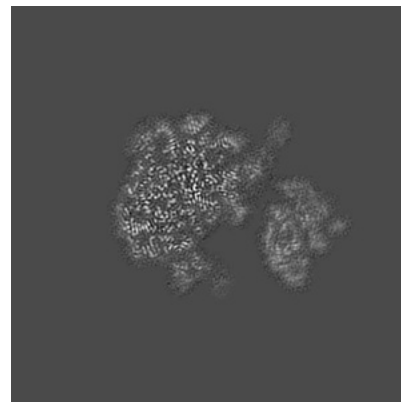
6.3.1 Primary map



X Index: 172



Y Index: 181



Z Index: 198

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 0.0731. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

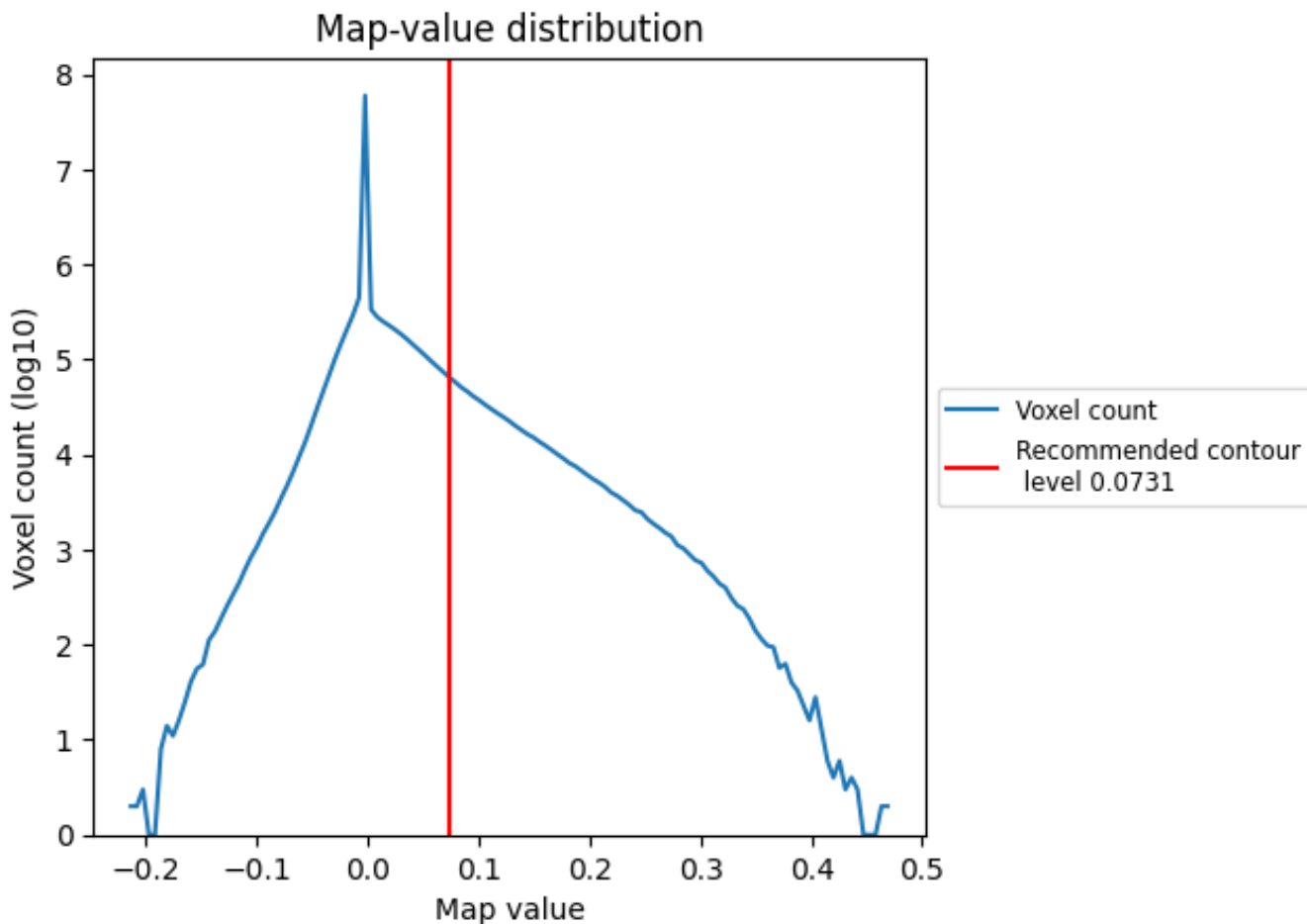
6.5 Mask visualisation

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

7 Map analysis [i](#)

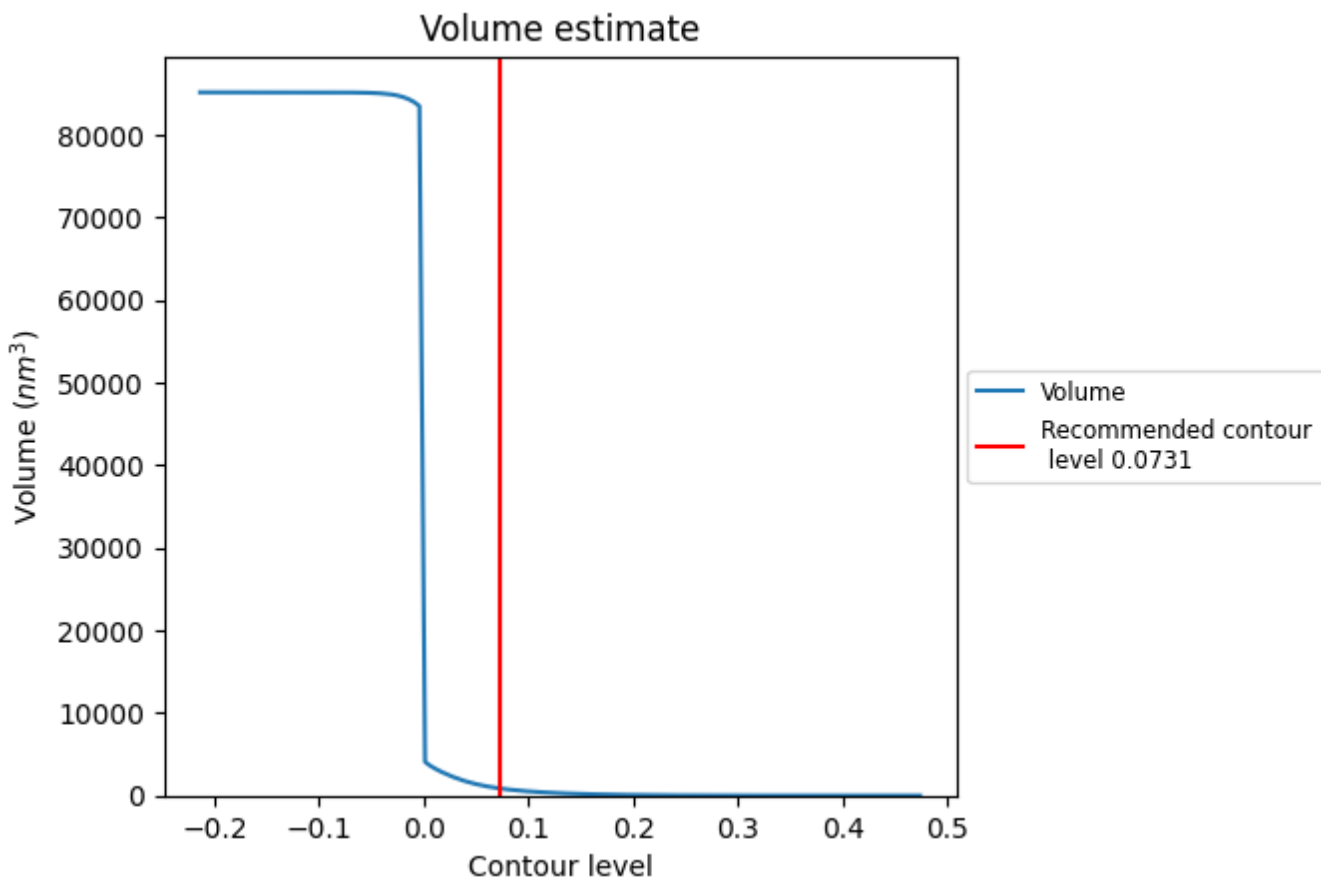
This section contains the results of statistical analysis of the map.

