



Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 01:29 pm GMT

PDB ID : 6SPF
EMDB ID : EMD-10284
Title : Pseudomonas aeruginosa 70s ribosome from an aminoglycoside resistant 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 : 2.89 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:

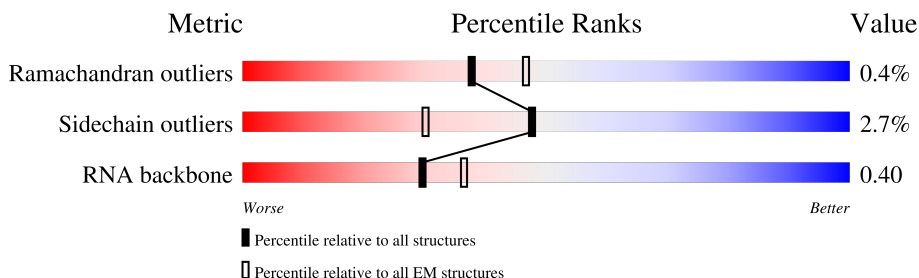
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.89 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	2888	
2	B	117	
3	C	271	
4	D	207	
5	E	199	
6	F	174	
7	G	169	
8	H	78	

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Mol	Chain	Length	Quality of chain
9	I	140	100% 98%
10	J	141	99%
11	K	120	97%
12	L	144	98%
13	M	136	99%
14	N	120	98%
15	O	115	38% 96%
16	P	114	97%
17	Q	117	97%
18	R	102	5% 95% 5%
19	S	110	98%
20	T	94	97%
21	U	103	6% 99%
22	V	188	97%
23	W	76	99%
24	X	77	99%
25	Y	60	98%
26	Z	57	96%
27	1	31	100% 100%
28	2	53	98%
29	3	50	44% 98%
30	4	44	98%
31	5	63	97%
32	6	38	97%
33	a	1521	32% 51% 38% 9%

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Mol	Chain	Length	Quality of chain
34	b	226	80% 94% ..
35	c	203	99% 100%
36	d	204	76% 98% .
37	e	150	70% 97% ..
38	f	100	87% 99% .
39	g	154	97% 98% .
40	h	129	58% 95% 5% .
41	i	126	91% 97% .
42	j	96	99% 99% .
43	k	115	83% 98% .
44	l	120	72% 97% .
45	m	110	93% 95% ..
46	n	98	98% 98% .
47	o	87	59% 91% 9%
48	p	78	46% 99% .
49	q	76	34% 96% .
50	r	56	82% 98% .
51	s	80	95% 96% ..
52	t	86	29% 100%
53	u	34	97% 100%

2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 138296 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 Pseudomonas aeruginosa strain PAO1 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2885	61899	27618	11351	20046	2884	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	174	1278	806	225	244	3	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	169	1264	795	233	234	2	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	GLY	deletion	UNP A0A2V3F3S9
G	?	-	TYR	deletion	UNP A0A2V3F3S9
G	?	-	LYS	deletion	UNP A0A2V3F3S9
G	?	-	ALA	deletion	UNP A0A2V3F3S9

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L11.

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

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	144	1063	653	214	193	3	0	0

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	136	1076	684	210	179	3	0	0

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	120	959	600	192	162	5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	114	901	567	171	162	1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	110	Total	C	N	O	S	0	0
			833	515	161	153	4		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	94	Total	C	N	O	S	0	0
			732	469	132	130	1		

- Molecule 21 is a protein called 50S ribosomal protein L24.

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

- Molecule 22 is a protein called 50S ribosomal protein L25.

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

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 23 is a protein called 50S ribosomal protein L27.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called Ribosomal protein uL29.

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

- Molecule 26 is a protein called 50S ribosomal protein L30.

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

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	31	Total	C	N	O	S	0	0
			232	144	40	45	3		

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	53	Total	C	N	O	S	0	0
			419	251	89	78	1		

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	3	50	Total	C	N	O	0	0
			408	262	74	72		

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	44	Total	C	N	O	S	0	0
			364	222	87	53	2		

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	63	Total	C	N	O	S	0	0
			502	311	107	81	3		

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	38	Total	C	N	O	S	0	0
			303	184	69	46	4		

- Molecule 33 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	1390	Total	C	N	O	P	0	0
			29826	13303	5479	9654	1390		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	101	A	G	conflict	GB 1378074500

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	221	Total	C	N	O	S	0	0
			1698	1070	309	310	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	203	Total	C	N	O	S	0	0
			1609	1017	303	284	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	204	Total	C	N	O	S	0	0
			1596	988	310	293	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	149	Total	C	N	O	S	0	0
			1092	687	202	197	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	100	Total	C	N	O	S	0	0
			802	497	152	149	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	80	ALA	TYR	conflict	UNP A0A069Q263

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	129	Total	C	N	O	S	0	0
			965	608	171	180	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	94	ALA	LYS	conflict	UNP E2RXT9

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	96	Total	C	N	O	S	0	0
			763	479	143	140	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	k	115	832	514	160	156	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	l	120	942	577	195	166	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	m	109	847	515	173	155	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	n	98	776	479	163	131	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	o	87	691	428	135	127	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	p	78	609	381	120	107	1	0	0

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	r	56	Total	C	N	O	0	0
			443	283	79	81		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	86	Total	C	N	O	S	0	0
			662	410	137	113	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
53	u	34	Total	C	N	O	0	0
			295	178	70	47		

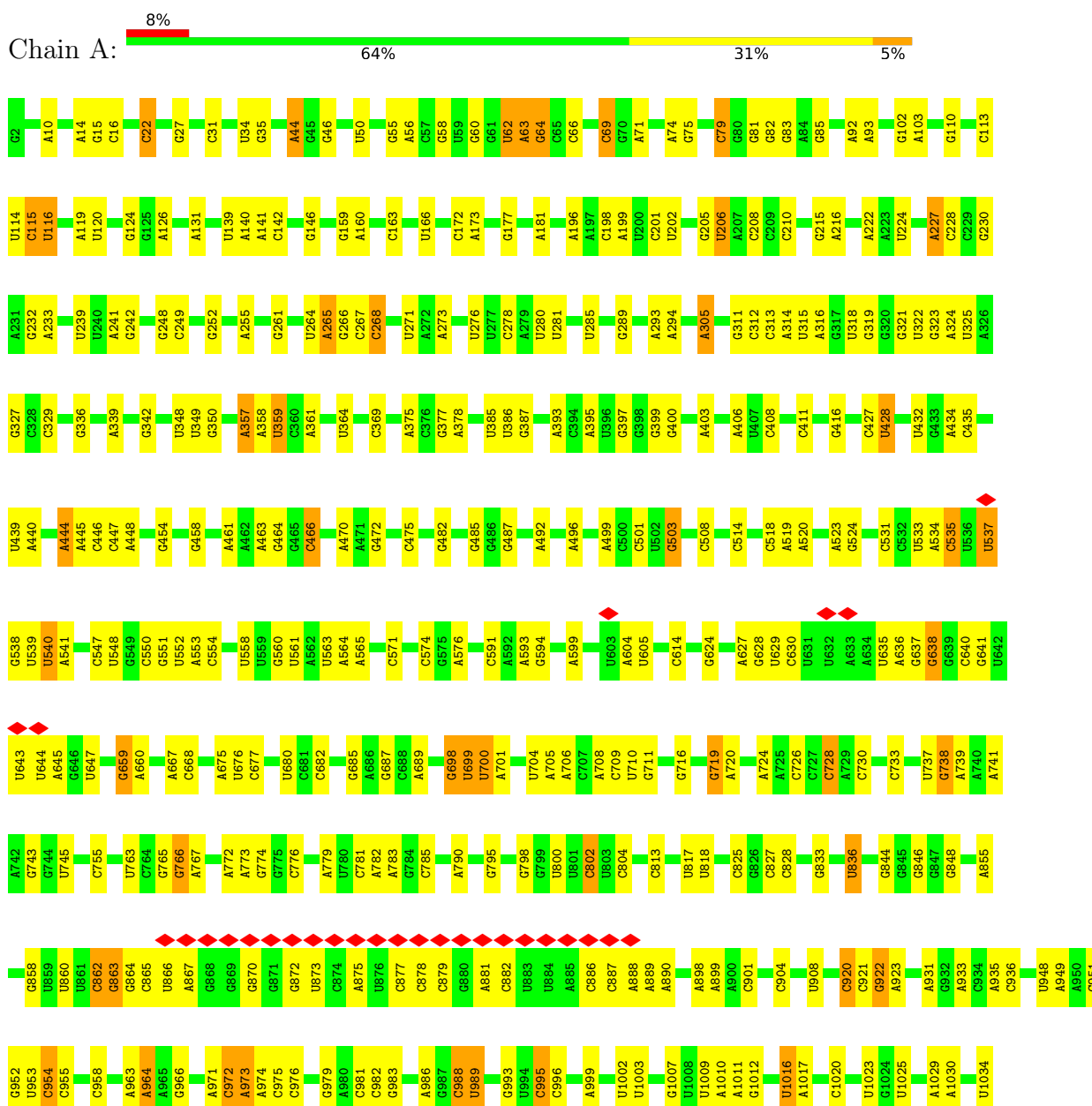
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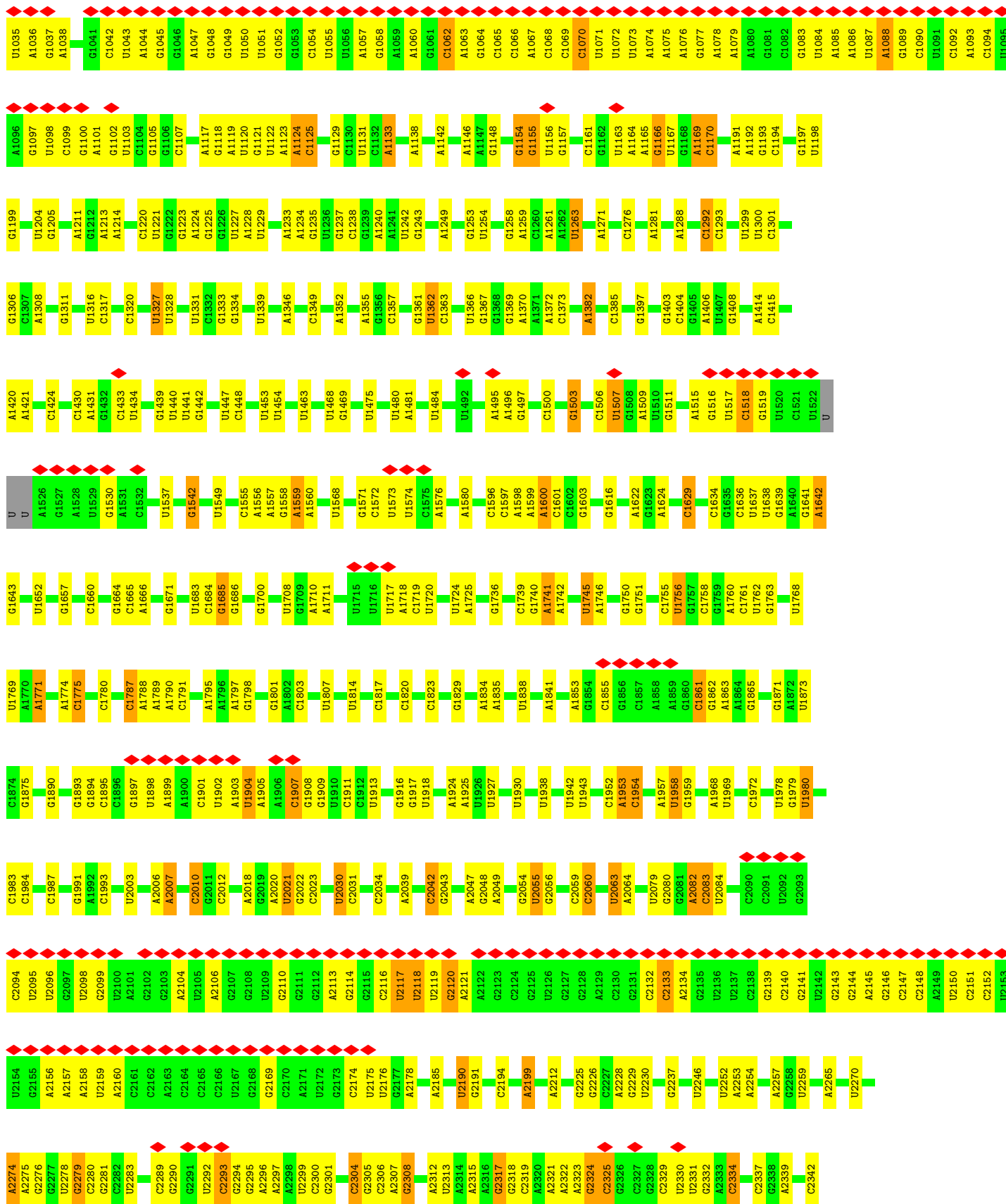
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u	46	ARG	LYS	conflict	UNP A0A069QC99

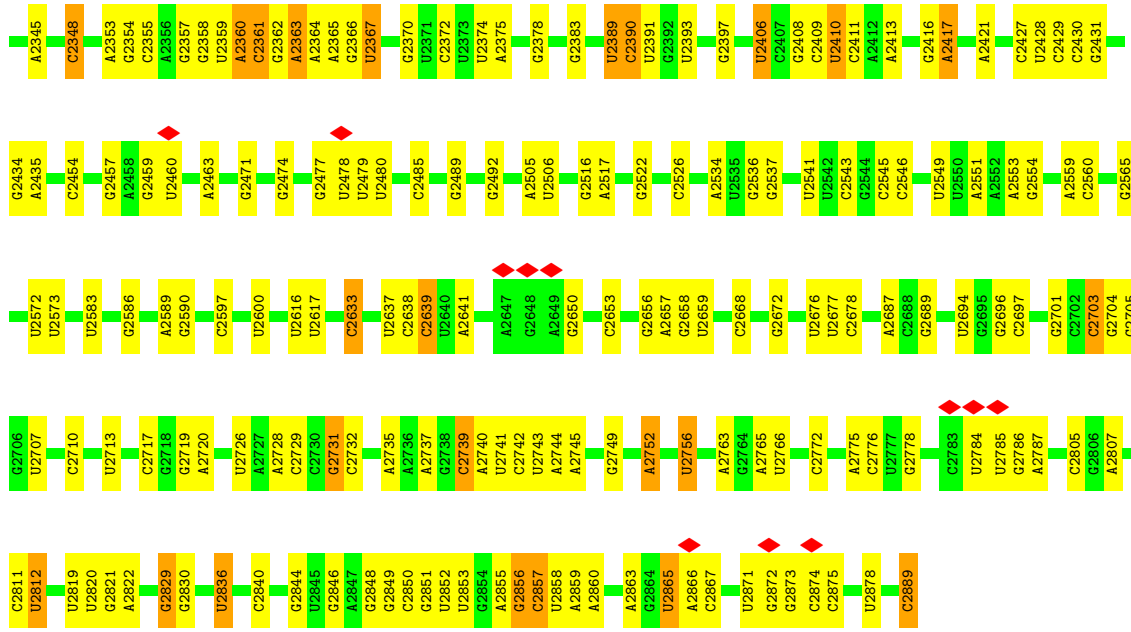
3 Residue-property plots

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.

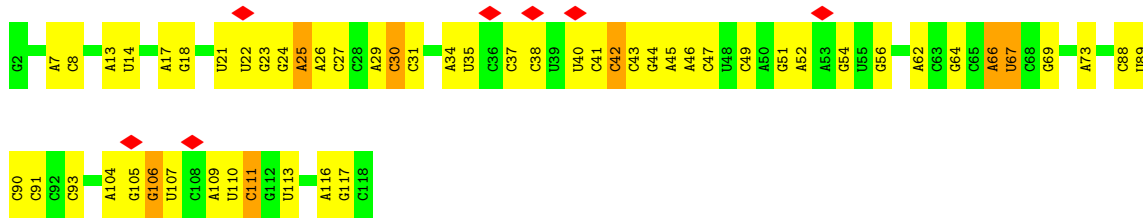
- Molecule 1: *Pseudomonas aeruginosa* strain PAO1 23S ribosomal RNA



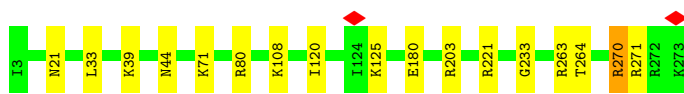
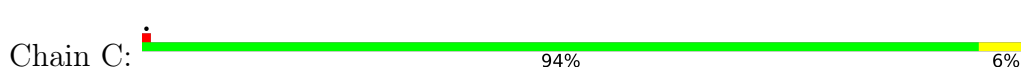




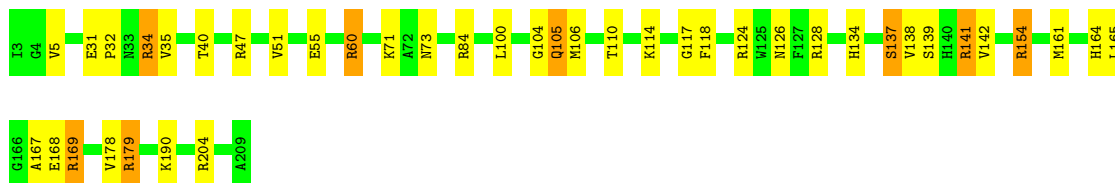
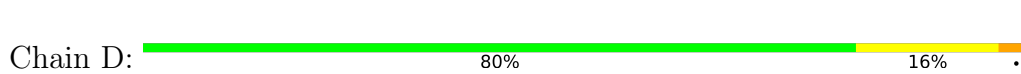
• Molecule 2: 5S rRNA



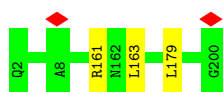
• Molecule 3: 50S ribosomal protein L2



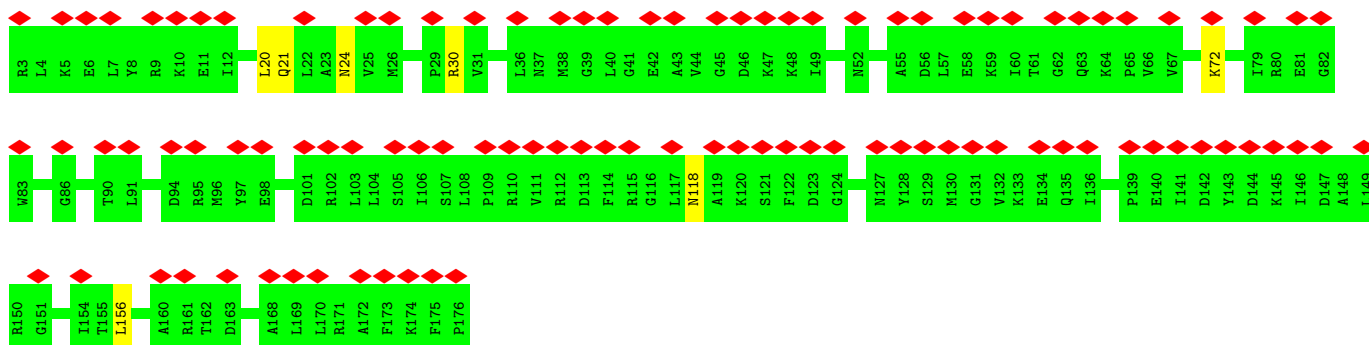
• Molecule 4: 50S ribosomal protein L3



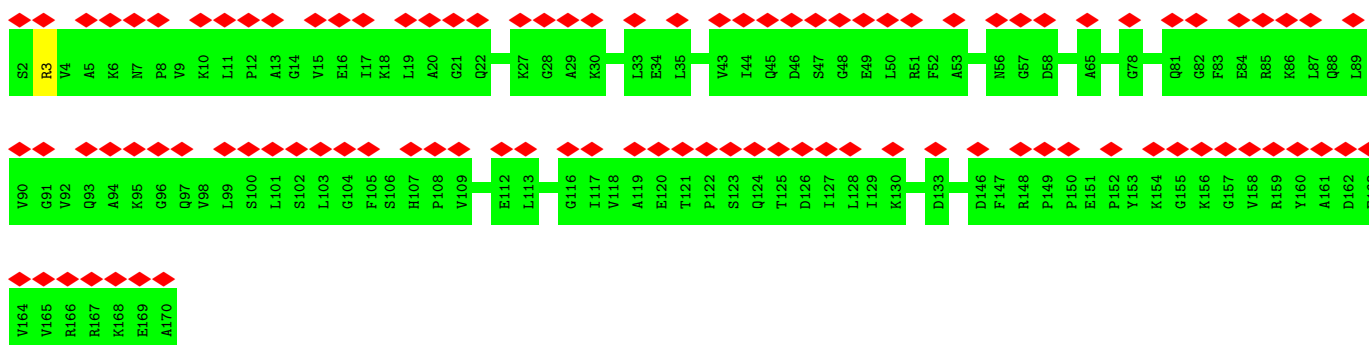
• Molecule 5: 50S ribosomal protein L4



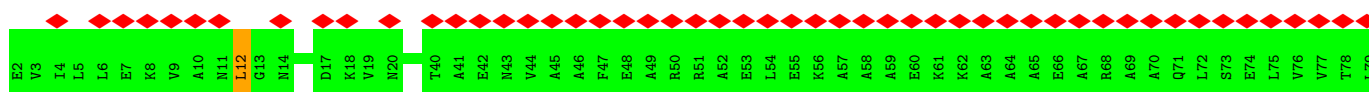
• Molecule 6: 50S ribosomal protein L5



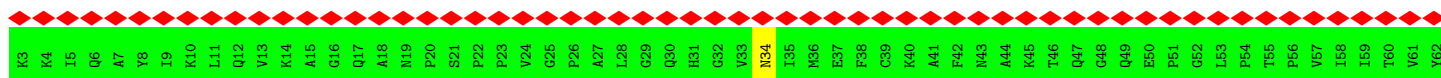
• Molecule 7: 50S ribosomal protein L6

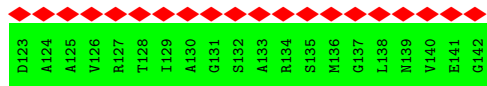
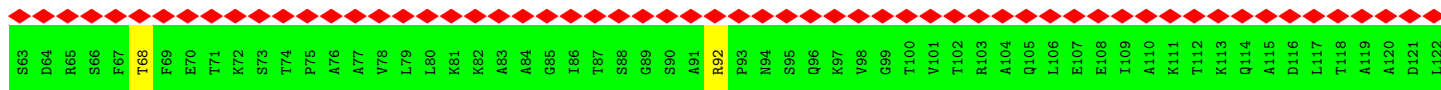