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.

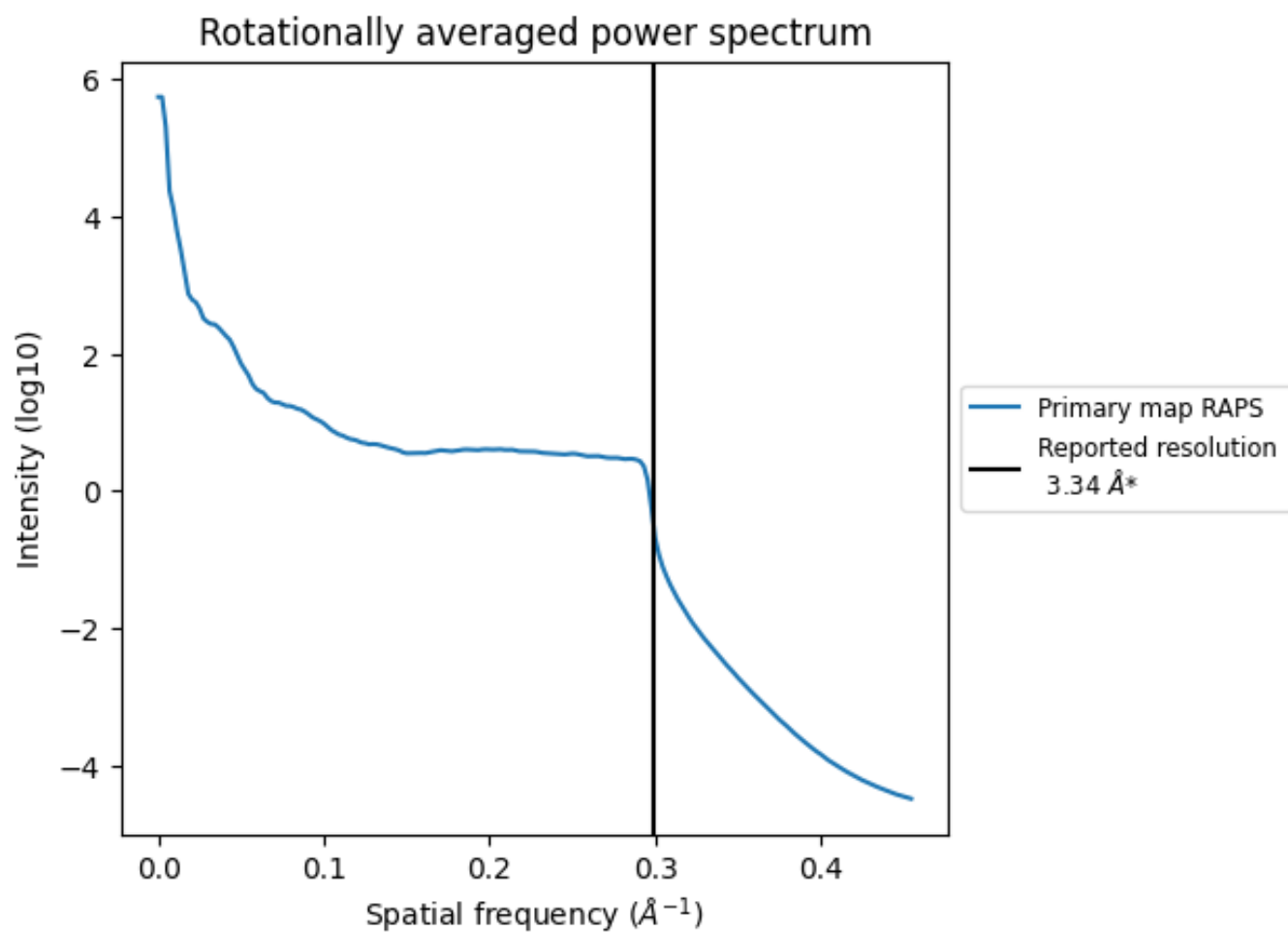
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 860 nm³; this corresponds to an approximate mass of 777 kDa.