• Molecule 8: 50S ribosomal protein L9

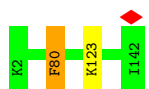


• Molecule 9: 50S ribosomal protein L11

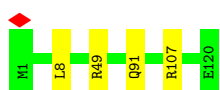




● Molecule 10: 50S ribosomal protein L13



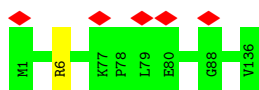
● Molecule 11: 50S ribosomal protein L14



● Molecule 12: 50S ribosomal protein L15



● Molecule 13: 50S ribosomal protein L16

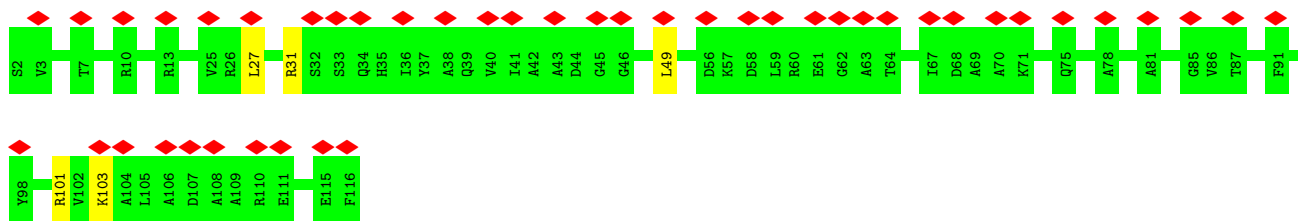


● Molecule 14: 50S ribosomal protein L17

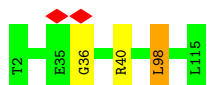


● Molecule 15: 50S ribosomal protein L18

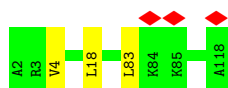




- Molecule 16: 50S ribosomal protein L19



- Molecule 17: 50S ribosomal protein L20



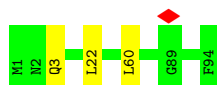
- Molecule 18: 50S ribosomal protein L21



- Molecule 19: 50S ribosomal protein L22

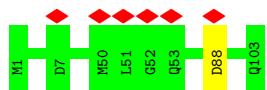


- Molecule 20: 50S ribosomal protein L23

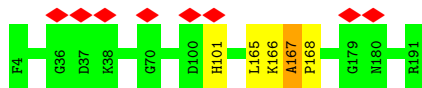


- Molecule 21: 50S ribosomal protein L24

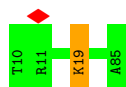




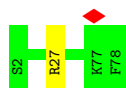
- Molecule 22: 50S ribosomal protein L25



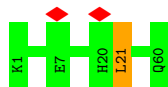
- Molecule 23: 50S ribosomal protein L27



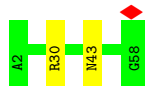
- Molecule 24: 50S ribosomal protein L28



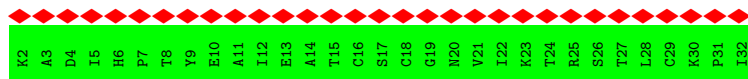
- Molecule 25: Ribosomal protein uL29



- Molecule 26: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L31

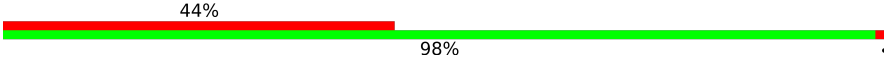


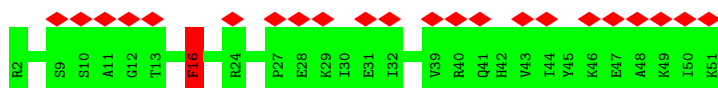
- Molecule 28: 50S ribosomal protein L32

Chain 2:  98%



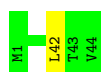
• Molecule 29: 50S ribosomal protein L33

Chain 3:  44% 98%



• Molecule 30: 50S ribosomal protein L34

Chain 4:  98%



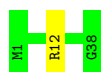
• Molecule 31: 50S ribosomal protein L35

Chain 5:  97%



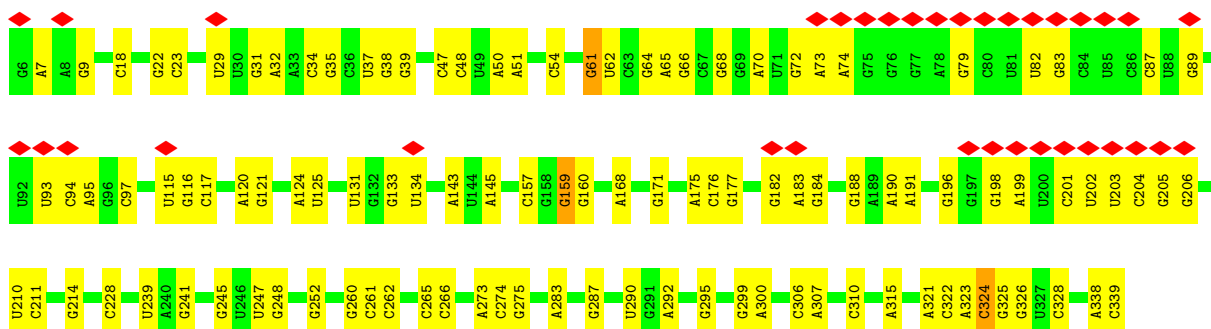
• Molecule 32: 50S ribosomal protein L36

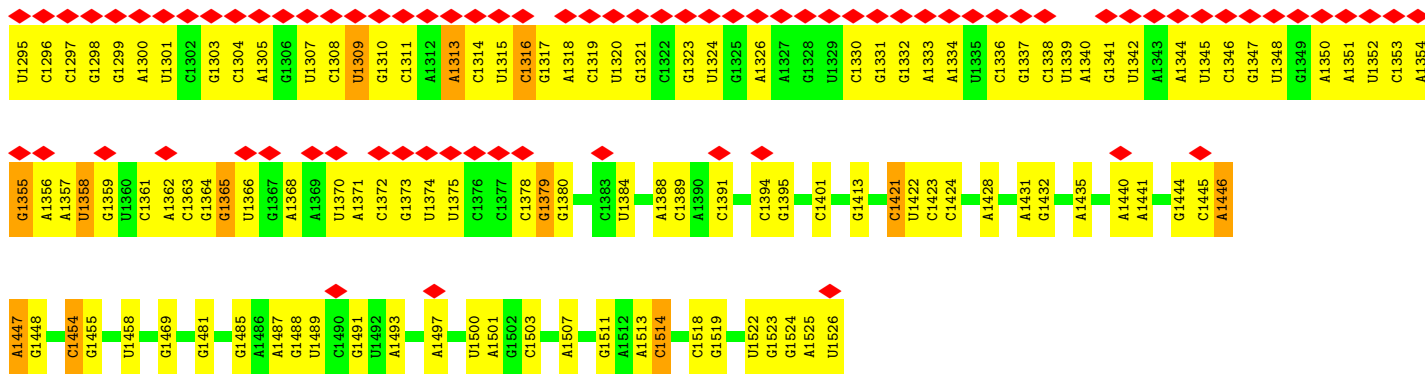
Chain 6:  97%



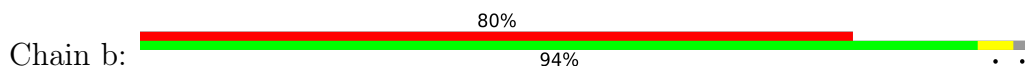
• Molecule 33: 16S rRNA

Chain a:  32% 51% 38% 9%

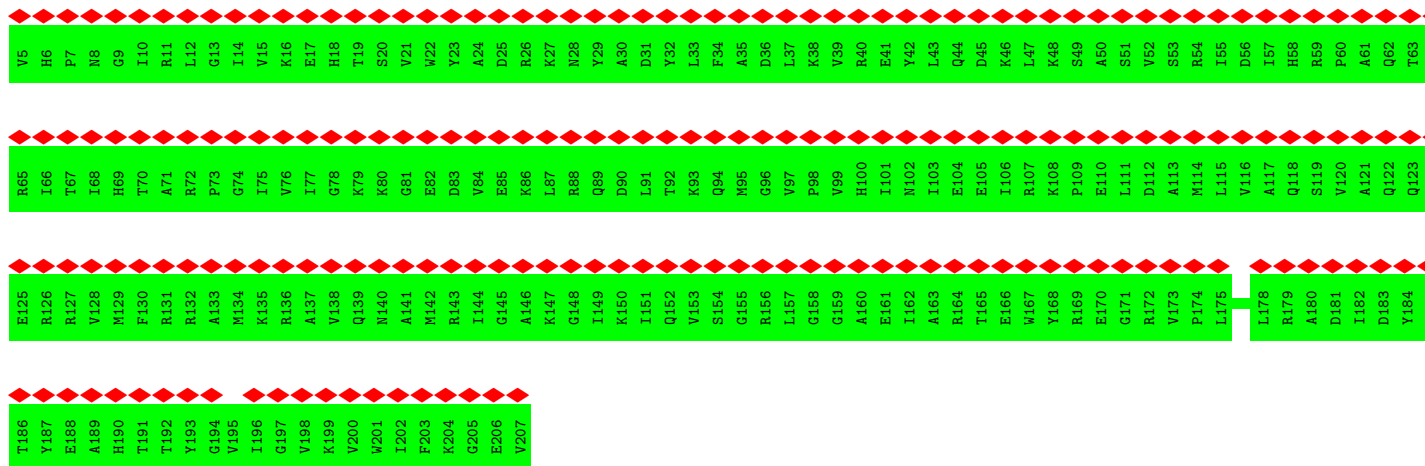




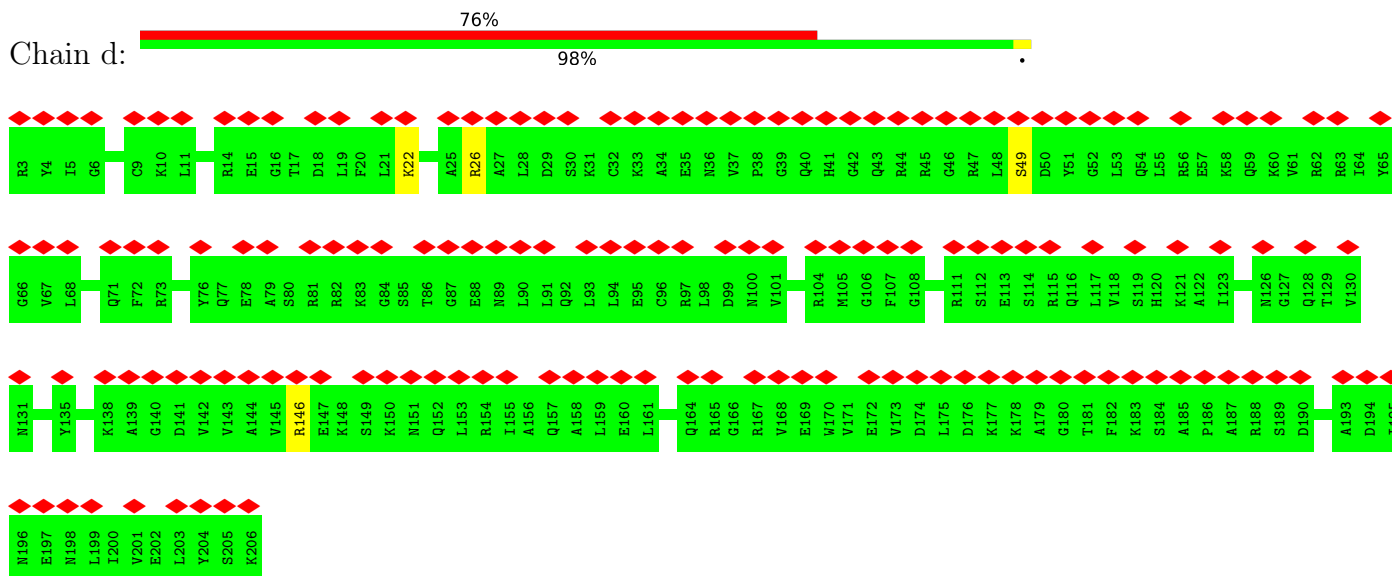
• Molecule 34: 30S ribosomal protein S2



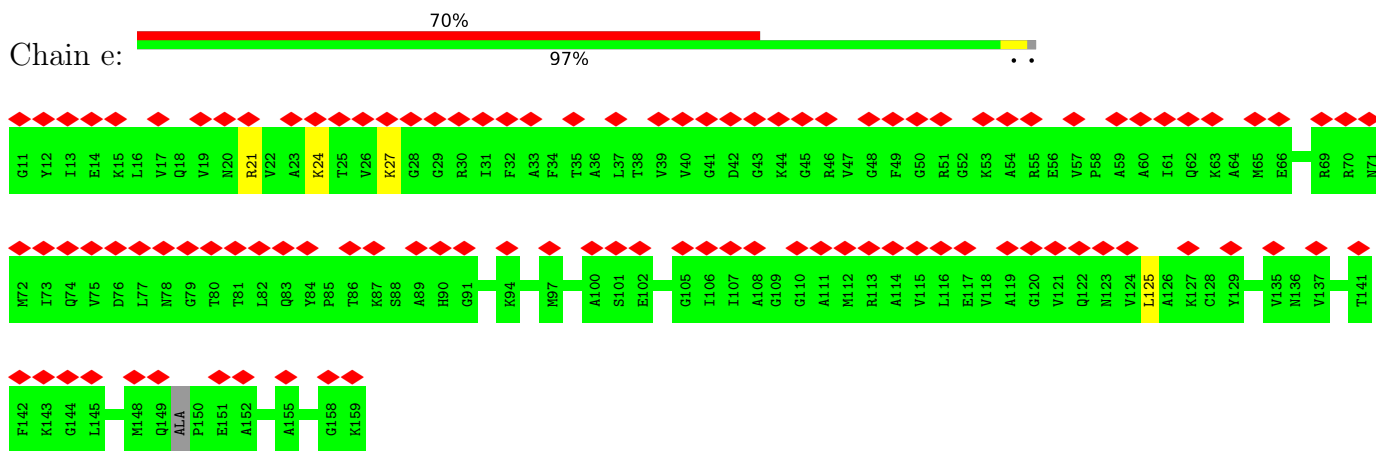
• Molecule 35: 30S ribosomal protein S3



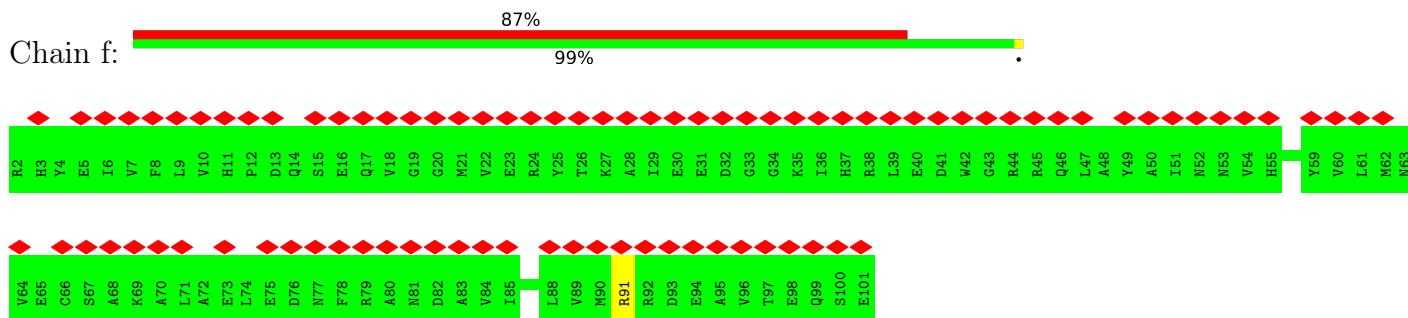
• Molecule 36: 30S ribosomal protein S4



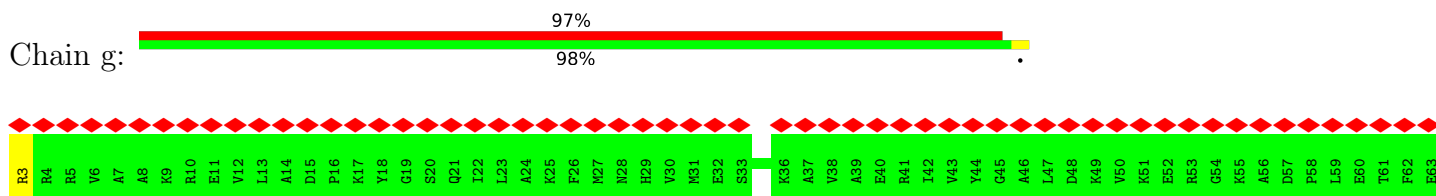
• Molecule 37: 30S ribosomal protein S5

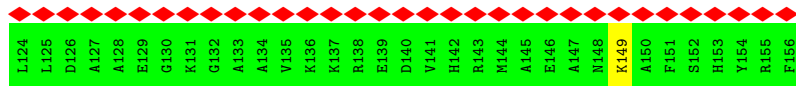
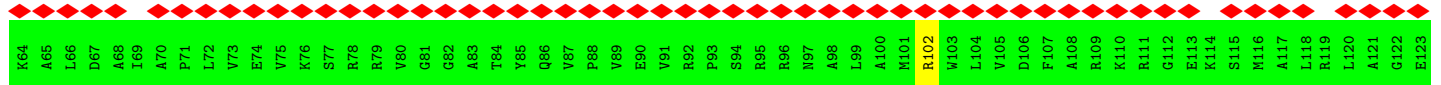


• Molecule 38: 30S ribosomal protein S6

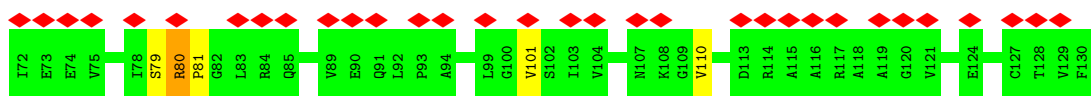
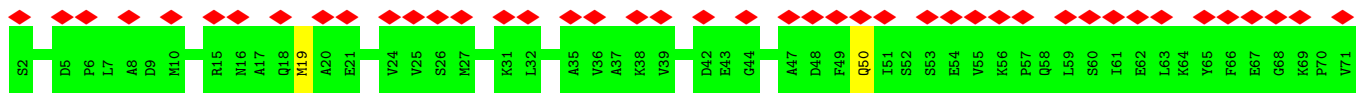
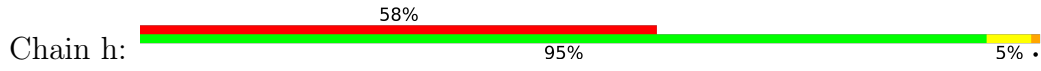


• Molecule 39: 30S ribosomal protein S7

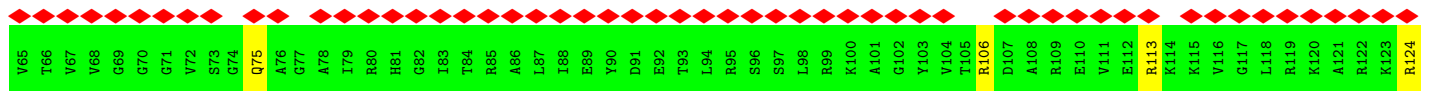
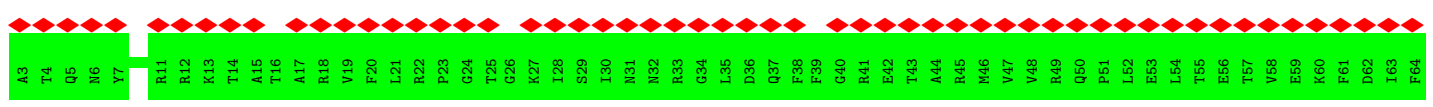
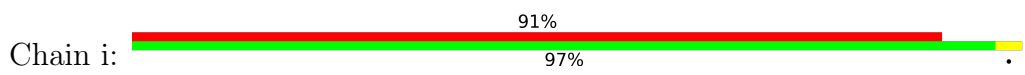




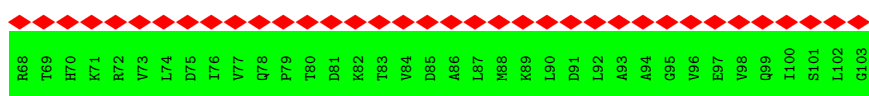
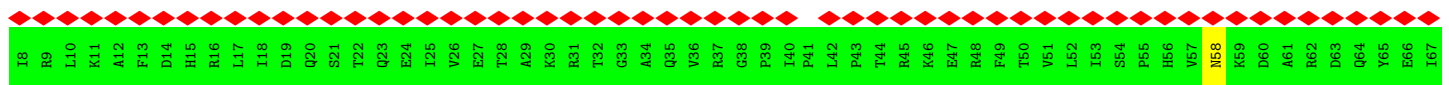
• Molecule 40: 30S ribosomal protein S8



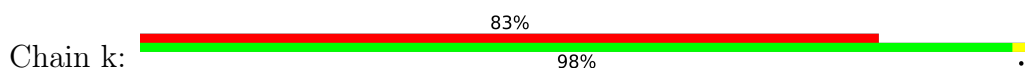
• Molecule 41: 30S ribosomal protein S9

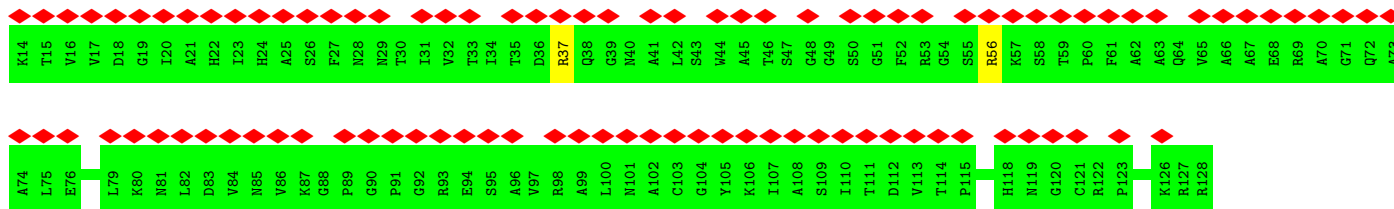


• Molecule 42: 30S ribosomal protein S10



• Molecule 43: 30S ribosomal protein S11





• Molecule 44: 30S ribosomal protein S12



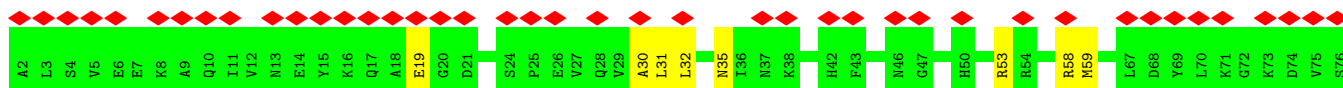
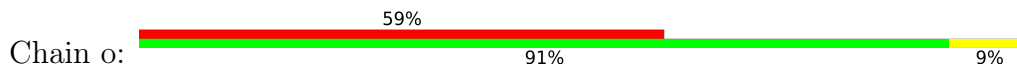
• Molecule 45: 30S ribosomal protein S13

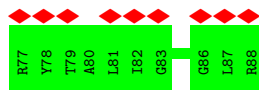


• Molecule 46: 30S ribosomal protein S14

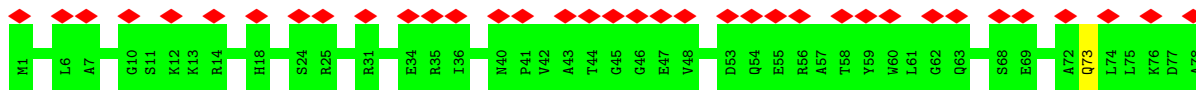


• Molecule 47: 30S ribosomal protein S15

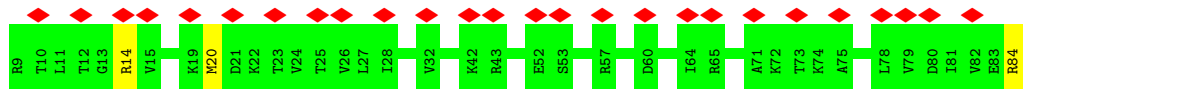




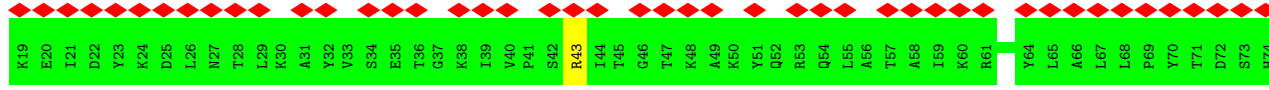
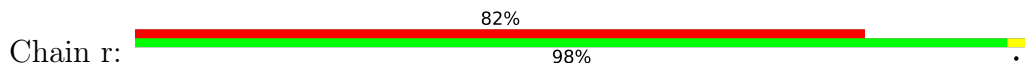
• Molecule 48: 30S ribosomal protein S16



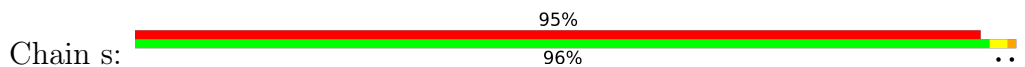
• Molecule 49: 30S ribosomal protein S17



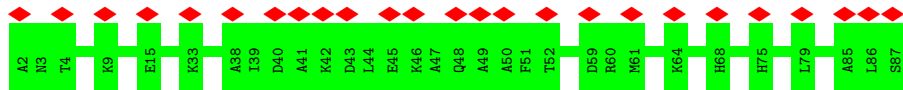
• Molecule 50: 30S ribosomal protein S18



• Molecule 51: 30S ribosomal protein S19



• Molecule 52: 30S ribosomal protein S20



• Molecule 53: 30S ribosomal protein S21



S34	R35	E36	F37	Y38	E39	K40	P41	T42	A43	E44	R45	R46	R47	K48	A49	A50	A51	A52	V53	K54	R55	H56	A57	K58	K59	V60	D61	R62	E63	Q64	R65	R66	R67
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	319022	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	0.788	Depositor
Minimum map value	-0.478	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.0491	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

5.1 Standard geometry

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	0.96	13/69320 (0.0%)	1.26	713/108135 (0.7%)
2	B	0.61	0/2789	1.23	26/4345 (0.6%)
3	C	0.54	0/2084	0.73	0/2800
4	D	0.59	0/1572	0.82	2/2118 (0.1%)
5	E	0.48	0/1529	0.70	1/2060 (0.0%)
6	F	0.32	0/1294	0.73	0/1754
7	G	0.30	0/1280	0.62	0/1726
8	H	0.30	0/580	0.60	1/781 (0.1%)
9	I	0.32	0/1041	0.66	0/1408
10	J	0.52	0/1148	0.66	1/1549 (0.1%)
11	K	0.58	0/931	0.74	1/1247 (0.1%)
12	L	0.48	0/1075	0.69	1/1432 (0.1%)
13	M	0.37	0/1096	0.60	0/1466
14	N	0.51	0/975	0.71	0/1304
15	O	0.33	0/888	0.74	2/1183 (0.2%)
16	P	0.52	0/910	0.72	1/1218 (0.1%)
17	Q	0.59	0/946	0.71	2/1257 (0.2%)
18	R	0.48	0/814	0.67	0/1091
19	S	0.49	0/837	0.64	0/1114
20	T	0.47	0/742	0.74	2/993 (0.2%)
21	U	0.39	0/809	0.65	0/1079
22	V	0.36	0/1420	0.71	1/1927 (0.1%)
23	W	0.51	0/582	0.87	1/773 (0.1%)
24	X	0.45	0/637	0.62	0/849
25	Y	0.36	0/471	0.71	1/630 (0.2%)
26	Z	0.46	0/449	0.67	0/602
27	1	0.27	0/235	0.51	0/318
28	2	0.51	0/425	0.66	1/568 (0.2%)
29	3	0.38	0/415	0.73	1/554 (0.2%)
30	4	0.60	0/367	0.84	1/482 (0.2%)
31	5	0.40	0/507	0.73	0/664
32	6	0.36	0/304	0.69	0/399
33	a	0.78	11/33391 (0.0%)	1.55	179/52073 (0.3%)
34	b	0.30	0/1724	0.64	2/2319 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	c	0.26	0/1638	0.56	0/2209
36	d	0.28	0/1615	0.60	0/2163
37	e	0.32	0/1106	0.66	0/1488
38	f	0.31	0/815	0.69	0/1098
39	g	0.30	0/1207	0.61	0/1616
40	h	0.29	0/976	0.66	0/1314
41	i	0.30	0/1006	0.65	0/1347
42	j	0.27	0/773	0.58	0/1045
43	k	0.28	0/848	0.57	0/1152
44	l	0.32	0/955	0.66	0/1280
45	m	0.28	0/853	0.66	1/1144 (0.1%)
46	n	0.29	0/786	0.60	0/1047
47	o	0.30	0/698	0.74	2/933 (0.2%)
48	p	0.31	0/620	0.65	0/835
49	q	0.28	0/627	0.59	0/844
50	r	0.27	0/450	0.53	0/608
51	s	4.72	1/649 (0.2%)	0.68	0/874
52	t	0.29	0/669	0.55	0/891
53	u	0.29	0/298	0.46	0/391
All	All	0.84	25/150176 (0.0%)	1.21	943/224497 (0.4%)

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
3	C	0	2
4	D	0	10
5	E	0	1
6	F	0	2
9	I	0	2
16	P	0	1
17	Q	0	1
18	R	0	1
22	V	0	3
29	3	0	1
36	d	0	1
40	h	0	3
41	i	0	1
44	l	0	1
45	m	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
46	n	0	1
47	o	0	1
48	p	0	1
51	s	0	1
All	All	0	36

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	s	3	ARG	CB-CG	120.12	4.76	1.52
33	a	1313	A	N3-C4	56.98	1.69	1.34
33	a	1313	A	C6-N1	52.01	1.72	1.35
33	a	1219	A	N9-C4	43.52	1.64	1.37
33	a	1313	A	C5-C4	41.61	1.67	1.38
33	a	1313	A	N1-C2	37.93	1.68	1.34
33	a	1313	A	C2-N3	37.19	1.67	1.33
33	a	1313	A	C5-C6	35.77	1.73	1.41
33	a	1219	A	N9-C8	-25.82	1.17	1.37
33	a	1219	A	N3-C4	20.39	1.47	1.34
33	a	1219	A	C8-N7	14.34	1.41	1.31
1	A	519	A	N9-C4	-9.04	1.32	1.37
1	A	1011	A	N9-C4	-7.97	1.33	1.37
1	A	1133	A	N9-C4	-7.12	1.33	1.37
33	a	1219	A	N7-C5	-6.73	1.35	1.39
1	A	2254	A	N9-C4	-6.56	1.33	1.37
1	A	2863	A	N9-C4	5.78	1.41	1.37
1	A	766	G	C2-N3	-5.59	1.28	1.32
1	A	519	A	N3-C4	-5.23	1.31	1.34
1	A	773	A	N9-C4	-5.10	1.34	1.37
1	A	1771	A	N7-C5	-5.09	1.36	1.39
1	A	1790	A	N9-C4	-5.09	1.34	1.37
1	A	1191	A	N9-C4	-5.07	1.34	1.37
1	A	1559	A	N9-C4	-5.07	1.34	1.37
1	A	560	G	N7-C5	-5.03	1.36	1.39