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

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

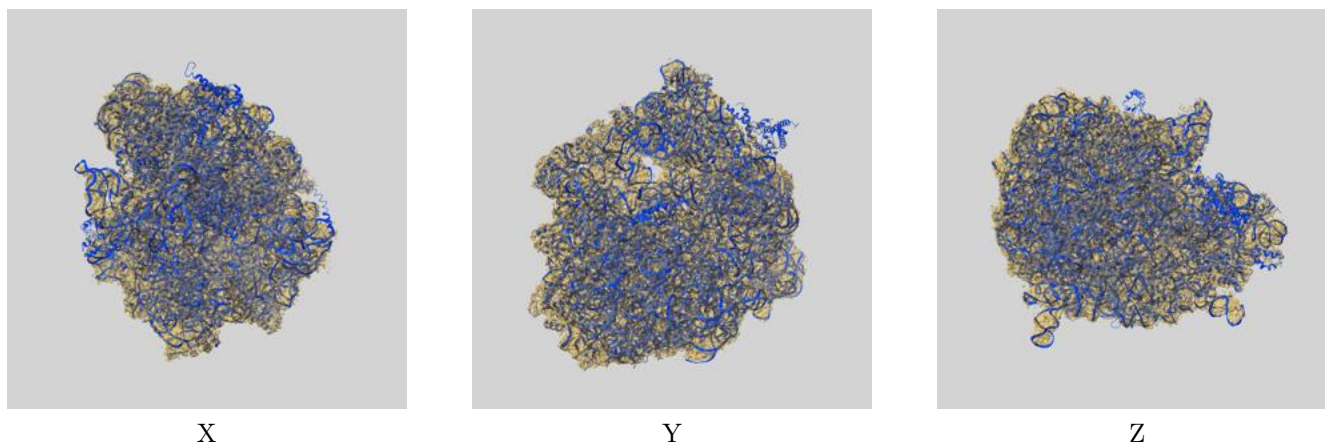
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

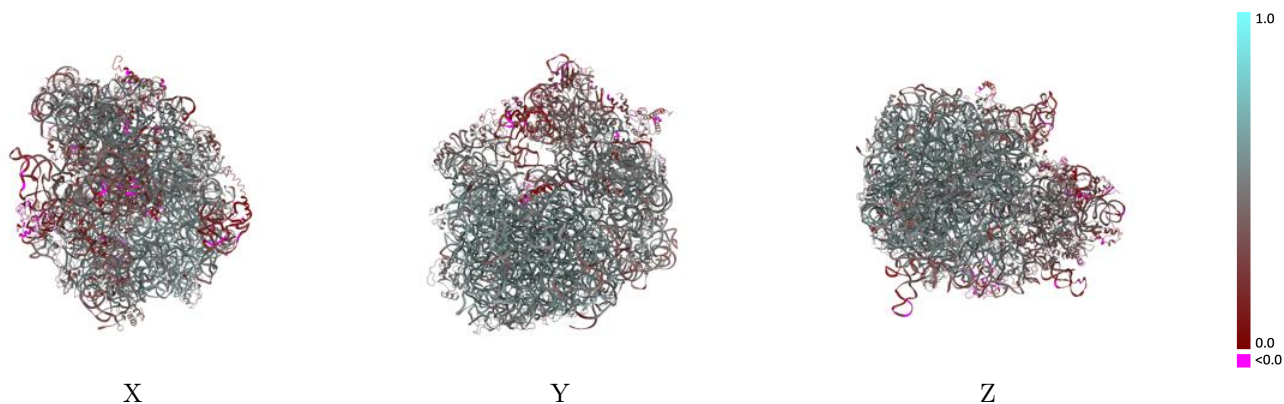
This section contains information regarding the fit between EMDB map EMD-10285 and PDB model 6SPG. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