All (943) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	1219	A	N7-C8-N9	-145.93	40.83	113.80
33	a	1219	A	C4-C5-N7	-137.41	42.00	110.70
33	a	1219	A	C8-N9-C4	-132.12	52.95	105.80
33	a	1219	A	C5-N7-C8	58.62	133.21	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	1219	A	C6-C5-N7	37.35	158.44	132.30
33	a	1313	A	N1-C2-N3	-35.36	111.62	129.30
33	a	1313	A	C2-N3-C4	30.18	125.69	110.60
33	a	1219	A	N3-C4-N9	20.63	143.91	127.40
33	a	1219	A	N9-C4-C5	-18.08	98.57	105.80
33	a	1219	A	C2-N3-C4	17.80	119.50	110.60
33	a	1219	A	C5-C6-N1	15.42	125.41	117.70
33	a	1219	A	C4-N9-C1'	15.38	153.98	126.30
33	a	1219	A	C8-N9-C1'	-14.81	101.05	127.70
33	a	1313	A	C6-N1-C2	14.74	127.44	118.60
33	a	1313	A	N7-C8-N9	14.53	121.07	113.80
33	a	1514	C	N1-C2-O2	13.89	127.23	118.90
33	a	1219	A	N3-C4-C5	-13.25	117.52	126.80
1	A	1154	G	C2-N3-C4	12.61	118.20	111.90
33	a	1313	A	N3-C4-N9	11.78	136.83	127.40
33	a	1514	C	C2-N1-C1'	11.78	131.76	118.80
33	a	1316	C	N1-C2-O2	11.66	125.90	118.90
1	A	540	U	N3-C2-O2	-11.53	114.13	122.20
1	A	540	U	N1-C2-O2	11.05	130.53	122.80
1	A	2410	U	N1-C2-O2	10.97	130.48	122.80
1	A	863	G	O5'-P-OP1	-10.89	95.90	105.70
1	A	1506	C	C6-N1-C2	-10.89	115.94	120.30
1	A	2410	U	C2-N1-C1'	10.84	130.71	117.70
1	A	1596	C	N1-C2-O2	10.81	125.38	118.90
1	A	2304	C	N1-C2-O2	10.70	125.32	118.90
1	A	1506	C	C2-N1-C1'	10.53	130.38	118.80
33	a	1514	C	N3-C2-O2	-10.44	114.59	121.90
1	A	818	U	N1-C2-O2	10.30	130.01	122.80
1	A	1506	C	N1-C2-O2	10.30	125.08	118.90
1	A	1154	G	N3-C4-C5	-10.19	123.50	128.60
1	A	2021	U	N3-C2-O2	-10.16	115.09	122.20
1	A	2304	C	C2-N1-C1'	10.07	129.88	118.80
1	A	1125	C	N1-C2-O2	10.02	124.91	118.90
1	A	1300	U	C2-N1-C1'	10.01	129.71	117.70
1	A	2830	G	N3-C2-N2	10.01	126.90	119.90
1	A	2830	G	N1-C2-N2	-9.90	107.29	116.20
1	A	2410	U	N3-C2-O2	-9.83	115.32	122.20
1	A	818	U	C2-N1-C1'	9.79	129.44	117.70
1	A	1125	C	N3-C2-O2	-9.71	115.10	121.90
1	A	265	A	O4'-C1'-N9	9.70	115.96	108.20
1	A	1968	A	N7-C8-N9	9.67	118.64	113.80
1	A	818	U	N3-C2-O2	-9.61	115.47	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	1316	C	N3-C2-O2	-9.58	115.19	121.90
1	A	2280	C	C5-C6-N1	9.54	125.77	121.00
1	A	519	A	C2-N3-C4	-9.49	105.85	110.60
1	A	535	C	N1-C2-O2	9.49	124.59	118.90
1	A	2280	C	C6-N1-C2	-9.40	116.54	120.30
1	A	503	G	O4'-C1'-N9	9.33	115.66	108.20
1	A	2031	C	C6-N1-C2	-9.29	116.58	120.30
1	A	2742	C	C2-N1-C1'	9.24	128.97	118.80
1	A	2653	C	C2-N1-C1'	9.24	128.96	118.80
1	A	2742	C	N1-C2-O2	9.21	124.42	118.90
1	A	1301	C	C5-C6-N1	9.19	125.60	121.00
1	A	1596	C	N3-C2-O2	-9.16	115.49	121.90
1	A	1154	G	N3-C4-N9	9.16	131.50	126.00
1	A	2367	U	N3-C2-O2	-9.06	115.86	122.20
1	A	773	A	N7-C8-N9	9.06	118.33	113.80
1	A	2357	G	N3-C4-C5	-9.05	124.07	128.60
33	a	1316	C	C2-N1-C1'	9.04	128.74	118.80
1	A	836	U	N3-C2-O2	-8.99	115.91	122.20
1	A	2857	C	N1-C2-O2	8.98	124.29	118.90
33	a	176	C	N1-C2-O2	8.98	124.28	118.90
33	a	1313	A	N9-C4-C5	-8.97	102.21	105.80
1	A	1506	C	N3-C2-O2	-8.95	115.64	121.90
1	A	2583	U	N3-C2-O2	-8.93	115.95	122.20
1	A	2830	G	N3-C4-N9	8.93	131.36	126.00
1	A	1009	U	C2-N1-C1'	8.92	128.40	117.70
1	A	1596	C	C2-N1-C1'	8.92	128.61	118.80
1	A	2653	C	N1-C2-O2	8.88	124.23	118.90
1	A	2863	A	C2-N3-C4	8.81	115.01	110.60
30	4	42	LEU	CA-CB-CG	8.81	135.56	115.30
1	A	1301	C	N1-C2-O2	8.66	124.10	118.90
1	A	773	A	C5-N7-C8	-8.66	99.57	103.90
1	A	519	A	N3-C4-N9	-8.61	120.51	127.40
1	A	2460	U	C2-N1-C1'	8.52	127.92	117.70
1	A	535	C	N3-C2-O2	-8.48	115.97	121.90
1	A	1968	A	C8-N9-C4	-8.45	102.42	105.80
1	A	2339	A	N1-C6-N6	-8.42	113.55	118.60
1	A	2710	C	C6-N1-C2	-8.40	116.94	120.30
1	A	1972	C	N1-C2-O2	8.35	123.91	118.90
33	a	1313	A	N3-C4-C5	-8.34	120.96	126.80
1	A	2857	C	C6-N1-C2	-8.34	116.96	120.30
47	o	31	LEU	CA-CB-CG	8.33	134.45	115.30
33	a	1219	A	N1-C2-N3	-8.31	125.15	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	1514	C	C6-N1-C1'	-8.30	110.84	120.80
1	A	359	U	N1-C2-O2	8.29	128.60	122.80
33	a	1024	U	C2-N1-C1'	8.29	127.65	117.70
33	a	576	U	C2-N1-C1'	8.29	127.64	117.70
1	A	1131	U	N3-C2-O2	-8.24	116.43	122.20
22	V	166	LYS	C-N-CA	8.24	142.31	121.70
1	A	2042	C	C2-N1-C1'	8.23	127.85	118.80
1	A	1572	C	N1-C2-O2	8.21	123.83	118.90
1	A	22	C	C6-N1-C2	-8.16	117.03	120.30
1	A	2583	U	C2-N1-C1'	8.13	127.46	117.70
1	A	2304	C	N3-C2-O2	-8.13	116.21	121.90
1	A	836	U	C2-N1-C1'	8.13	127.45	117.70
33	a	1313	A	C4-C5-N7	-8.12	106.64	110.70
1	A	115	C	N1-C2-O2	8.10	123.76	118.90
1	A	988	C	N1-C2-O2	8.10	123.76	118.90
1	A	2812	U	N3-C2-O2	-8.10	116.53	122.20
25	Y	21	LEU	CA-CB-CG	8.10	133.93	115.30
1	A	1506	C	C5-C6-N1	8.09	125.05	121.00
33	a	748	C	C2-N1-C1'	8.09	127.70	118.80
1	A	2865	U	C2-N1-C1'	8.09	127.41	117.70
33	a	369	U	C2-N1-C1'	8.07	127.38	117.70
1	A	1050	U	C2-N1-C1'	8.06	127.38	117.70
1	A	293	A	N7-C8-N9	8.06	117.83	113.80
1	A	2541	U	C2-N1-C1'	8.06	127.37	117.70
1	A	2849	G	N3-C4-C5	-8.03	124.59	128.60
1	A	1745	U	N3-C2-O2	-8.02	116.59	122.20
1	A	1131	U	N1-C2-O2	8.01	128.41	122.80
1	A	1300	U	N1-C2-O2	8.01	128.41	122.80
1	A	2653	C	N3-C2-O2	-8.01	116.30	121.90
1	A	1011	A	N3-C4-N9	-8.00	121.00	127.40
1	A	113	C	C2-N1-C1'	8.00	127.60	118.80
1	A	2830	G	C4-N9-C1'	7.99	136.89	126.50
1	A	2460	U	N1-C2-O2	7.99	128.39	122.80
1	A	836	U	N1-C2-O2	7.99	128.39	122.80
1	A	1020	C	C2-N1-C1'	7.98	127.58	118.80
1	A	348	U	C2-N1-C1'	7.96	127.25	117.70
1	A	1301	C	C6-N1-C2	-7.94	117.12	120.30
1	A	2259	U	N3-C2-O2	-7.91	116.66	122.20
1	A	2742	C	N3-C2-O2	-7.91	116.36	121.90
1	A	972	C	N3-C2-O2	-7.89	116.38	121.90
1	A	2021	U	N1-C2-O2	7.89	128.32	122.80
1	A	1131	U	C2-N1-C1'	7.89	127.17	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	748	C	N1-C2-O2	7.89	123.63	118.90
1	A	2357	G	C8-N9-C4	-7.88	103.25	106.40
1	A	862	C	N1-C2-O2	7.87	123.62	118.90
1	A	198	C	C5-C6-N1	7.86	124.93	121.00
1	A	1107	C	N1-C2-O2	7.86	123.61	118.90
1	A	800	U	C5-C6-N1	7.85	126.63	122.70
1	A	2304	C	C6-N1-C2	-7.85	117.16	120.30
1	A	2357	G	C4-N9-C1'	7.83	136.68	126.50
1	A	2367	U	N1-C2-O2	7.83	128.28	122.80
1	A	1107	C	C2-N1-C1'	7.82	127.40	118.80
1	A	738	G	O4'-C1'-N9	7.81	114.45	108.20
1	A	359	U	N3-C2-O2	-7.78	116.76	122.20
1	A	2812	U	C2-N1-C1'	7.75	127.00	117.70
1	A	1745	U	N1-C2-O2	7.75	128.22	122.80
1	A	2812	U	N1-C2-O2	7.74	128.22	122.80
33	a	324	C	N1-C2-O2	7.74	123.54	118.90
1	A	1938	U	N3-C2-O2	-7.74	116.78	122.20
1	A	862	C	C6-N1-C2	-7.72	117.21	120.30
33	a	576	U	N3-C2-O2	-7.72	116.80	122.20
1	A	63	A	O5'-P-OP2	-7.72	98.75	105.70
1	A	964	A	N7-C8-N9	7.72	117.66	113.80
34	b	101	LEU	CA-CB-CG	7.71	133.03	115.30
1	A	1300	U	N3-C2-O2	-7.69	116.82	122.20
1	A	862	C	N3-C2-O2	-7.62	116.57	121.90
33	a	1316	C	C6-N1-C2	-7.60	117.26	120.30
1	A	2857	C	C2-N1-C1'	7.58	127.14	118.80
1	A	198	C	C6-N1-C2	-7.58	117.27	120.30
33	a	176	C	C6-N1-C2	-7.57	117.27	120.30
1	A	1671	G	N7-C8-N9	7.55	116.88	113.10
33	a	1020	G	C4-N9-C1'	7.55	136.31	126.50
1	A	1385	C	N1-C2-O2	7.54	123.43	118.90
1	A	981	C	C6-N1-C2	-7.54	117.28	120.30
33	a	262	C	N1-C2-O2	7.54	123.42	118.90
1	A	293	A	C8-N9-C4	-7.53	102.79	105.80
33	a	1358	U	C2-N1-C1'	7.53	126.73	117.70
33	a	1204	C	N1-C2-O2	7.52	123.41	118.90
1	A	2653	C	C6-N1-C2	-7.52	117.29	120.30
1	A	2849	G	C2-N3-C4	7.51	115.66	111.90
1	A	519	A	N3-C4-C5	7.50	132.05	126.80
1	A	1301	C	C2-N1-C1'	7.50	127.05	118.80
1	A	2830	G	C8-N9-C1'	-7.47	117.29	127.00
1	A	2410	U	C6-N1-C1'	-7.46	110.75	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	1424	C	N1-C2-O2	7.46	123.38	118.90
1	A	1107	C	N3-C2-O2	-7.46	116.68	121.90
1	A	540	U	C2-N1-C1'	7.45	126.64	117.70
33	a	176	C	C2-N1-C1'	7.44	126.99	118.80
1	A	348	U	N1-C2-O2	7.44	128.01	122.80
1	A	1572	C	C2-N1-C1'	7.44	126.98	118.80
33	a	176	C	N3-C2-O2	-7.42	116.70	121.90
1	A	1557	A	C8-N9-C4	7.42	108.77	105.80
1	A	2367	U	C2-N1-C1'	7.41	126.59	117.70
1	A	2003	U	C2-N1-C1'	7.41	126.59	117.70
1	A	981	C	C5-C6-N1	7.39	124.69	121.00
1	A	113	C	N3-C2-O2	-7.39	116.73	121.90
33	a	1514	C	C6-N1-C2	-7.38	117.35	120.30
1	A	2460	U	N3-C2-O2	-7.36	117.05	122.20
1	A	2042	C	N1-C2-O2	7.35	123.31	118.90
17	Q	18	LEU	CA-CB-CG	7.35	132.20	115.30
1	A	1011	A	C2-N3-C4	-7.34	106.93	110.60
1	A	2254	A	N3-C4-N9	-7.34	121.53	127.40
1	A	126	A	O4'-C1'-N9	7.33	114.07	108.20
1	A	2361	C	C5-C6-N1	7.33	124.67	121.00
33	a	34	C	C2-N1-C1'	7.31	126.84	118.80
1	A	1741	A	O4'-C1'-N9	7.30	114.04	108.20
1	A	2199	A	N7-C8-N9	7.30	117.45	113.80
1	A	989	U	N1-C2-O2	7.29	127.91	122.80
1	A	2361	C	C6-N1-C2	-7.28	117.39	120.30
1	A	2857	C	N3-C2-O2	-7.27	116.81	121.90
1	A	1671	G	C8-N9-C4	-7.26	103.50	106.40
1	A	1622	A	N7-C8-N9	7.26	117.43	113.80
1	A	2830	G	N9-C4-C5	-7.25	102.50	105.40
1	A	955	C	C6-N1-C2	-7.23	117.41	120.30
1	A	69	C	N1-C2-O2	7.22	123.23	118.90
1	A	818	U	C6-N1-C1'	-7.22	111.10	121.20
1	A	1166	G	P-O3'-C3'	7.21	128.36	119.70
1	A	79	C	C6-N1-C2	-7.21	117.42	120.30
1	A	548	U	O5'-P-OP1	-7.21	99.21	105.70
1	A	1009	U	N3-C2-O2	-7.21	117.15	122.20
1	A	535	C	C2-N1-C1'	7.21	126.73	118.80
1	A	974	A	O4'-C1'-N9	7.20	113.96	108.20
2	B	18	G	C5-C6-O6	-7.19	124.29	128.60
33	a	159	G	P-O3'-C3'	7.17	128.31	119.70
1	A	69	C	C5-C6-N1	7.16	124.58	121.00
1	A	359	U	C2-N1-C1'	7.16	126.29	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2252	U	N3-C2-O2	-7.16	117.19	122.20
1	A	2633	C	C6-N1-C2	-7.16	117.44	120.30
1	A	2836	U	N3-C2-O2	-7.15	117.19	122.20
1	A	2829	G	C4-C5-N7	-7.14	107.94	110.80
1	A	2710	C	C5-C6-N1	7.13	124.57	121.00
1	A	1125	C	C6-N1-C2	-7.12	117.45	120.30
1	A	773	A	C8-N9-C4	-7.11	102.95	105.80
1	A	922	G	C4-N9-C1'	7.11	135.75	126.50
1	A	2021	U	C2-N1-C1'	7.09	126.21	117.70
1	A	958	C	C6-N1-C2	-7.08	117.47	120.30
1	A	348	U	N3-C2-O2	-7.07	117.25	122.20
1	A	920	C	P-O3'-C3'	7.07	128.19	119.70
1	A	2374	U	C2-N1-C1'	7.07	126.18	117.70
1	A	2830	G	C4-C5-N7	7.06	113.62	110.80
33	a	1020	G	N3-C4-C5	-7.04	125.08	128.60
1	A	2836	U	N1-C2-O2	7.04	127.73	122.80
1	A	115	C	N3-C2-O2	-6.99	117.01	121.90
33	a	34	C	N1-C2-O2	6.99	123.09	118.90
1	A	2583	U	N1-C2-O2	6.98	127.69	122.80
1	A	1503	G	N3-C4-C5	-6.98	125.11	128.60
1	A	971	A	O4'-C1'-N9	6.97	113.78	108.20
1	A	1938	U	C2-N1-C1'	6.97	126.06	117.70
1	A	728	C	N1-C2-O2	6.97	123.08	118.90
20	T	22	LEU	CA-CB-CG	6.96	131.31	115.30
33	a	1227	G	C4-N9-C1'	6.96	135.55	126.50
1	A	1972	C	N3-C2-O2	-6.96	117.03	121.90
1	A	264	U	O4'-C1'-N1	6.95	113.76	108.20
1	A	1943	U	N1-C2-O2	6.92	127.65	122.80
1	A	475	C	C5-C6-N1	6.92	124.46	121.00
1	A	2867	C	N1-C2-O2	6.90	123.04	118.90
2	B	25	A	P-O3'-C3'	6.89	127.97	119.70
1	A	2849	G	N3-C4-N9	6.89	130.13	126.00
1	A	1622	A	C5-N7-C8	-6.88	100.46	103.90
1	A	2060	C	N1-C2-O2	6.88	123.03	118.90
33	a	1216	G	N3-C4-C5	-6.87	125.16	128.60
1	A	988	C	N3-C2-O2	-6.87	117.09	121.90
1	A	1596	C	C6-N1-C1'	-6.85	112.58	120.80
1	A	113	C	N1-C2-O2	6.85	123.01	118.90
2	B	18	G	C6-C5-N7	-6.85	126.29	130.40
1	A	641	G	C6-C5-N7	6.83	134.50	130.40
1	A	2849	G	C4-N9-C1'	6.83	135.38	126.50
33	a	369	U	N3-C2-O2	-6.82	117.43	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	728	C	N3-C2-O2	-6.82	117.13	121.90
1	A	2541	U	N1-C2-O2	6.80	127.56	122.80
11	K	91	GLN	C-N-CA	6.80	138.70	121.70
33	a	369	U	N1-C2-O2	6.80	127.56	122.80
33	a	1024	U	N1-C2-O2	6.78	127.54	122.80
33	a	1358	U	N1-C2-O2	6.78	127.54	122.80
1	A	22	C	C5-C6-N1	6.76	124.38	121.00
1	A	62	U	OP2-P-O3'	6.76	120.08	105.20
1	A	547	C	C6-N1-C2	-6.76	117.59	120.30
1	A	1787	C	N3-C2-O2	-6.76	117.17	121.90
33	a	1060	C	C2-N1-C1'	6.75	126.23	118.80
1	A	1125	C	C2-N1-C1'	6.75	126.22	118.80
1	A	2830	G	C6-C5-N7	-6.73	126.36	130.40
1	A	2836	U	C2-N1-C1'	6.72	125.77	117.70
33	a	1142	U	C2-N1-C1'	6.72	125.77	117.70
33	a	324	C	N3-C2-O2	-6.71	117.20	121.90
1	A	1791	C	C6-N1-C2	-6.71	117.62	120.30
33	a	34	C	N3-C2-O2	-6.70	117.21	121.90
1	A	1009	U	N1-C2-O2	6.69	127.48	122.80
33	a	673	U	C2-N1-C1'	6.68	125.72	117.70
1	A	2526	C	N1-C2-O2	6.68	122.91	118.90
1	A	1958	U	C2-N1-C1'	6.67	125.71	117.70
2	B	42	C	C2-N1-C1'	6.67	126.14	118.80
33	a	1514	C	C5-C6-N1	6.66	124.33	121.00
1	A	2374	U	N3-C2-O2	-6.66	117.54	122.20
1	A	1943	U	N3-C2-O2	-6.66	117.54	122.20
1	A	922	G	N3-C4-N9	6.65	129.99	126.00
33	a	262	C	N3-C2-O2	-6.65	117.25	121.90
1	A	428	U	C5-C6-N1	6.63	126.02	122.70
1	A	113	C	C6-N1-C2	-6.63	117.65	120.30
1	A	1300	U	C6-N1-C1'	-6.63	111.92	121.20
1	A	2304	C	C6-N1-C1'	-6.63	112.85	120.80
1	A	1369	G	O4'-C1'-N9	6.62	113.50	108.20
1	A	1048	G	P-O3'-C3'	6.62	127.64	119.70
33	a	576	U	N1-C2-O2	6.61	127.43	122.80
33	a	1020	G	N3-C4-N9	6.61	129.97	126.00
1	A	16	C	N1-C2-O2	6.59	122.85	118.90
1	A	2339	A	N9-C4-C5	6.59	108.44	105.80
1	A	1011	A	N3-C4-C5	6.58	131.41	126.80
33	a	1227	G	N3-C4-C5	-6.58	125.31	128.60
1	A	1987	C	C6-N1-C2	-6.56	117.67	120.30
1	A	1572	C	N3-C2-O2	-6.56	117.31	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1958	U	N1-C2-O2	6.56	127.39	122.80
1	A	2003	U	N3-C2-O2	-6.56	117.61	122.20
5	E	179	LEU	CA-CB-CG	6.56	130.38	115.30
1	A	16	C	C6-N1-C2	-6.55	117.68	120.30
1	A	954	C	C6-N1-C2	-6.55	117.68	120.30
1	A	2541	U	N3-C2-O2	-6.55	117.62	122.20
1	A	2865	U	N3-C2-O2	-6.54	117.62	122.20
1	A	1629	C	N3-C2-O2	-6.54	117.32	121.90
1	A	1913	U	C2-N1-C1'	6.54	125.55	117.70
33	a	159	G	OP1-P-O3'	6.53	119.56	105.20
1	A	1980	U	N3-C2-O2	-6.51	117.64	122.20
1	A	2811	C	C6-N1-C2	-6.51	117.69	120.30
1	A	2742	C	C6-N1-C1'	-6.50	112.99	120.80
1	A	682	C	N1-C2-O2	6.50	122.80	118.90
1	A	2304	C	C5-C6-N1	6.50	124.25	121.00
1	A	116	U	N1-C2-O2	6.50	127.35	122.80
1	A	2811	C	C5-C6-N1	6.50	124.25	121.00
1	A	700	U	N1-C2-O2	6.49	127.34	122.80
1	A	1775	C	C6-N1-C2	-6.49	117.70	120.30
33	a	465	U	C2-N1-C1'	6.49	125.48	117.70
1	A	2060	C	N3-C2-O2	-6.48	117.36	121.90
1	A	640	C	C6-N1-C2	-6.48	117.71	120.30
33	a	1227	G	N3-C4-N9	6.48	129.89	126.00
33	a	1446	A	OP1-P-O3'	6.47	119.44	105.20
1	A	698	G	C4-N9-C1'	6.47	134.91	126.50
1	A	1745	U	C2-N1-C1'	6.47	125.47	117.70
1	A	2329	C	C6-N1-C2	-6.47	117.71	120.30
20	T	60	LEU	CB-CG-CD2	-6.47	100.00	111.00
33	a	306	C	N1-C2-O2	6.45	122.77	118.90
1	A	973	A	C4-C5-N7	6.44	113.92	110.70
1	A	2259	U	C2-N1-C1'	6.44	125.43	117.70
1	A	2006	A	N1-C2-N3	-6.43	126.09	129.30
1	A	1671	G	C6-C5-N7	-6.42	126.55	130.40
2	B	27	C	C6-N1-C2	-6.41	117.74	120.30
1	A	1938	U	N1-C2-O2	6.40	127.28	122.80
1	A	2339	A	C5-C6-N6	6.39	128.81	123.70
1	A	2391	U	N1-C2-O2	6.39	127.28	122.80
15	O	49	LEU	CA-CB-CG	6.39	130.00	115.30
1	A	1107	C	C6-N1-C2	-6.39	117.75	120.30
33	a	1446	A	P-O3'-C3'	6.38	127.35	119.70
1	A	475	C	C6-N1-C2	-6.37	117.75	120.30
17	Q	18	LEU	CB-CG-CD2	-6.37	100.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1930	U	C2-N1-C1'	6.37	125.34	117.70
1	A	1918	U	C5-C6-N1	6.37	125.88	122.70
1	A	2042	C	N3-C2-O2	-6.36	117.45	121.90
1	A	69	C	C2-N1-C1'	6.35	125.79	118.80
2	B	18	G	N1-C6-O6	6.35	123.71	119.90
33	a	748	C	N3-C2-O2	-6.35	117.45	121.90
1	A	554	C	C6-N1-C2	-6.34	117.76	120.30
1	A	2417	A	C2-N3-C4	6.34	113.77	110.60
1	A	62	U	P-O3'-C3'	6.34	127.31	119.70
1	A	1629	C	N1-C2-O2	6.33	122.70	118.90
1	A	2199	A	C8-N9-C4	-6.33	103.27	105.80
33	a	1216	G	N3-C4-N9	6.32	129.79	126.00
1	A	1363	C	C5-C6-N1	6.32	124.16	121.00
1	A	2274	A	P-O3'-C3'	6.31	127.28	119.70
1	A	2546	C	C6-N1-C2	-6.31	117.78	120.30
2	B	42	C	N1-C2-O2	6.31	122.69	118.90
1	A	1088	A	P-O3'-C3'	6.30	127.27	119.70
1	A	1020	C	N1-C2-O2	6.30	122.68	118.90
1	A	1761	C	C6-N1-C2	-6.30	117.78	120.30
1	A	1930	U	N3-C2-O2	-6.29	117.80	122.20
1	A	2389	U	P-O3'-C3'	6.29	127.25	119.70
1	A	1500	C	N1-C2-O2	6.29	122.67	118.90
1	A	2857	C	C5-C6-N1	6.29	124.14	121.00
1	A	2254	A	N3-C4-C5	6.28	131.19	126.80
1	A	733	C	C6-N1-C2	-6.27	117.79	120.30
1	A	973	A	O4'-C1'-N9	6.27	113.21	108.20
1	A	726	C	C6-N1-C2	-6.27	117.79	120.30
1	A	1020	C	N3-C2-O2	-6.26	117.52	121.90
1	A	922	G	N3-C4-C5	-6.25	125.47	128.60
1	A	1790	A	C5-N7-C8	-6.25	100.78	103.90
33	a	1216	G	C4-N9-C1'	6.24	134.61	126.50
1	A	1301	C	N3-C2-O2	-6.24	117.54	121.90
1	A	2875	C	C5-C6-N1	6.23	124.11	121.00
33	a	1447	A	O5'-P-OP1	-6.22	100.10	105.70
1	A	1088	A	C2-N3-C4	6.21	113.71	110.60
1	A	614	C	C6-N1-C2	-6.21	117.81	120.30
1	A	641	G	C4-C5-N7	-6.21	108.32	110.80
33	a	1355	G	C4-N9-C1'	6.21	134.57	126.50
33	a	1358	U	N3-C2-O2	-6.21	117.86	122.20
1	A	1220	C	C6-N1-C2	-6.20	117.82	120.30
1	A	1506	C	C6-N1-C1'	-6.20	113.37	120.80
1	A	321	G	O4'-C1'-N9	6.19	113.15	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1133	A	N3-C4-C5	6.19	131.13	126.80
1	A	293	A	C5-N7-C8	-6.19	100.81	103.90
1	A	2252	U	C2-N1-C1'	6.18	125.12	117.70
33	a	203	U	N3-C2-O2	-6.18	117.88	122.20
1	A	2363	A	N1-C6-N6	6.17	122.30	118.60
1	A	699	U	N3-C2-O2	-6.17	117.88	122.20
33	a	399	U	C5-C6-N1	6.17	125.78	122.70
1	A	863	G	N7-C8-N9	6.16	116.18	113.10
1	A	640	C	N3-C2-O2	-6.16	117.59	121.90
1	A	1434	U	C4-C5-C6	6.15	123.39	119.70
1	A	210	C	N1-C2-O2	6.12	122.57	118.90
1	A	1755	C	N1-C2-O2	6.12	122.57	118.90
1	A	2374	U	C4-C5-C6	6.12	123.37	119.70
1	A	2739	C	N1-C2-O2	6.12	122.57	118.90
1	A	922	G	C8-N9-C1'	-6.11	119.05	127.00
1	A	1671	G	C4-N9-C1'	6.11	134.45	126.50
33	a	1489	U	C2-N1-C1'	6.11	125.03	117.70
1	A	1671	G	C5-N7-C8	-6.11	101.25	104.30
1	A	1155	G	C4-C5-N7	6.11	113.24	110.80
1	A	1050	U	C5-C6-N1	6.11	125.75	122.70
47	o	32	LEU	CA-CB-CG	6.10	129.34	115.30
33	a	262	C	C6-N1-C2	-6.10	117.86	120.30
1	A	2315	A	C6-N1-C2	6.09	122.25	118.60
1	A	773	A	C4-C5-N7	6.09	113.74	110.70
1	A	989	U	N3-C2-O2	-6.09	117.94	122.20
15	O	27	LEU	CA-CB-CG	6.09	129.30	115.30
1	A	574	C	N3-C4-C5	6.08	124.33	121.90
1	A	726	C	C5-C6-N1	6.08	124.04	121.00
1	A	2391	U	N3-C2-O2	-6.07	117.95	122.20
1	A	776	C	C6-N1-C2	-6.07	117.87	120.30
2	B	25	A	OP1-P-O3'	6.07	118.56	105.20
1	A	1382	A	O4'-C1'-N9	6.07	113.05	108.20
1	A	92	A	O4'-C1'-N9	6.06	113.05	108.20
33	a	1173	A	C2-N3-C4	6.06	113.63	110.60
1	A	206	U	N3-C2-O2	-6.06	117.96	122.20
1	A	2865	U	N1-C2-O2	6.06	127.04	122.80
33	a	893	C	C6-N1-C2	-6.06	117.88	120.30
1	A	2199	A	C5-N7-C8	-6.06	100.87	103.90
1	A	533	U	N1-C2-O2	6.04	127.03	122.80
1	A	973	A	C5-N7-C8	-6.04	100.88	103.90
1	A	2325	C	N1-C2-O2	6.04	122.52	118.90
33	a	674	C	N1-C2-O2	6.03	122.52	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	901	C	N1-C2-O2	6.03	122.52	118.90
33	a	1060	C	N1-C2-O2	6.03	122.52	118.90
1	A	1062	C	N1-C2-O2	6.03	122.52	118.90
1	A	2348	C	N1-C2-O2	6.02	122.51	118.90
33	a	1489	U	N1-C2-O2	6.02	127.02	122.80
1	A	964	A	O4'-C1'-N9	6.02	113.02	108.20
1	A	1671	G	C4-C5-N7	6.02	113.21	110.80
1	A	955	C	C5-C6-N1	6.01	124.01	121.00
1	A	2133	C	C2-N1-C1'	6.01	125.42	118.80
1	A	964	A	C5-N7-C8	-6.01	100.89	103.90
1	A	2023	C	C6-N1-C2	-6.01	117.90	120.30
1	A	1787	C	N1-C2-O2	6.00	122.50	118.90
1	A	2429	C	N1-C2-O2	6.00	122.50	118.90
1	A	1503	G	N3-C4-N9	6.00	129.60	126.00
1	A	79	C	C5-C6-N1	6.00	124.00	121.00
1	A	503	G	C4-N9-C1'	-6.00	118.71	126.50
1	A	1790	A	N7-C8-N9	5.99	116.80	113.80
1	A	2889	C	N1-C2-O2	5.99	122.50	118.90
1	A	44	A	O4'-C1'-N9	5.99	112.99	108.20
1	A	2308	G	C4-N9-C1'	5.99	134.29	126.50
1	A	2430	C	C6-N1-C2	-5.99	117.91	120.30
2	B	27	C	N1-C2-O2	5.99	122.49	118.90
16	P	98	LEU	CB-CG-CD1	-5.99	100.82	111.00
33	a	1219	A	N1-C6-N6	-5.99	115.01	118.60
33	a	465	U	N3-C2-O2	-5.98	118.01	122.20
1	A	201	C	N1-C2-O2	5.97	122.48	118.90
1	A	699	U	N1-C2-O2	5.97	126.98	122.80
33	a	477	C	N1-C2-O2	5.97	122.48	118.90
1	A	2007	A	N1-C2-N3	-5.97	126.31	129.30
2	B	30	C	C6-N1-C2	-5.97	117.91	120.30
1	A	1972	C	C6-N1-C2	-5.96	117.91	120.30
1	A	2278	U	O4'-C1'-N1	5.96	112.97	108.20
1	A	66	C	C6-N1-C2	-5.96	117.92	120.30
4	D	165	LEU	C-N-CA	-5.96	109.79	122.30
33	a	720	C	C6-N1-C2	-5.96	117.92	120.30
33	a	1234	U	C2-N1-C1'	5.95	124.84	117.70
1	A	2082	A	O4'-C1'-N9	5.95	112.96	108.20
12	L	38	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	995	C	C6-N1-C2	-5.94	117.92	120.30
2	B	42	C	C6-N1-C2	-5.93	117.93	120.30
33	a	1215	G	C4-N9-C1'	5.93	134.21	126.50
1	A	503	G	C8-N9-C1'	5.93	134.71	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	A	P-O3'-C3'	5.92	126.81	119.70
1	A	1009	U	C6-N1-C1'	-5.92	112.91	121.20
1	A	2863	A	N3-C4-N9	5.92	132.14	127.40
1	A	2805	C	N3-C2-O2	-5.92	117.76	121.90
1	A	2118	U	C2-N1-C1'	5.92	124.80	117.70
1	A	2257	A	O4'-C1'-N9	5.91	112.93	108.20
1	A	116	U	N3-C2-O2	-5.91	118.06	122.20
1	A	2293	C	C2-N1-C1'	5.91	125.30	118.80
1	A	1968	A	C4-N9-C1'	5.90	136.93	126.30
1	A	1070	C	P-O3'-C3'	5.90	126.78	119.70
33	a	1020	G	C8-N9-C1'	-5.90	119.33	127.00
33	a	1215	G	N3-C4-C5	-5.89	125.65	128.60
1	A	22	C	N1-C2-O2	5.89	122.44	118.90
1	A	2194	C	C6-N1-C2	-5.89	117.94	120.30
1	A	2653	C	C6-N1-C1'	-5.89	113.73	120.80
1	A	1020	C	C6-N1-C1'	-5.89	113.73	120.80
1	A	1010	A	O4'-C1'-N9	5.89	112.91	108.20
1	A	2360	A	C2-N3-C4	5.88	113.54	110.60
1	A	1756	U	N1-C2-O2	5.88	126.92	122.80
1	A	2731	G	P-O3'-C3'	5.88	126.76	119.70
1	A	2010	C	C6-N1-C2	-5.87	117.95	120.30
1	A	2863	A	N3-C4-C5	-5.87	122.69	126.80
1	A	785	C	C6-N1-C2	-5.87	117.95	120.30
1	A	2194	C	N1-C2-O2	5.87	122.42	118.90
1	A	2279	G	O4'-C1'-N9	5.87	112.90	108.20
33	a	893	C	P-O3'-C3'	5.87	126.74	119.70
1	A	518	C	C2-N1-C1'	5.87	125.25	118.80
1	A	1652	U	N3-C2-O2	-5.87	118.09	122.20
33	a	203	U	C2-N1-C1'	5.87	124.74	117.70
1	A	16	C	N3-C2-O2	-5.86	117.80	121.90
1	A	1050	U	O4'-C1'-N1	5.86	112.89	108.20
33	a	512	C	P-O3'-C3'	5.86	126.73	119.70
1	A	1170	C	C6-N1-C2	-5.86	117.96	120.30
1	A	2865	U	C6-N1-C1'	-5.85	113.00	121.20
1	A	1424	C	N1-C2-O2	5.85	122.41	118.90
1	A	1599	A	C5-N7-C8	-5.85	100.97	103.90
1	A	813	C	C6-N1-C2	-5.85	117.96	120.30
33	a	1234	U	N1-C2-O2	5.85	126.89	122.80
33	a	1024	U	N3-C2-O2	-5.84	118.11	122.20
1	A	879	C	N1-C2-O2	5.84	122.40	118.90
1	A	1634	C	N1-C2-O2	5.83	122.40	118.90
1	A	552	U	C6-N1-C2	-5.83	117.50	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	80	PHE	CB-CG-CD1	5.83	124.88	120.80
1	A	408	C	N1-C2-O2	5.82	122.39	118.90
1	A	766	G	N7-C8-N9	5.82	116.01	113.10
33	a	1155	C	C6-N1-C2	-5.81	117.98	120.30
1	A	1642	A	P-O3'-C3'	5.80	126.67	119.70
1	A	1622	A	O4'-C1'-N9	5.79	112.83	108.20
33	a	1316	C	C6-N1-C1'	-5.79	113.85	120.80
33	a	1204	C	C2-N1-C1'	5.78	125.16	118.80
1	A	357	A	C8-N9-C4	-5.77	103.49	105.80
33	a	203	U	N1-C2-O2	5.77	126.84	122.80
1	A	785	C	C5-C6-N1	5.77	123.89	121.00
1	A	550	C	C5-C6-N1	5.77	123.88	121.00
1	A	1317	C	N1-C2-O2	5.77	122.36	118.90
33	a	729	C	C6-N1-C2	-5.77	117.99	120.30
1	A	2042	C	C6-N1-C1'	-5.76	113.88	120.80
1	A	1557	A	N7-C8-N9	-5.76	110.92	113.80
1	A	976	C	N1-C2-O2	5.76	122.36	118.90
1	A	535	C	C6-N1-C2	-5.76	118.00	120.30
2	B	111	C	N1-C2-O2	5.76	122.35	118.90
1	A	2361	C	C2-N1-C1'	5.75	125.13	118.80
1	A	1790	A	C2-N3-C4	-5.75	107.72	110.60
1	A	1958	U	N3-C2-O2	-5.75	118.18	122.20
33	a	34	C	P-O3'-C3'	5.75	126.60	119.70
1	A	2023	C	N3-C2-O2	-5.75	117.88	121.90
2	B	18	G	C4-C5-N7	5.75	113.10	110.80
1	A	1088	A	OP1-P-O3'	5.74	117.84	105.20
1	A	2742	C	C6-N1-C2	-5.74	118.00	120.30
1	A	540	U	P-O3'-C3'	5.74	126.59	119.70
1	A	2849	G	C8-N9-C1'	-5.74	119.54	127.00
33	a	1204	C	C6-N1-C2	-5.73	118.01	120.30
1	A	537	U	O4'-C1'-N1	5.73	112.79	108.20
33	a	1204	C	N3-C2-O2	-5.73	117.89	121.90
1	A	519	A	C8-N9-C1'	5.73	138.01	127.70
1	A	1629	C	C6-N1-C2	-5.73	118.01	120.30
33	a	479	U	P-O3'-C3'	5.73	126.57	119.70
1	A	2851	G	C6-C5-N7	-5.72	126.97	130.40
33	a	306	C	N3-C2-O2	-5.72	117.89	121.90
1	A	1221	U	N3-C2-O2	-5.72	118.20	122.20
1	A	202	U	N3-C2-O2	-5.71	118.20	122.20
1	A	1918	U	C2-N1-C1'	5.71	124.56	117.70
1	A	1756	U	N3-C2-O2	-5.71	118.20	122.20
33	a	465	U	N1-C2-O2	5.71	126.80	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1930	U	N1-C2-O2	5.70	126.79	122.80
1	A	2374	U	C6-N1-C1'	-5.70	113.22	121.20
1	A	1616	G	N7-C8-N9	5.70	115.95	113.10
1	A	2703	C	C6-N1-C2	-5.70	118.02	120.30
33	a	159	G	O4'-C1'-N9	5.70	112.76	108.20
1	A	2325	C	C6-N1-C2	-5.70	118.02	120.30
33	a	18	C	C6-N1-C2	-5.70	118.02	120.30
33	a	176	C	C5-C6-N1	5.69	123.85	121.00
33	a	1155	C	N1-C2-O2	5.69	122.31	118.90
1	A	773	A	N1-C6-N6	5.68	122.01	118.60
1	A	1154	G	C5-C6-N1	5.68	114.34	111.50
1	A	1780	C	C6-N1-C2	-5.68	118.03	120.30
1	A	2339	A	C6-C5-N7	5.68	136.27	132.30
33	a	773	C	C6-N1-C2	-5.68	118.03	120.30
1	A	1616	G	C6-C5-N7	-5.67	127.00	130.40
1	A	2390	C	C6-N1-C2	-5.67	118.03	120.30
1	A	1161	C	N1-C2-O2	5.67	122.30	118.90
1	A	698	G	C8-N9-C1'	-5.66	119.64	127.00
1	A	1320	C	C6-N1-C2	-5.66	118.03	120.30
45	m	24	GLY	N-CA-C	5.66	127.25	113.10
33	a	748	C	C6-N1-C1'	-5.66	114.01	120.80
1	A	1155	G	C5-C6-O6	-5.66	125.21	128.60
1	A	1263	U	N1-C2-O2	5.64	126.75	122.80
1	A	2726	U	N3-C2-O2	-5.64	118.25	122.20
33	a	1215	G	N3-C4-N9	5.64	129.38	126.00
33	a	777	C	C6-N1-C2	-5.63	118.05	120.30
1	A	2063	U	N1-C2-O2	5.62	126.74	122.80
33	a	1063	C	N1-C2-O2	5.62	122.27	118.90
33	a	1248	G	C4-N9-C1'	5.61	133.80	126.50
1	A	629	U	N3-C2-O2	-5.61	118.27	122.20
1	A	682	C	N3-C2-O2	-5.61	117.97	121.90
1	A	2717	C	C6-N1-C2	-5.61	118.06	120.30
1	A	659	G	C4-N9-C1'	5.60	133.78	126.50
2	B	18	G	N3-C4-N9	5.60	129.36	126.00
1	A	1009	U	O4'-C1'-N1	5.60	112.68	108.20
2	B	30	C	N1-C2-O2	5.60	122.26	118.90
1	A	1050	U	N3-C2-O2	-5.59	118.28	122.20
1	A	863	G	OP1-P-OP2	5.59	127.98	119.60
33	a	378	G	P-O3'-C3'	5.59	126.41	119.70
1	A	519	A	C8-N9-C4	-5.59	103.57	105.80
1	A	1050	U	N1-C2-O2	5.59	126.71	122.80
1	A	700	U	N3-C2-O2	-5.58	118.29	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	A	C5-N7-C8	-5.58	101.11	103.90
1	A	312	C	N1-C2-O2	5.58	122.25	118.90
1	A	66	C	N3-C2-O2	-5.58	117.99	121.90
1	A	783	A	C8-N9-C4	-5.58	103.57	105.80
1	A	2703	C	N3-C2-O2	-5.58	118.00	121.90
1	A	172	C	N1-C2-O2	5.58	122.25	118.90
1	A	1468	U	C2-N1-C1'	5.58	124.39	117.70
1	A	659	G	C8-N9-C1'	-5.57	119.76	127.00
1	A	964	A	C4-N9-C1'	5.57	136.33	126.30
33	a	673	U	N1-C2-O2	5.57	126.70	122.80
1	A	1016	U	P-O3'-C3'	5.57	126.38	119.70
1	A	2697	C	N3-C2-O2	-5.57	118.00	121.90
33	a	324	C	C6-N1-C2	-5.57	118.07	120.30
1	A	1954	C	C6-N1-C2	-5.56	118.08	120.30
2	B	106	G	C6-C5-N7	-5.56	127.06	130.40
1	A	2726	U	N1-C2-O2	5.55	126.69	122.80
33	a	744	C	N1-C2-O2	5.55	122.23	118.90
2	B	66	A	P-O3'-C3'	5.55	126.36	119.70
1	A	1385	C	N3-C2-O2	-5.55	118.02	121.90
1	A	2729	C	N1-C2-O2	5.55	122.23	118.90
1	A	202	U	N1-C2-O2	5.55	126.68	122.80
1	A	2252	U	N1-C2-O2	5.54	126.68	122.80
33	a	34	C	C6-N1-C2	-5.54	118.08	120.30
1	A	305	A	O4'-C1'-N9	5.54	112.63	108.20
1	A	2410	U	C5-C6-N1	5.54	125.47	122.70
1	A	1362	U	O4'-C1'-N1	5.54	112.63	108.20
1	A	804	C	C6-N1-C2	-5.53	118.09	120.30
1	A	2315	A	N1-C2-N3	-5.53	126.53	129.30
1	A	2460	U	C6-N1-C1'	-5.53	113.45	121.20
1	A	177	G	O4'-C1'-N9	5.53	112.62	108.20
1	A	393	A	O4'-C1'-N9	5.53	112.62	108.20
1	A	1161	C	C5-C6-N1	5.53	123.76	121.00
1	A	2083	C	C6-N1-C2	-5.53	118.09	120.30
1	A	2254	A	C4-C5-C6	-5.52	114.24	117.00
33	a	1024	U	C5-C6-N1	5.52	125.46	122.70
1	A	27	G	N9-C4-C5	5.52	107.61	105.40
34	b	144	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	2339	A	N3-C4-N9	-5.52	122.98	127.40
1	A	27	G	N3-C4-N9	-5.52	122.69	126.00
1	A	2541	U	O4'-C1'-N1	5.52	112.61	108.20
1	A	741	A	O4'-C1'-N9	5.51	112.61	108.20
33	a	61	G	O4'-C1'-N9	5.51	112.61	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2059	C	C5-C6-N1	5.51	123.75	121.00
33	a	1122	C	C6-N1-C2	-5.51	118.10	120.30
1	A	1254	U	N3-C2-O2	-5.51	118.34	122.20
2	B	31	C	C6-N1-C2	-5.51	118.10	120.30
1	A	958	C	N1-C2-O2	5.50	122.20	118.90
28	2	38	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	638	G	N3-C2-N2	-5.50	116.05	119.90
1	A	2406	U	N1-C2-O2	5.50	126.65	122.80
1	A	1599	A	C4-C5-N7	5.49	113.44	110.70
1	A	630	C	C6-N1-C2	-5.49	118.11	120.30
1	A	2118	U	N1-C2-O2	5.48	126.64	122.80
1	A	2324	G	N1-C6-O6	5.48	123.19	119.90
1	A	798	G	N3-C4-N9	-5.48	122.71	126.00
1	A	972	C	C2-N1-C1'	5.48	124.83	118.80
1	A	1968	A	C5-N7-C8	-5.48	101.16	103.90
1	A	2829	G	C6-C5-N7	5.48	133.69	130.40
1	A	440	A	O5'-P-OP1	-5.47	100.77	105.70
1	A	550	C	C6-N1-C2	-5.47	118.11	120.30
1	A	933	A	O4'-C1'-N9	5.47	112.58	108.20
1	A	1263	U	N3-C2-O2	-5.47	118.37	122.20
1	A	2703	C	N1-C2-O2	5.47	122.18	118.90
33	a	1227	G	C8-N9-C1'	-5.47	119.89	127.00
1	A	677	C	N3-C2-O2	-5.46	118.08	121.90
1	A	2012	C	C5-C6-N1	5.46	123.73	121.00
1	A	641	G	N9-C4-C5	5.46	107.58	105.40
2	B	88	C	C2-N1-C1'	5.45	124.80	118.80
1	A	1953	A	N7-C8-N9	5.45	116.52	113.80
1	A	2875	C	C6-N1-C2	-5.45	118.12	120.30
1	A	1293	C	N1-C2-O2	5.45	122.17	118.90
1	A	1363	C	N1-C2-O2	5.45	122.17	118.90
1	A	2254	A	C8-N9-C1'	5.45	137.50	127.70
1	A	2355	C	C5-C4-N4	-5.45	116.39	120.20
1	A	1448	C	C6-N1-C2	-5.44	118.12	120.30
1	A	2390	C	N1-C2-O2	5.44	122.17	118.90
1	A	1719	C	N1-C2-O2	5.44	122.17	118.90
1	A	2526	C	N3-C2-O2	-5.44	118.09	121.90
1	A	1671	G	O4'-C1'-N9	5.44	112.55	108.20
1	A	2889	C	N3-C2-O2	-5.44	118.09	121.90
1	A	677	C	C6-N1-C2	-5.43	118.13	120.30
33	a	893	C	C5-C6-N1	5.43	123.72	121.00
1	A	1599	A	O4'-C1'-N9	5.43	112.54	108.20
1	A	800	U	C6-N1-C2	-5.42	117.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1161	C	C6-N1-C2	-5.42	118.13	120.30
1	A	974	A	N1-C6-N6	-5.41	115.35	118.60
1	A	508	C	N1-C2-O2	5.41	122.15	118.90
1	A	550	C	N1-C2-O2	5.41	122.14	118.90
1	A	1453	U	N3-C2-O2	-5.41	118.42	122.20
1	A	1622	A	C8-N9-C4	-5.41	103.64	105.80
1	A	828	C	N1-C2-O2	5.40	122.14	118.90
1	A	982	C	N3-C4-N4	-5.40	114.22	118.00
1	A	728	C	C2-N1-C1'	5.39	124.73	118.80
33	a	1233	A	C2-N3-C4	5.39	113.30	110.60
1	A	1357	C	C6-N1-C2	-5.39	118.14	120.30
1	A	2526	C	C2-N1-C1'	5.39	124.73	118.80
1	A	922	G	C2-N3-C4	5.39	114.60	111.90
1	A	1873	U	N3-C2-O2	-5.39	118.43	122.20
1	A	1194	C	C6-N1-C2	-5.39	118.15	120.30
1	A	369	C	C6-N1-C2	-5.38	118.15	120.30
1	A	2357	G	C8-N9-C1'	-5.38	120.00	127.00
1	A	519	A	C5-N7-C8	-5.38	101.21	103.90
1	A	1601	C	N1-C2-O2	5.38	122.13	118.90
2	B	27	C	N3-C2-O2	-5.38	118.13	121.90
1	A	1980	U	N1-C2-O2	5.38	126.57	122.80
33	a	1195	A	C2-N3-C4	5.38	113.29	110.60
1	A	115	C	C6-N1-C2	-5.37	118.15	120.30
8	H	12	LEU	CA-CB-CG	5.37	127.65	115.30
2	B	42	C	N3-C2-O2	-5.37	118.14	121.90
1	A	971	A	N7-C8-N9	5.36	116.48	113.80
1	A	1953	A	C5-N7-C8	-5.36	101.22	103.90
1	A	1197	G	N3-C4-C5	5.36	131.28	128.60
1	A	1741	A	N7-C8-N9	5.35	116.48	113.80
1	A	1385	C	C2-N1-C1'	5.35	124.69	118.80
1	A	1453	U	N1-C2-O2	5.35	126.55	122.80
1	A	1011	A	C8-N9-C1'	5.34	137.32	127.70
1	A	2012	C	C6-N1-C2	-5.34	118.16	120.30
1	A	2805	C	N1-C2-O2	5.34	122.11	118.90
33	a	1061	A	P-O3'-C3'	5.34	126.11	119.70
33	a	1365	G	C4-N9-C1'	5.34	133.44	126.50
33	a	131	U	C2-N1-C1'	5.34	124.10	117.70
1	A	1500	C	N3-C2-O2	-5.33	118.17	121.90
33	a	479	U	OP1-P-O3'	5.33	116.94	105.20
33	a	1024	U	C6-N1-C1'	-5.33	113.73	121.20
1	A	69	C	C6-N1-C2	-5.32	118.17	120.30
1	A	1507	U	N1-C2-O2	-5.32	119.07	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	93	C	C6-N1-C2	-5.32	118.17	120.30
33	a	1489	U	N3-C2-O2	-5.32	118.47	122.20
1	A	411	C	C6-N1-C2	-5.32	118.17	120.30
1	A	2329	C	N3-C2-O2	-5.32	118.18	121.90
1	A	958	C	C5-C6-N1	5.32	123.66	121.00
33	a	794	G	P-O3'-C3'	5.31	126.08	119.70
1	A	1133	A	N3-C4-N9	-5.31	123.15	127.40
1	A	1518	C	C5-C6-N1	5.31	123.66	121.00
1	A	64	G	N7-C8-N9	5.30	115.75	113.10
1	A	825	C	N1-C2-O2	5.30	122.08	118.90
33	a	1316	C	C5-C6-N1	5.30	123.65	121.00
1	A	591	C	N1-C2-O2	5.30	122.08	118.90
1	A	1327	U	N3-C2-O2	-5.30	118.49	122.20
1	A	466	C	C5-C6-N1	5.30	123.65	121.00
1	A	1292	C	N3-C2-O2	-5.29	118.20	121.90
1	A	444	A	P-O3'-C3'	5.29	126.05	119.70
1	A	2756	U	N3-C2-O2	-5.29	118.50	122.20
1	A	862	C	P-O3'-C3'	-5.29	113.36	119.70
33	a	1228	C	C6-N1-C2	-5.29	118.19	120.30
1	A	783	A	N7-C8-N9	5.28	116.44	113.80
1	A	2639	C	N1-C2-O2	5.28	122.07	118.90
1	A	836	U	C6-N1-C1'	-5.28	113.81	121.20
1	A	1169	A	P-O3'-C3'	5.28	126.04	119.70
1	A	2031	C	C5-C6-N1	5.28	123.64	121.00
4	D	165	LEU	CA-C-N	5.28	126.75	116.20
1	A	964	A	C8-N9-C4	-5.27	103.69	105.80
1	A	348	U	C6-N1-C1'	-5.27	113.82	121.20
1	A	766	G	C8-N9-C4	-5.27	104.29	106.40
1	A	1758	C	C6-N1-C2	-5.27	118.19	120.30
1	A	1823	C	N1-C2-O2	5.27	122.06	118.90
33	a	1216	G	C8-N9-C1'	-5.27	120.15	127.00
33	a	1253	C	C6-N1-C2	-5.27	118.19	120.30
2	B	30	C	C5-C6-N1	5.26	123.63	121.00
1	A	66	C	N1-C2-O2	5.26	122.06	118.90
1	A	357	A	N7-C8-N9	5.26	116.43	113.80
1	A	2583	U	C6-N1-C1'	-5.26	113.84	121.20
1	A	427	C	N1-C2-O2	5.25	122.05	118.90
1	A	1020	C	O4'-C1'-N1	5.25	112.40	108.20
1	A	1756	U	C5-C6-N1	5.25	125.33	122.70
1	A	66	C	C2-N1-C1'	5.25	124.57	118.80
1	A	719	G	C4-N9-C1'	5.25	133.32	126.50
1	A	1211	A	O4'-C1'-N9	5.25	112.40	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1913	U	O4'-C1'-N1	5.24	112.39	108.20
1	A	2363	A	C4-C5-N7	5.24	113.32	110.70
33	a	508	C	N1-C2-O2	5.24	122.05	118.90
1	A	2541	U	C6-N1-C1'	-5.24	113.86	121.20
1	A	201	C	N3-C2-O2	-5.24	118.23	121.90
1	A	210	C	N3-C2-O2	-5.24	118.23	121.90
1	A	1363	C	C6-N1-C2	-5.24	118.20	120.30
1	A	1762	U	N3-C2-O2	-5.24	118.53	122.20
1	A	2812	U	O4'-C1'-N1	5.24	112.39	108.20
1	A	1979	G	O4'-C1'-N9	-5.24	104.01	108.20
1	A	2030	U	C5-C6-N1	5.24	125.32	122.70
1	A	1660	C	N1-C2-O2	5.23	122.04	118.90
1	A	630	C	O4'-C1'-N1	5.23	112.38	108.20
1	A	1317	C	N3-C2-O2	-5.23	118.24	121.90
1	A	2120	G	C4-N9-C1'	5.23	133.30	126.50
33	a	310	C	C6-N1-C2	-5.23	118.21	120.30
1	A	996	C	C6-N1-C2	-5.23	118.21	120.30
1	A	2850	C	C6-N1-C2	-5.23	118.21	120.30
1	A	411	C	N1-C2-O2	5.22	122.03	118.90
1	A	1154	G	C4-N9-C1'	5.22	133.29	126.50
1	A	1790	A	O4'-C1'-N9	5.22	112.38	108.20
1	A	828	C	N3-C2-O2	-5.22	118.24	121.90
33	a	1122	C	P-O3'-C3'	5.22	125.97	119.70
1	A	285	U	N1-C2-O2	5.22	126.45	122.80
33	a	765	G	N3-C4-C5	-5.22	125.99	128.60
1	A	1572	C	C6-N1-C1'	-5.21	114.54	120.80
1	A	2653	C	C5-C6-N1	5.21	123.61	121.00
1	A	1616	G	C4-C5-N7	5.21	112.89	110.80
1	A	463	A	O4'-C1'-N9	5.21	112.37	108.20
1	A	508	C	N3-C2-O2	-5.21	118.25	121.90
33	a	1155	C	C5-C6-N1	5.21	123.61	121.00
1	A	208	C	C6-N1-C2	-5.21	118.22	120.30
1	A	1817	C	C5-C6-N1	5.21	123.60	121.00
33	a	1379	G	P-O3'-C3'	5.21	125.95	119.70
33	a	613	U	P-O3'-C3'	5.20	125.94	119.70
33	a	1142	U	N1-C2-O2	5.20	126.44	122.80
33	a	1204	C	C5-C6-N1	5.20	123.60	121.00
33	a	1249	G	P-O3'-C3'	5.20	125.94	119.70
1	A	790	A	N9-C4-C5	-5.20	103.72	105.80
1	A	923	A	O4'-C1'-N9	5.20	112.36	108.20
1	A	571	C	C5-C6-N1	5.19	123.60	121.00
1	A	2390	C	C5-C6-N1	5.19	123.60	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	1101	C	N1-C2-O2	5.19	122.02	118.90
1	A	1907	C	O5'-P-OP1	5.19	116.93	110.70
33	a	765	G	C4-N9-C1'	5.18	133.24	126.50
1	A	2059	C	C6-N1-C2	-5.18	118.23	120.30
33	a	1421	C	C6-N1-C2	-5.18	118.23	120.30
1	A	2324	G	C5-C6-O6	-5.18	125.49	128.60
1	A	2190	U	C2-N1-C1'	5.18	123.91	117.70
1	A	2230	U	N3-C2-O2	-5.18	118.58	122.20
1	A	2406	U	N3-C2-O2	-5.17	118.58	122.20
1	A	2003	U	N1-C2-O2	5.17	126.42	122.80
33	a	1454	C	C6-N1-C2	-5.17	118.23	120.30
1	A	2633	C	C5-C6-N1	5.17	123.58	121.00
1	A	1300	U	C5-C6-N1	5.17	125.28	122.70
1	A	1311	G	O4'-C1'-N9	5.16	112.33	108.20
1	A	591	C	N3-C2-O2	-5.16	118.29	121.90
1	A	1542	G	N7-C8-N9	5.16	115.68	113.10
1	A	1791	C	C5-C6-N1	5.16	123.58	121.00
1	A	361	A	O4'-C1'-N9	-5.16	104.07	108.20
1	A	514	C	C6-N1-C2	-5.16	118.24	120.30
1	A	432	U	N3-C2-O2	-5.15	118.59	122.20
1	A	2752	A	C2-N3-C4	5.15	113.17	110.60
33	a	1219	A	C5-C6-N6	-5.15	119.58	123.70
1	A	1987	C	C5-C6-N1	5.15	123.57	121.00
1	A	2042	C	C6-N1-C2	-5.15	118.24	120.30
1	A	547	C	C5-C6-N1	5.14	123.57	121.00
33	a	513	C	N1-C2-O2	5.14	121.99	118.90
33	a	1431	A	P-O3'-C3'	5.14	125.87	119.70
1	A	463	A	N7-C8-N9	5.14	116.37	113.80
1	A	2034	C	N1-C2-O2	5.14	121.99	118.90
33	a	328	C	C6-N1-C2	-5.14	118.24	120.30
1	A	1434	U	N3-C4-C5	-5.14	111.52	114.60
1	A	2863	A	C4-N9-C1'	5.14	135.55	126.30
1	A	126	A	N7-C8-N9	5.14	116.37	113.80
1	A	2840	C	C6-N1-C2	-5.14	118.25	120.30
1	A	2334	C	C6-N1-C2	-5.14	118.25	120.30
1	A	501	C	C6-N1-C2	-5.13	118.25	120.30
1	A	629	U	N1-C2-O2	5.13	126.39	122.80
1	A	766	G	C5-N7-C8	-5.13	101.74	104.30
1	A	1622	A	C4-C5-N7	5.13	113.27	110.70
1	A	393	A	N7-C8-N9	5.13	116.36	113.80
1	A	1191	A	O4'-C1'-N9	5.12	112.30	108.20
1	A	1503	G	C2-N3-C4	5.12	114.46	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	668	C	N3-C2-O2	-5.12	118.32	121.90
1	A	1124	A	P-O3'-C3'	5.12	125.84	119.70
33	a	1020	G	C8-N9-C4	-5.12	104.35	106.40
1	A	227	A	OP1-P-O3'	5.12	116.46	105.20
1	A	641	G	N1-C6-O6	-5.12	116.83	119.90
1	A	827	C	C5-C6-N1	5.12	123.56	121.00
33	a	576	U	C6-N1-C1'	-5.12	114.04	121.20
33	a	1309	U	C2-N1-C1'	5.12	123.84	117.70
1	A	1774	A	C2-N3-C4	5.11	113.16	110.60
1	A	1873	U	N1-C2-O2	5.11	126.38	122.80
1	A	428	U	C6-N1-C2	-5.11	117.93	121.00
1	A	1292	C	N1-C2-O2	5.11	121.97	118.90
1	A	2363	A	C5-C6-N6	-5.11	119.61	123.70
2	B	88	C	N1-C2-O2	5.11	121.97	118.90
1	A	552	U	C5-C6-N1	5.11	125.25	122.70
1	A	668	C	N1-C2-O2	5.11	121.97	118.90
33	a	1245	A	C2-N3-C4	5.11	113.15	110.60
1	A	518	C	C6-N1-C2	-5.11	118.26	120.30
1	A	411	C	C2-N1-C1'	5.10	124.41	118.80
1	A	802	C	C5-C6-N1	5.10	123.55	121.00
1	A	974	A	C2-N3-C4	5.10	113.15	110.60
1	A	2339	A	C8-N9-C1'	5.10	136.89	127.70
2	B	31	C	C5-C6-N1	5.10	123.55	121.00
1	A	1198	U	C2-N1-C1'	5.10	123.82	117.70
1	A	933	A	C5-N7-C8	-5.10	101.35	103.90
1	A	1993	C	C6-N1-C2	-5.10	118.26	120.30
1	A	2856	G	C8-N9-C4	-5.10	104.36	106.40
1	A	1801	G	N1-C2-N2	-5.10	111.61	116.20
33	a	369	U	C6-N1-C1'	-5.09	114.07	121.20
33	a	1424	C	C2-N1-C1'	5.09	124.40	118.80
1	A	1600	A	N7-C8-N9	5.09	116.35	113.80
1	A	531	C	N3-C2-O2	-5.09	118.34	121.90
1	A	741	A	N7-C8-N9	5.09	116.35	113.80
1	A	2653	C	O4'-C1'-N1	5.09	112.27	108.20
1	A	369	C	N1-C2-O2	5.09	121.95	118.90
33	a	1234	U	N3-C2-O2	-5.09	118.64	122.20
33	a	1355	G	N3-C4-N9	5.09	129.05	126.00
1	A	1666	A	N1-C2-N3	-5.09	126.76	129.30
1	A	2118	U	N3-C2-O2	-5.09	118.64	122.20
1	A	2063	U	N3-C2-O2	-5.08	118.64	122.20
1	A	982	C	C2-N3-C4	-5.08	117.36	119.90
1	A	2325	C	N3-C2-O2	-5.08	118.35	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2526	C	C6-N1-C2	-5.08	118.27	120.30
1	A	1301	C	C4-C5-C6	-5.08	114.86	117.40
33	a	617	C	C6-N1-C2	-5.08	118.27	120.30
33	a	1355	G	C8-N9-C1'	-5.07	120.40	127.00
1	A	285	U	N3-C2-O2	-5.07	118.65	122.20
1	A	1861	C	N1-C2-O2	5.07	121.94	118.90
1	A	2583	U	O4'-C1'-N1	5.07	112.26	108.20
1	A	2117	U	C2-N1-C1'	5.07	123.78	117.70
33	a	795	U	N1-C2-O2	5.07	126.35	122.80
23	W	19	LYS	CA-C-O	-5.06	109.47	120.10
1	A	2079	U	N3-C2-O2	-5.06	118.66	122.20
1	A	268	C	C6-N1-C2	-5.06	118.28	120.30
29	3	16	PHE	CB-CA-C	5.06	120.52	110.40
1	A	972	C	N1-C2-O2	5.06	121.94	118.90
1	A	2055	U	C5-C6-N1	5.06	125.23	122.70
1	A	2357	G	C4-C5-N7	-5.06	108.78	110.80
33	a	748	C	C6-N1-C2	-5.06	118.28	120.30
1	A	638	G	C4-N9-C1'	-5.05	119.93	126.50
1	A	1370	A	C5-N7-C8	-5.05	101.37	103.90
1	A	2279	G	C8-N9-C4	-5.05	104.38	106.40
33	a	1216	G	C2-N3-C4	5.05	114.42	111.90
1	A	1755	C	N3-C2-O2	-5.05	118.37	121.90
1	A	2729	C	N3-C2-O2	-5.05	118.37	121.90
1	A	1904	U	N3-C2-O2	-5.04	118.67	122.20
1	A	2357	G	N3-C4-N9	5.04	129.03	126.00
1	A	113	C	C6-N1-C1'	-5.04	114.75	120.80
1	A	2023	C	N1-C2-O2	5.04	121.92	118.90
1	A	2678	C	C6-N1-C2	-5.04	118.28	120.30
1	A	198	C	C2-N1-C1'	5.04	124.34	118.80
33	a	572	C	C6-N1-C2	-5.04	118.28	120.30
1	A	1685	G	C4-N9-C1'	5.04	133.05	126.50
2	B	67	U	C5-C6-N1	5.04	125.22	122.70
1	A	1634	C	N3-C2-O2	-5.03	118.38	121.90
1	A	2363	A	C5-N7-C8	-5.03	101.38	103.90
1	A	1088	A	N3-C4-N9	5.03	131.43	127.40
1	A	1507	U	C6-N1-C1'	5.03	128.24	121.20
1	A	2194	C	C2-N1-C1'	5.03	124.33	118.80
1	A	2362	G	N3-C4-N9	-5.03	122.98	126.00
33	a	1454	C	N1-C2-O2	5.03	121.92	118.90
1	A	2317	G	P-O3'-C3'	5.03	125.73	119.70
1	A	728	C	C6-N1-C2	-5.02	118.29	120.30
1	A	1170	C	C5-C6-N1	5.02	123.51	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	310	C	N1-C2-O2	5.02	121.91	118.90
1	A	629	U	C6-N1-C2	-5.02	117.99	121.00
1	A	659	G	N3-C4-N9	5.02	129.01	126.00
1	A	1221	U	N1-C2-O2	5.02	126.31	122.80
1	A	1907	C	O5'-P-OP2	-5.02	101.18	105.70
1	A	802	C	C6-N1-C2	-5.01	118.29	120.30
1	A	1814	U	N1-C2-O2	5.01	126.31	122.80
1	A	2430	C	C5-C6-N1	5.01	123.50	121.00
1	A	31	C	C6-N1-C2	-5.01	118.30	120.30
1	A	1197	G	C4-C5-N7	5.01	112.80	110.80
1	A	22	C	C2-N1-C1'	5.01	124.31	118.80
1	A	730	C	N1-C2-O2	5.00	121.90	118.90
1	A	971	A	C5-N7-C8	-5.00	101.40	103.90
1	A	1088	A	C5'-C4'-C3'	5.00	124.01	116.00
33	a	782	U	C2-N1-C1'	5.00	123.70	117.70