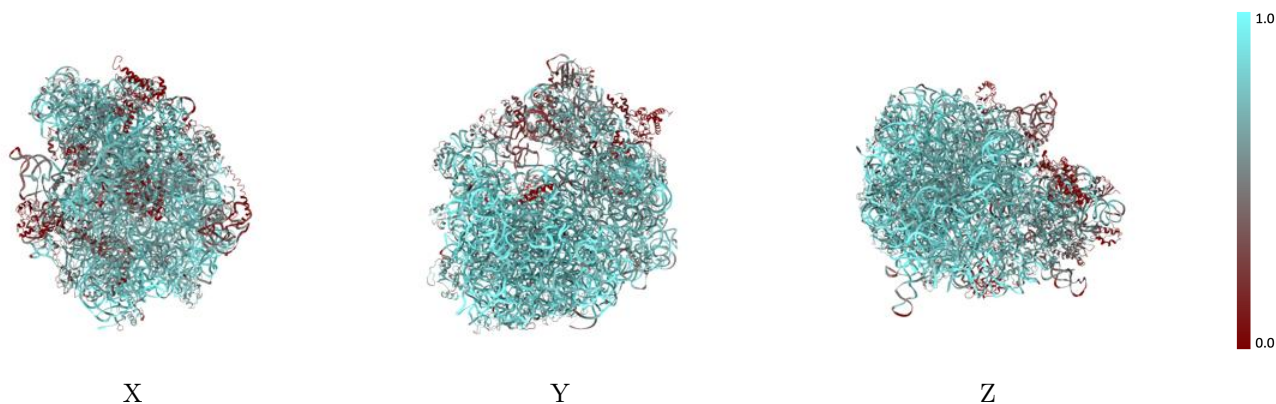
The images above show the 3D surface view of the map at the recommended contour level 0.0731 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