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	3	16	PHE	Peptide
3	C	270	ARG	Sidechain
3	C	271	ARG	Sidechain
4	D	124	ARG	Sidechain
4	D	128	ARG	Sidechain
4	D	141	ARG	Sidechain
4	D	154	ARG	Sidechain
4	D	169	ARG	Sidechain
4	D	179	ARG	Sidechain
4	D	204	ARG	Sidechain
4	D	34	ARG	Sidechain
4	D	60	ARG	Sidechain
4	D	84	ARG	Sidechain
5	E	163	LEU	Peptide
6	F	24	ASN	Peptide
6	F	72	LYS	Peptide
9	I	34	ASN	Peptide
9	I	68	THR	Peptide
16	P	36	GLY	Peptide
17	Q	83	LEU	Peptide
18	R	51	LEU	Peptide
22	V	101	HIS	Peptide

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Mol	Chain	Res	Type	Group
22	V	165	LEU	Peptide
22	V	167	ALA	Peptide
36	d	49	SER	Peptide
40	h	110	VAL	Peptide
40	h	79	SER	Peptide
40	h	80	ARG	Peptide
41	i	75	GLN	Peptide
44	l	108	LYS	Peptide
45	m	101	ARG	Peptide
45	m	26	GLY	Peptide
46	n	51	GLN	Peptide
47	o	30	ALA	Peptide
48	p	73	GLN	Peptide
51	s	44	MET	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	
3	C	269/271 (99%)	239 (89%)	28 (10%)	2 (1%)	22	54
4	D	205/207 (99%)	176 (86%)	19 (9%)	10 (5%)	2	8
5	E	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
6	F	172/174 (99%)	138 (80%)	34 (20%)	0	100	100
7	G	167/169 (99%)	152 (91%)	15 (9%)	0	100	100
8	H	76/78 (97%)	70 (92%)	6 (8%)	0	100	100
9	I	138/140 (99%)	118 (86%)	20 (14%)	0	100	100
10	J	139/141 (99%)	129 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
12	L	142/144 (99%)	132 (93%)	10 (7%)	0	100	100
13	M	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
14	N	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
15	O	113/115 (98%)	96 (85%)	17 (15%)	0	100	100
16	P	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
17	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
18	R	100/102 (98%)	91 (91%)	8 (8%)	1 (1%)	15	45
19	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
20	T	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	14	42
21	U	101/103 (98%)	90 (89%)	10 (10%)	1 (1%)	15	45
22	V	186/188 (99%)	158 (85%)	26 (14%)	2 (1%)	14	42
23	W	74/76 (97%)	60 (81%)	13 (18%)	1 (1%)	11	36
24	X	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
25	Y	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
26	Z	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
27	1	29/31 (94%)	26 (90%)	3 (10%)	0	100	100
28	2	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
29	3	48/50 (96%)	36 (75%)	12 (25%)	0	100	100
30	4	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
31	5	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
32	6	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
34	b	217/226 (96%)	199 (92%)	18 (8%)	0	100	100
35	c	201/203 (99%)	174 (87%)	27 (13%)	0	100	100
36	d	202/204 (99%)	177 (88%)	25 (12%)	0	100	100
37	e	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
38	f	98/100 (98%)	88 (90%)	10 (10%)	0	100	100
39	g	152/154 (99%)	134 (88%)	18 (12%)	0	100	100
40	h	127/129 (98%)	111 (87%)	14 (11%)	2 (2%)	9	32
41	i	124/126 (98%)	107 (86%)	17 (14%)	0	100	100
42	j	94/96 (98%)	81 (86%)	13 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	k	113/115 (98%)	95 (84%)	18 (16%)	0	100	100
44	l	118/120 (98%)	100 (85%)	17 (14%)	1 (1%)	19	51
45	m	105/110 (96%)	92 (88%)	13 (12%)	0	100	100
46	n	96/98 (98%)	81 (84%)	15 (16%)	0	100	100
47	o	85/87 (98%)	78 (92%)	6 (7%)	1 (1%)	13	40
48	p	76/78 (97%)	68 (90%)	8 (10%)	0	100	100
49	q	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
50	r	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
51	s	78/80 (98%)	59 (76%)	19 (24%)	0	100	100
52	t	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
53	u	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5608/5719 (98%)	5018 (90%)	568 (10%)	22 (0%)	38	66

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	120	ILE
4	D	105	GLN
4	D	134	HIS
20	T	3	GLN
22	V	167	ALA
22	V	168	PRO
40	h	80	ARG
4	D	117	GLY
4	D	167	ALA
21	U	88	ASP
4	D	73	ASN
4	D	164	HIS
40	h	81	PRO
47	o	19	GLU
4	D	55	GLU
18	R	52	PRO
23	W	19	LYS
44	l	109	ASP
3	C	233	GLY
4	D	32	PRO
4	D	137	SER
4	D	104	GLY

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	
3	C	206/212 (97%)	192 (93%)	14 (7%)	16	42
4	D	157/159 (99%)	129 (82%)	28 (18%)	2	5
5	E	155/157 (99%)	154 (99%)	1 (1%)	86	96
6	F	122/149 (82%)	117 (96%)	5 (4%)	30	64
7	G	131/135 (97%)	130 (99%)	1 (1%)	81	94
8	H	55/55 (100%)	54 (98%)	1 (2%)	59	85
9	I	108/108 (100%)	107 (99%)	1 (1%)	78	93
10	J	118/118 (100%)	116 (98%)	2 (2%)	60	86
11	K	100/100 (100%)	97 (97%)	3 (3%)	41	75
12	L	105/106 (99%)	103 (98%)	2 (2%)	57	84
13	M	109/109 (100%)	108 (99%)	1 (1%)	78	93
14	N	99/99 (100%)	97 (98%)	2 (2%)	55	82
15	O	86/86 (100%)	83 (96%)	3 (4%)	36	70
16	P	96/96 (100%)	94 (98%)	2 (2%)	53	81
17	Q	87/87 (100%)	86 (99%)	1 (1%)	73	92
18	R	82/86 (95%)	79 (96%)	3 (4%)	34	68
19	S	87/87 (100%)	85 (98%)	2 (2%)	50	80
20	T	77/79 (98%)	77 (100%)	0	100	100
21	U	88/88 (100%)	88 (100%)	0	100	100
22	V	144/153 (94%)	144 (100%)	0	100	100
23	W	56/56 (100%)	56 (100%)	0	100	100
24	X	65/66 (98%)	64 (98%)	1 (2%)	65	87
25	Y	51/53 (96%)	50 (98%)	1 (2%)	55	82
26	Z	48/48 (100%)	46 (96%)	2 (4%)	30	63
27	1	27/27 (100%)	27 (100%)	0	100	100
28	2	45/46 (98%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	3	44/46 (96%)	43 (98%)	1 (2%)	50	80
30	4	37/37 (100%)	37 (100%)	0	100	100
31	5	53/54 (98%)	51 (96%)	2 (4%)	33	67
32	6	33/34 (97%)	32 (97%)	1 (3%)	41	75
34	b	174/188 (93%)	167 (96%)	7 (4%)	31	65
35	c	163/169 (96%)	163 (100%)	0	100	100
36	d	166/173 (96%)	163 (98%)	3 (2%)	59	85
37	e	108/109 (99%)	104 (96%)	4 (4%)	34	68
38	f	81/85 (95%)	80 (99%)	1 (1%)	71	91
39	g	116/120 (97%)	113 (97%)	3 (3%)	46	77
40	h	104/107 (97%)	101 (97%)	3 (3%)	42	76
41	i	102/102 (100%)	99 (97%)	3 (3%)	42	76
42	j	85/85 (100%)	84 (99%)	1 (1%)	71	91
43	k	83/87 (95%)	81 (98%)	2 (2%)	49	79
44	l	104/104 (100%)	102 (98%)	2 (2%)	57	84
45	m	91/92 (99%)	90 (99%)	1 (1%)	73	92
46	n	78/80 (98%)	77 (99%)	1 (1%)	69	90
47	o	73/73 (100%)	69 (94%)	4 (6%)	21	53
48	p	61/63 (97%)	61 (100%)	0	100	100
49	q	70/70 (100%)	67 (96%)	3 (4%)	29	62
50	r	46/48 (96%)	45 (98%)	1 (2%)	52	81
51	s	69/71 (97%)	67 (97%)	2 (3%)	42	76
52	t	68/68 (100%)	68 (100%)	0	100	100
53	u	28/28 (100%)	28 (100%)	0	100	100
All	All	4541/4658 (98%)	4420 (97%)	121 (3%)	48	77

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	21	ASN
3	C	33	LEU
3	C	39	LYS
3	C	44	ASN
3	C	71	LYS

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Mol	Chain	Res	Type
3	C	80	ARG
3	C	108	LYS
3	C	125	LYS
3	C	180	GLU
3	C	203	ARG
3	C	221	ARG
3	C	263	ARG
3	C	264	THR
3	C	270	ARG
4	D	5	VAL
4	D	31	GLU
4	D	34	ARG
4	D	35	VAL
4	D	40	THR
4	D	47	ARG
4	D	51	VAL
4	D	60	ARG
4	D	71	LYS
4	D	100	LEU
4	D	105	GLN
4	D	106	MET
4	D	110	THR
4	D	114	LYS
4	D	118	PHE
4	D	126	ASN
4	D	137	SER
4	D	138	VAL
4	D	139	SER
4	D	141	ARG
4	D	142	VAL
4	D	154	ARG
4	D	161	MET
4	D	168	GLU
4	D	169	ARG
4	D	178	VAL
4	D	179	ARG
4	D	190	LYS
5	E	161	ARG
6	F	20	LEU
6	F	21	GLN
6	F	30	ARG
6	F	118	ASN

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Mol	Chain	Res	Type
6	F	156	LEU
7	G	3	ARG
8	H	12	LEU
9	I	92	ARG
10	J	80	PHE
10	J	123	LYS
11	K	8	LEU
11	K	49	ARG
11	K	107	ARG
12	L	7	ARG
12	L	78	ARG
13	M	6	ARG
14	N	2	ARG
14	N	95	LEU
15	O	31	ARG
15	O	101	ARG
15	O	103	LYS
16	P	40	ARG
16	P	98	LEU
17	Q	4	VAL
18	R	21	LYS
18	R	43	ASN
18	R	58	LYS
19	S	82	LEU
19	S	92	ARG
24	X	27	ARG
25	Y	21	LEU
26	Z	30	ARG
26	Z	43	ASN
29	3	16	PHE
31	5	13	ARG
31	5	50	ASN
32	6	12	ARG
34	b	36	ASN
34	b	42	ASN
34	b	49	MET
34	b	51	ASN
34	b	117	LEU
34	b	170	ARG
34	b	190	ASN
36	d	22	LYS
36	d	26	ARG

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Mol	Chain	Res	Type
36	d	146	ARG
37	e	21	ARG
37	e	24	LYS
37	e	27	LYS
37	e	125	LEU
38	f	91	ARG
39	g	3	ARG
39	g	102	ARG
39	g	149	LYS
40	h	19	MET
40	h	50	GLN
40	h	101	VAL
41	i	106	ARG
41	i	113	ARG
41	i	124	ARG
42	j	58	ASN
43	k	37	ARG
43	k	56	ARG
44	l	15	MET
44	l	51	LYS
45	m	40	ASN
46	n	75	ARG
47	o	35	ASN
47	o	53	ARG
47	o	58	ARG
47	o	59	MET
49	q	14	ARG
49	q	20	MET
49	q	84	ARG
50	r	43	ARG
51	s	29	LYS
51	s	44	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	21	ASN
3	C	261	ASN
4	D	33	ASN
4	D	37	GLN
4	D	68	HIS
4	D	95	GLN

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Mol	Chain	Res	Type
4	D	105	GLN
4	D	148	GLN
4	D	150	GLN
5	E	6	ASN
7	G	23	GLN
7	G	45	GLN
7	G	59	GLN
7	G	139	GLN
10	J	77	HIS
11	K	5	GLN
17	Q	37	GLN
18	R	43	ASN
18	R	83	HIS
19	S	61	ASN
19	S	102	HIS
20	T	14	HIS
21	U	48	ASN
22	V	129	HIS
23	W	12	ASN
23	W	29	GLN
23	W	35	ASN
23	W	57	HIS
24	X	34	GLN
25	Y	58	ASN
26	Z	13	ASN
26	Z	33	HIS
26	Z	43	ASN
31	5	50	ASN
34	b	3	GLN
34	b	36	ASN
34	b	51	ASN
34	b	120	GLN
34	b	190	ASN
35	c	28	ASN
36	d	116	GLN
38	f	37	HIS
39	g	28	ASN
40	h	107	ASN
41	i	81	HIS
42	j	58	ASN
43	k	72	GLN
44	l	5	ASN

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Mol	Chain	Res	Type
44	l	25	GLN
44	l	59	ASN
44	l	72	HIS
45	m	14	HIS
45	m	40	ASN
47	o	28	GLN
47	o	35	ASN
47	o	42	HIS
47	o	61	ASN
48	p	54	GLN
50	r	52	GLN
51	s	57	HIS
52	t	21	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2883/2888 (99%)	817 (28%)	36 (1%)
2	B	116/117 (99%)	48 (41%)	4 (3%)
33	a	1382/1521 (90%)	573 (41%)	0
All	All	4381/4526 (96%)	1438 (32%)	40 (0%)

All (1438) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	14	A
1	A	15	G
1	A	22	C
1	A	34	U
1	A	35	G
1	A	44	A
1	A	46	G
1	A	50	U
1	A	55	G
1	A	56	A
1	A	58	G
1	A	60	G
1	A	62	U
1	A	63	A
1	A	64	G

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Mol	Chain	Res	Type
1	A	69	C
1	A	71	A
1	A	74	A
1	A	75	G
1	A	79	C
1	A	82	G
1	A	83	G
1	A	85	G
1	A	93	A
1	A	102	G
1	A	103	A
1	A	110	G
1	A	114	U
1	A	115	C
1	A	116	U
1	A	119	A
1	A	120	U
1	A	124	G
1	A	131	A
1	A	139	U
1	A	140	A
1	A	141	A
1	A	142	C
1	A	146	G
1	A	160	A
1	A	163	C
1	A	166	U
1	A	173	A
1	A	181	A
1	A	196	A
1	A	199	A
1	A	205	G
1	A	206	U
1	A	215	G
1	A	216	A
1	A	222	A
1	A	224	U
1	A	227	A
1	A	228	C
1	A	230	G
1	A	232	G
1	A	233	A

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Mol	Chain	Res	Type
1	A	239	U
1	A	241	A
1	A	242	G
1	A	248	G
1	A	249	C
1	A	252	G
1	A	255	A
1	A	261	G
1	A	265	A
1	A	266	G
1	A	267	C
1	A	268	C
1	A	271	U
1	A	273	A
1	A	276	U
1	A	278	C
1	A	280	U
1	A	281	U
1	A	289	G
1	A	294	A
1	A	305	A
1	A	311	G
1	A	313	C
1	A	315	U
1	A	316	A
1	A	318	U
1	A	319	G
1	A	322	U
1	A	323	G
1	A	324	A
1	A	325	U
1	A	327	G
1	A	329	C
1	A	336	G
1	A	339	A
1	A	342	G
1	A	349	U
1	A	350	G
1	A	357	A
1	A	358	A
1	A	359	U
1	A	364	U

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Mol	Chain	Res	Type
1	A	375	A
1	A	377	G
1	A	378	A
1	A	385	U
1	A	386	U
1	A	387	G
1	A	395	A
1	A	397	G
1	A	400	G
1	A	403	A
1	A	406	A
1	A	416	G
1	A	428	U
1	A	435	C
1	A	439	U
1	A	445	A
1	A	446	C
1	A	447	C
1	A	448	A
1	A	454	G
1	A	458	G
1	A	461	A
1	A	464	G
1	A	466	C
1	A	470	A
1	A	472	G
1	A	482	G
1	A	485	G
1	A	487	G
1	A	492	A
1	A	496	A
1	A	499	A
1	A	520	A
1	A	523	A
1	A	524	G
1	A	534	A
1	A	535	C
1	A	537	U
1	A	538	G
1	A	539	U
1	A	540	U
1	A	541	A

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Mol	Chain	Res	Type
1	A	553	A
1	A	558	U
1	A	561	U
1	A	563	U
1	A	564	A
1	A	565	A
1	A	576	A
1	A	593	A
1	A	594	G
1	A	599	A
1	A	604	A
1	A	605	U
1	A	624	G
1	A	627	A
1	A	628	G
1	A	635	U
1	A	636	A
1	A	637	G
1	A	638	G
1	A	643	U
1	A	644	U
1	A	645	A
1	A	647	U
1	A	659	G
1	A	660	A
1	A	667	A
1	A	675	A
1	A	676	U
1	A	680	U
1	A	685	G
1	A	687	G
1	A	689	A
1	A	698	G
1	A	699	U
1	A	700	U
1	A	701	A
1	A	704	U
1	A	705	A
1	A	706	A
1	A	708	A
1	A	709	C
1	A	710	U

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Mol	Chain	Res	Type
1	A	711	G
1	A	716	G
1	A	719	G
1	A	720	A
1	A	724	A
1	A	728	C
1	A	737	U
1	A	738	G
1	A	739	A
1	A	743	G
1	A	745	U
1	A	755	C
1	A	763	U
1	A	765	G
1	A	766	G
1	A	767	A
1	A	772	A
1	A	774	G
1	A	779	A
1	A	781	C
1	A	782	A
1	A	795	G
1	A	802	C
1	A	817	U
1	A	833	G
1	A	836	U
1	A	844	G
1	A	846	G
1	A	848	G
1	A	855	A
1	A	858	G
1	A	860	U
1	A	862	C
1	A	863	G
1	A	864	G
1	A	865	C
1	A	866	U
1	A	867	A
1	A	870	G
1	A	872	G
1	A	873	U
1	A	875	A

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Mol	Chain	Res	Type
1	A	877	C
1	A	878	C
1	A	881	A
1	A	882	C
1	A	886	C
1	A	887	C
1	A	888	A
1	A	889	A
1	A	890	A
1	A	898	A
1	A	899	A
1	A	904	C
1	A	908	U
1	A	921	C
1	A	922	G
1	A	931	A
1	A	935	A
1	A	936	C
1	A	948	U
1	A	949	A
1	A	951	C
1	A	952	G
1	A	954	C
1	A	963	A
1	A	964	A
1	A	966	G
1	A	972	C
1	A	973	A
1	A	975	C
1	A	979	G
1	A	983	G
1	A	986	A
1	A	988	C
1	A	989	U
1	A	993	G
1	A	995	C
1	A	999	A
1	A	1002	U
1	A	1003	U
1	A	1007	G
1	A	1012	G
1	A	1016	U

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Mol	Chain	Res	Type
1	A	1017	A
1	A	1023	U
1	A	1025	U
1	A	1029	A
1	A	1030	A
1	A	1034	U
1	A	1035	U
1	A	1036	A
1	A	1037	G
1	A	1038	A
1	A	1042	C
1	A	1043	U
1	A	1044	A
1	A	1045	G
1	A	1047	A
1	A	1049	G
1	A	1051	U
1	A	1052	G
1	A	1054	C
1	A	1055	U
1	A	1057	A
1	A	1058	G
1	A	1060	A
1	A	1062	C
1	A	1063	A
1	A	1064	G
1	A	1065	C
1	A	1066	C
1	A	1067	A
1	A	1068	C
1	A	1069	C
1	A	1070	C
1	A	1071	U
1	A	1072	U
1	A	1073	U
1	A	1074	A
1	A	1075	A
1	A	1076	A
1	A	1077	G
1	A	1078	A
1	A	1079	A
1	A	1083	G

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Mol	Chain	Res	Type
1	A	1084	U
1	A	1085	A
1	A	1086	A
1	A	1087	U
1	A	1088	A
1	A	1089	G
1	A	1090	C
1	A	1092	C
1	A	1093	A
1	A	1094	C
1	A	1097	G
1	A	1098	U
1	A	1099	C
1	A	1100	G
1	A	1101	A
1	A	1102	G
1	A	1103	U
1	A	1105	G
1	A	1117	A
1	A	1118	G
1	A	1119	A
1	A	1120	U
1	A	1121	G
1	A	1122	U
1	A	1123	A
1	A	1124	A
1	A	1125	C
1	A	1129	G
1	A	1133	A
1	A	1138	A
1	A	1142	A
1	A	1146	A
1	A	1148	G
1	A	1154	G
1	A	1155	G
1	A	1156	U
1	A	1157	G
1	A	1163	U
1	A	1164	A
1	A	1165	A
1	A	1166	G
1	A	1167	U