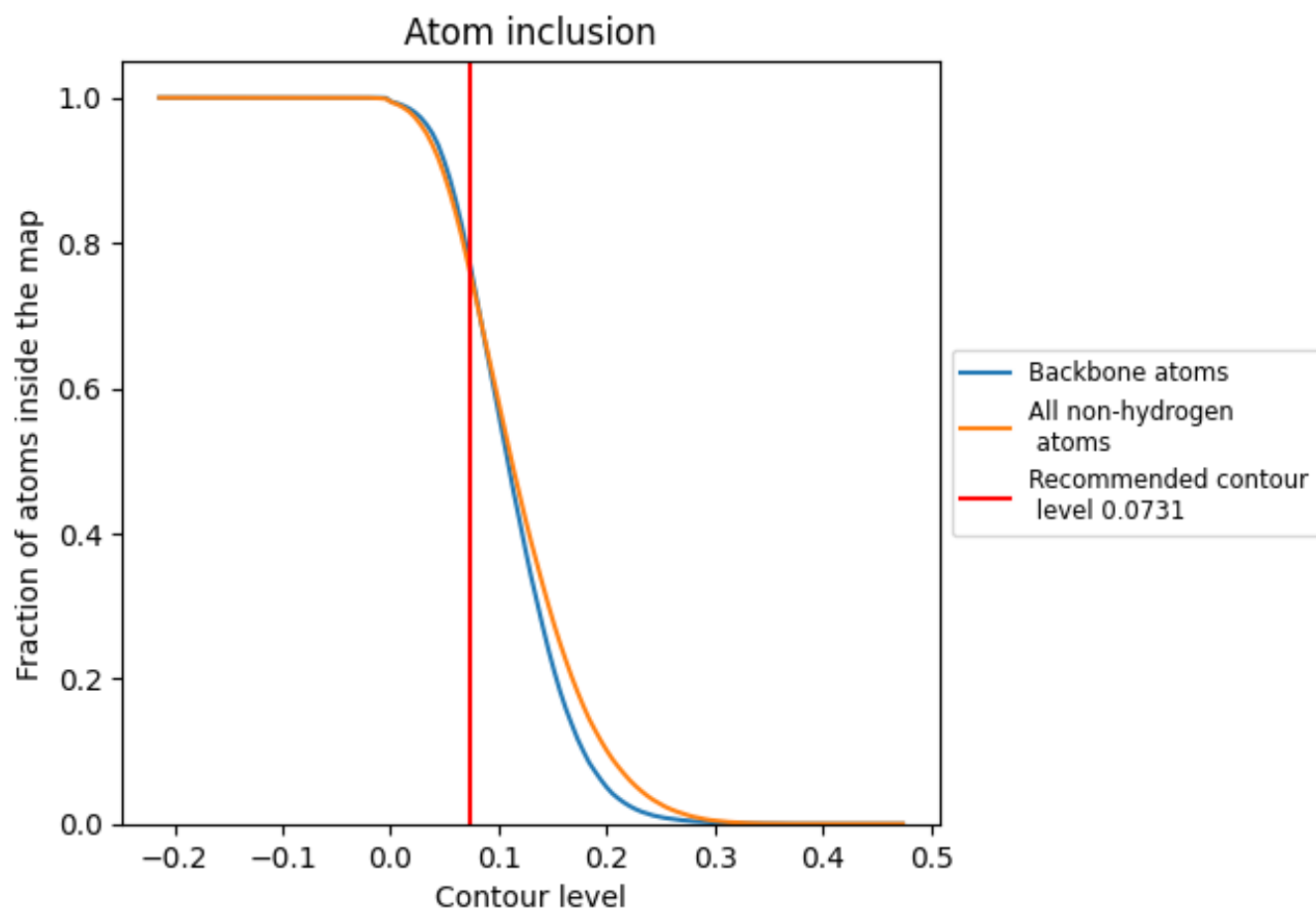
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0731).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% 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 (0.0731) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7638	 0.4680
1	 0.3100	 0.2040
2	 0.7255	 0.4890
3	 0.5848	 0.4370
4	 0.7813	 0.5540
5	 0.7286	 0.5340
6	 0.7405	 0.5280
A	 0.8694	 0.5150
B	 0.8658	 0.4590
C	 0.7328	 0.5270
D	 0.7646	 0.5160
E	 0.7128	 0.5070
F	 0.5048	 0.3360
G	 0.5812	 0.4190
H	 0.0634	 0.1670
I	 0.0217	 0.0610
J	 0.7500	 0.5160
K	 0.6343	 0.4910
L	 0.7167	 0.4960
M	 0.6838	 0.5070
N	 0.7791	 0.5280
O	 0.6420	 0.4240
P	 0.6632	 0.4910
Q	 0.7998	 0.5380
R	 0.7267	 0.5050
S	 0.6890	 0.5120
T	 0.6681	 0.4960
U	 0.6315	 0.4290
V	 0.5493	 0.4370
W	 0.7750	 0.5120
X	 0.7105	 0.5070
Y	 0.7162	 0.4810
Z	 0.7021	 0.5120
a	 0.8209	 0.4470
b	 0.0858	 0.2710



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Chain	Atom inclusion	Q-score
c	 0.4537	 0.3630
d	 0.5748	 0.4100
e	 0.5996	 0.4350
f	 0.5187	 0.3580
g	 0.2528	 0.2470
h	 0.6397	 0.4680
i	 0.3491	 0.2610
j	 0.3110	 0.2880
k	 0.5814	 0.4300
l	 0.5958	 0.4610
m	 0.3176	 0.2210
n	 0.4592	 0.3570
o	 0.6447	 0.4480
p	 0.7223	 0.4740
q	 0.6187	 0.4380
r	 0.5456	 0.4150
s	 0.2882	 0.2430
t	 0.6928	 0.4610
u	 0.3279	 0.3450