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Mol	Chain	Res	Type
1	A	1170	C
1	A	1192	A
1	A	1193	G
1	A	1199	G
1	A	1204	U
1	A	1205	G
1	A	1214	A
1	A	1223	G
1	A	1224	A
1	A	1225	G
1	A	1227	U
1	A	1228	A
1	A	1229	U
1	A	1233	A
1	A	1234	A
1	A	1235	G
1	A	1237	G
1	A	1238	C
1	A	1240	A
1	A	1242	U
1	A	1243	G
1	A	1249	A
1	A	1253	G
1	A	1258	G
1	A	1259	A
1	A	1261	A
1	A	1263	U
1	A	1271	A
1	A	1276	C
1	A	1281	A
1	A	1288	A
1	A	1292	C
1	A	1299	U
1	A	1306	G
1	A	1308	A
1	A	1316	U
1	A	1327	U
1	A	1328	U
1	A	1331	U
1	A	1333	G
1	A	1334	G
1	A	1339	U

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Mol	Chain	Res	Type
1	A	1346	A
1	A	1349	C
1	A	1352	A
1	A	1355	A
1	A	1361	G
1	A	1362	U
1	A	1366	U
1	A	1367	G
1	A	1372	A
1	A	1373	C
1	A	1382	A
1	A	1397	G
1	A	1403	G
1	A	1404	C
1	A	1406	A
1	A	1408	G
1	A	1414	A
1	A	1415	C
1	A	1420	A
1	A	1421	A
1	A	1430	C
1	A	1433	C
1	A	1439	G
1	A	1440	U
1	A	1441	U
1	A	1442	G
1	A	1447	U
1	A	1454	U
1	A	1463	U
1	A	1469	G
1	A	1475	U
1	A	1480	U
1	A	1481	A
1	A	1484	U
1	A	1495	A
1	A	1496	A
1	A	1497	G
1	A	1503	G
1	A	1507	U
1	A	1509	A
1	A	1511	G
1	A	1515	A

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Mol	Chain	Res	Type
1	A	1516	G
1	A	1517	U
1	A	1518	C
1	A	1519	G
1	A	1530	G
1	A	1537	U
1	A	1542	G
1	A	1549	U
1	A	1555	C
1	A	1556	A
1	A	1558	G
1	A	1559	A
1	A	1560	A
1	A	1568	U
1	A	1571	G
1	A	1573	U
1	A	1574	U
1	A	1576	A
1	A	1580	A
1	A	1597	C
1	A	1598	A
1	A	1600	A
1	A	1603	G
1	A	1624	A
1	A	1629	C
1	A	1636	C
1	A	1637	U
1	A	1638	U
1	A	1639	G
1	A	1641	G
1	A	1643	G
1	A	1657	G
1	A	1664	G
1	A	1665	C
1	A	1683	U
1	A	1684	C
1	A	1685	G
1	A	1686	G
1	A	1700	G
1	A	1708	U
1	A	1710	A
1	A	1711	A

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Mol	Chain	Res	Type
1	A	1717	U
1	A	1718	A
1	A	1720	U
1	A	1724	U
1	A	1725	A
1	A	1736	G
1	A	1739	C
1	A	1740	G
1	A	1741	A
1	A	1742	A
1	A	1745	U
1	A	1746	A
1	A	1750	G
1	A	1751	G
1	A	1756	U
1	A	1760	A
1	A	1763	G
1	A	1768	U
1	A	1769	U
1	A	1771	A
1	A	1775	C
1	A	1787	C
1	A	1788	A
1	A	1789	A
1	A	1795	A
1	A	1797	A
1	A	1798	G
1	A	1803	C
1	A	1807	U
1	A	1820	C
1	A	1829	G
1	A	1834	A
1	A	1835	A
1	A	1838	U
1	A	1841	A
1	A	1853	A
1	A	1855	C
1	A	1861	C
1	A	1862	G
1	A	1863	A
1	A	1865	G
1	A	1871	G

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Mol	Chain	Res	Type
1	A	1875	G
1	A	1890	G
1	A	1894	G
1	A	1895	C
1	A	1897	G
1	A	1898	U
1	A	1899	A
1	A	1901	C
1	A	1902	U
1	A	1903	A
1	A	1904	U
1	A	1905	A
1	A	1907	C
1	A	1908	G
1	A	1909	G
1	A	1911	C
1	A	1916	G
1	A	1917	G
1	A	1924	A
1	A	1925	A
1	A	1927	U
1	A	1942	U
1	A	1952	C
1	A	1953	A
1	A	1954	C
1	A	1957	A
1	A	1958	U
1	A	1959	G
1	A	1969	U
1	A	1978	U
1	A	1980	U
1	A	1983	C
1	A	1984	C
1	A	1991	G
1	A	2007	A
1	A	2010	C
1	A	2018	A
1	A	2020	A
1	A	2021	U
1	A	2022	G
1	A	2030	U
1	A	2039	A

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Mol	Chain	Res	Type
1	A	2042	C
1	A	2043	G
1	A	2047	A
1	A	2048	G
1	A	2049	A
1	A	2054	G
1	A	2055	U
1	A	2056	G
1	A	2060	C
1	A	2063	U
1	A	2064	A
1	A	2080	G
1	A	2082	A
1	A	2083	C
1	A	2084	U
1	A	2094	C
1	A	2095	U
1	A	2096	U
1	A	2098	U
1	A	2099	G
1	A	2104	A
1	A	2106	A
1	A	2110	G
1	A	2113	A
1	A	2114	G
1	A	2116	C
1	A	2117	U
1	A	2118	U
1	A	2119	U
1	A	2120	G
1	A	2121	A
1	A	2132	C
1	A	2133	C
1	A	2134	A
1	A	2139	G
1	A	2140	C
1	A	2141	G
1	A	2143	G
1	A	2144	G
1	A	2145	A
1	A	2146	G
1	A	2147	C

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Mol	Chain	Res	Type
1	A	2148	C
1	A	2150	U
1	A	2151	C
1	A	2152	C
1	A	2156	A
1	A	2157	A
1	A	2158	A
1	A	2159	U
1	A	2160	A
1	A	2169	G
1	A	2174	C
1	A	2175	U
1	A	2176	U
1	A	2178	A
1	A	2185	A
1	A	2190	U
1	A	2191	G
1	A	2199	A
1	A	2212	A
1	A	2225	G
1	A	2226	G
1	A	2229	G
1	A	2237	G
1	A	2246	U
1	A	2253	A
1	A	2265	A
1	A	2270	U
1	A	2274	A
1	A	2275	A
1	A	2276	G
1	A	2279	G
1	A	2281	G
1	A	2283	U
1	A	2289	C
1	A	2290	G
1	A	2292	U
1	A	2293	C
1	A	2294	G
1	A	2295	G
1	A	2296	A
1	A	2297	A
1	A	2299	U

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Mol	Chain	Res	Type
1	A	2300	C
1	A	2301	G
1	A	2304	C
1	A	2305	G
1	A	2306	C
1	A	2307	A
1	A	2308	G
1	A	2312	A
1	A	2313	U
1	A	2318	G
1	A	2319	C
1	A	2321	A
1	A	2322	A
1	A	2323	A
1	A	2324	G
1	A	2325	C
1	A	2330	U
1	A	2331	U
1	A	2332	G
1	A	2334	C
1	A	2337	C
1	A	2342	C
1	A	2345	A
1	A	2348	C
1	A	2353	A
1	A	2354	G
1	A	2358	G
1	A	2359	U
1	A	2360	A
1	A	2361	C
1	A	2363	A
1	A	2364	A
1	A	2365	A
1	A	2366	G
1	A	2367	U
1	A	2370	G
1	A	2372	C
1	A	2375	A
1	A	2378	G
1	A	2383	G
1	A	2389	U
1	A	2390	C

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Mol	Chain	Res	Type
1	A	2393	U
1	A	2397	G
1	A	2406	U
1	A	2409	C
1	A	2410	U
1	A	2411	C
1	A	2413	A
1	A	2416	G
1	A	2417	A
1	A	2421	A
1	A	2427	C
1	A	2428	U
1	A	2431	G
1	A	2434	G
1	A	2435	A
1	A	2454	C
1	A	2457	G
1	A	2459	G
1	A	2463	A
1	A	2471	G
1	A	2474	G
1	A	2477	G
1	A	2478	U
1	A	2479	U
1	A	2480	U
1	A	2485	C
1	A	2489	G
1	A	2492	G
1	A	2505	A
1	A	2506	U
1	A	2516	G
1	A	2517	A
1	A	2522	G
1	A	2534	A
1	A	2537	G
1	A	2543	C
1	A	2545	C
1	A	2549	U
1	A	2551	A
1	A	2553	A
1	A	2554	G
1	A	2559	A

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Mol	Chain	Res	Type
1	A	2560	C
1	A	2565	G
1	A	2572	U
1	A	2573	U
1	A	2586	G
1	A	2589	A
1	A	2590	G
1	A	2597	C
1	A	2600	U
1	A	2616	U
1	A	2617	U
1	A	2633	C
1	A	2637	U
1	A	2638	C
1	A	2639	C
1	A	2641	A
1	A	2650	G
1	A	2656	G
1	A	2657	A
1	A	2658	G
1	A	2659	U
1	A	2668	C
1	A	2672	G
1	A	2676	U
1	A	2677	U
1	A	2687	A
1	A	2689	G
1	A	2694	U
1	A	2696	G
1	A	2701	G
1	A	2704	G
1	A	2705	G
1	A	2707	U
1	A	2713	U
1	A	2719	G
1	A	2720	A
1	A	2728	A
1	A	2731	G
1	A	2732	C
1	A	2735	A
1	A	2737	A
1	A	2739	C

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Mol	Chain	Res	Type
1	A	2740	A
1	A	2741	U
1	A	2744	A
1	A	2745	A
1	A	2749	G
1	A	2752	A
1	A	2756	U
1	A	2763	A
1	A	2765	A
1	A	2766	U
1	A	2772	C
1	A	2775	A
1	A	2776	C
1	A	2778	G
1	A	2784	U
1	A	2785	U
1	A	2786	G
1	A	2787	A
1	A	2807	A
1	A	2812	U
1	A	2819	U
1	A	2820	U
1	A	2821	G
1	A	2822	A
1	A	2829	G
1	A	2836	U
1	A	2844	G
1	A	2846	G
1	A	2848	G
1	A	2852	U
1	A	2853	U
1	A	2855	A
1	A	2856	G
1	A	2857	C
1	A	2858	U
1	A	2859	A
1	A	2860	A
1	A	2865	U
1	A	2866	A
1	A	2871	U
1	A	2872	G
1	A	2873	G

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Mol	Chain	Res	Type
1	A	2874	C
1	A	2878	U
1	A	2889	C
2	B	7	A
2	B	8	C
2	B	13	A
2	B	14	U
2	B	17	A
2	B	21	U
2	B	22	U
2	B	23	G
2	B	24	G
2	B	25	A
2	B	26	A
2	B	29	A
2	B	30	C
2	B	35	U
2	B	37	C
2	B	38	C
2	B	40	U
2	B	41	C
2	B	42	C
2	B	43	C
2	B	44	G
2	B	45	A
2	B	46	A
2	B	47	C
2	B	49	C
2	B	51	G
2	B	52	A
2	B	54	G
2	B	56	G
2	B	62	A
2	B	64	G
2	B	66	A
2	B	67	U
2	B	69	G
2	B	73	A
2	B	89	U
2	B	90	C
2	B	91	C
2	B	104	A

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Mol	Chain	Res	Type
2	B	105	G
2	B	106	G
2	B	107	U
2	B	109	A
2	B	110	U
2	B	111	C
2	B	113	U
2	B	116	A
2	B	117	G
33	a	7	A
33	a	9	G
33	a	22	G
33	a	23	C
33	a	29	U
33	a	31	G
33	a	32	A
33	a	35	G
33	a	37	U
33	a	38	G
33	a	39	G
33	a	47	C
33	a	48	C
33	a	50	A
33	a	51	A
33	a	54	C
33	a	61	G
33	a	62	U
33	a	64	G
33	a	65	A
33	a	66	G
33	a	68	G
33	a	70	A
33	a	72	G
33	a	73	A
33	a	74	A
33	a	79	G
33	a	82	U
33	a	83	G
33	a	87	C
33	a	89	G
33	a	93	U
33	a	94	C

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Mol	Chain	Res	Type
33	a	95	A
33	a	97	C
33	a	115	U
33	a	116	G
33	a	117	C
33	a	120	A
33	a	121	G
33	a	124	A
33	a	125	U
33	a	133	G
33	a	134	U
33	a	143	A
33	a	145	A
33	a	157	C
33	a	159	G
33	a	160	G
33	a	168	A
33	a	171	G
33	a	175	A
33	a	177	G
33	a	182	G
33	a	183	A
33	a	184	G
33	a	188	G
33	a	190	A
33	a	191	A
33	a	196	G
33	a	198	G
33	a	199	A
33	a	201	C
33	a	202	U
33	a	204	C
33	a	205	G
33	a	206	G
33	a	210	U
33	a	211	C
33	a	214	G
33	a	228	C
33	a	239	U
33	a	241	G
33	a	245	G
33	a	247	U

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Mol	Chain	Res	Type
33	a	248	G
33	a	252	G
33	a	260	G
33	a	261	C
33	a	265	C
33	a	266	C
33	a	273	A
33	a	274	C
33	a	275	G
33	a	283	A
33	a	287	G
33	a	290	U
33	a	292	A
33	a	295	G
33	a	299	G
33	a	300	A
33	a	307	A
33	a	315	A
33	a	321	A
33	a	322	C
33	a	323	A
33	a	324	C
33	a	325	G
33	a	326	G
33	a	338	A
33	a	339	C
33	a	341	G
33	a	342	G
33	a	345	G
33	a	346	C
33	a	348	G
33	a	350	A
33	a	353	G
33	a	361	U
33	a	362	U
33	a	363	G
33	a	366	C
33	a	367	A
33	a	370	G
33	a	372	G
33	a	373	C
33	a	378	G

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Mol	Chain	Res	Type
33	a	379	C
33	a	382	G
33	a	388	G
33	a	389	C
33	a	391	A
33	a	392	U
33	a	393	G
33	a	395	C
33	a	399	U
33	a	400	G
33	a	431	U
33	a	433	U
33	a	440	G
33	a	441	G
33	a	445	A
33	a	450	C
33	a	451	A
33	a	452	G
33	a	456	G
33	a	457	U
33	a	458	U
33	a	459	A
33	a	461	U
33	a	462	A
33	a	463	C
33	a	469	U
33	a	470	G
33	a	475	G
33	a	479	U
33	a	480	U
33	a	482	C
33	a	489	A
33	a	490	A
33	a	491	U
33	a	492	A
33	a	493	A
33	a	497	C
33	a	499	G
33	a	500	G
33	a	501	C
33	a	502	U
33	a	503	A

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Mol	Chain	Res	Type
33	a	504	A
33	a	505	C
33	a	506	U
33	a	509	G
33	a	512	C
33	a	513	C
33	a	519	C
33	a	520	C
33	a	521	G
33	a	524	G
33	a	525	U
33	a	526	A
33	a	527	A
33	a	530	C
33	a	532	A
33	a	536	G
33	a	538	G
33	a	539	C
33	a	541	A
33	a	542	G
33	a	552	G
33	a	553	A
33	a	556	U
33	a	558	C
33	a	560	G
33	a	562	G
33	a	566	A
33	a	567	A
33	a	570	C
33	a	571	G
33	a	573	G
33	a	575	G
33	a	582	G
33	a	593	U
33	a	599	U
33	a	601	A
33	a	607	C
33	a	609	G
33	a	613	U
33	a	614	C
33	a	619	U
33	a	622	G

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Mol	Chain	Res	Type
33	a	627	G
33	a	635	A
33	a	636	A
33	a	644	G
33	a	647	A
33	a	650	G
33	a	654	G
33	a	656	U
33	a	658	G
33	a	659	A
33	a	660	G
33	a	665	G
33	a	667	G
33	a	670	A
33	a	674	C
33	a	675	C
33	a	705	A
33	a	709	A
33	a	710	A
33	a	711	C
33	a	712	A
33	a	715	A
33	a	717	U
33	a	726	C
33	a	727	G
33	a	728	A
33	a	734	U
33	a	737	A
33	a	741	A
33	a	746	G
33	a	747	A
33	a	749	A
33	a	757	G
33	a	762	A
33	a	763	G
33	a	764	C
33	a	766	U
33	a	771	A
33	a	775	A
33	a	776	A
33	a	777	C
33	a	778	A

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Mol	Chain	Res	Type
33	a	779	G
33	a	781	A
33	a	785	G
33	a	787	U
33	a	788	A
33	a	790	C
33	a	791	C
33	a	794	G
33	a	795	U
33	a	797	G
33	a	808	A
33	a	809	A
33	a	810	A
33	a	811	C
33	a	814	U
33	a	815	G
33	a	822	A
33	a	823	G
33	a	826	G
33	a	829	G
33	a	830	G
33	a	838	G
33	a	839	A
33	a	840	G
33	a	845	U
33	a	849	G
33	a	851	C
33	a	858	A
33	a	861	G
33	a	864	A
33	a	866	A
33	a	867	A
33	a	870	C
33	a	883	A
33	a	884	G
33	a	894	A
33	a	896	G
33	a	902	A
33	a	908	A
33	a	920	G
33	a	921	G
33	a	928	C

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Mol	Chain	Res	Type
33	a	929	A
33	a	931	A
33	a	997	G
33	a	998	A
33	a	1004	C
33	a	1007	G
33	a	1008	A
33	a	1009	G
33	a	1011	U
33	a	1013	G
33	a	1015	U
33	a	1017	G
33	a	1019	U
33	a	1021	C
33	a	1025	C
33	a	1026	G
33	a	1028	G
33	a	1032	U
33	a	1039	C
33	a	1041	G
33	a	1043	U
33	a	1044	G
33	a	1046	U
33	a	1047	G
33	a	1048	C
33	a	1049	A
33	a	1050	U
33	a	1051	G
33	a	1052	G
33	a	1053	C
33	a	1061	A
33	a	1062	G
33	a	1069	U
33	a	1073	G
33	a	1078	G
33	a	1079	U
33	a	1082	G
33	a	1088	G
33	a	1089	U
33	a	1090	C
33	a	1094	U
33	a	1095	A

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Mol	Chain	Res	Type
33	a	1100	G
33	a	1101	C
33	a	1105	A
33	a	1113	C
33	a	1115	U
33	a	1116	U
33	a	1117	A
33	a	1118	G
33	a	1119	U
33	a	1120	U
33	a	1121	A
33	a	1123	C
33	a	1124	A
33	a	1125	G
33	a	1126	C
33	a	1127	A
33	a	1130	U
33	a	1132	G
33	a	1133	G
33	a	1134	G
33	a	1135	U
33	a	1137	G
33	a	1139	C
33	a	1140	A
33	a	1141	C
33	a	1142	U
33	a	1143	C
33	a	1145	A
33	a	1146	A
33	a	1148	G
33	a	1149	A
33	a	1150	G
33	a	1151	A
33	a	1152	C
33	a	1153	U
33	a	1154	G
33	a	1159	U
33	a	1162	C
33	a	1163	A
33	a	1165	A
33	a	1167	C
33	a	1171	G

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Mol	Chain	Res	Type
33	a	1172	G
33	a	1173	A
33	a	1174	A
33	a	1175	G
33	a	1176	G
33	a	1177	U
33	a	1189	C
33	a	1190	A
33	a	1191	A
33	a	1192	G
33	a	1193	U
33	a	1194	C
33	a	1195	A
33	a	1196	U
33	a	1197	C
33	a	1199	U
33	a	1200	G
33	a	1204	C
33	a	1205	U
33	a	1206	U
33	a	1207	A
33	a	1208	C
33	a	1209	G
33	a	1210	G
33	a	1211	C
33	a	1212	C
33	a	1213	A
33	a	1214	G
33	a	1215	G
33	a	1217	C
33	a	1218	U
33	a	1219	A
33	a	1221	A
33	a	1224	C
33	a	1225	G
33	a	1227	G
33	a	1228	C
33	a	1229	U
33	a	1230	A
33	a	1231	C
33	a	1232	A
33	a	1233	A

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Mol	Chain	Res	Type
33	a	1234	U
33	a	1235	G
33	a	1236	G
33	a	1237	U
33	a	1239	G
33	a	1240	G
33	a	1242	A
33	a	1243	C
33	a	1244	A
33	a	1245	A
33	a	1246	A
33	a	1247	G
33	a	1250	U
33	a	1251	U
33	a	1252	G
33	a	1254	C
33	a	1255	A
33	a	1256	A
33	a	1257	G
33	a	1258	C
33	a	1259	C
33	a	1260	G
33	a	1261	C
33	a	1263	A
33	a	1264	G
33	a	1265	G
33	a	1266	U
33	a	1267	G
33	a	1268	G
33	a	1272	U
33	a	1273	A
33	a	1274	A
33	a	1275	U
33	a	1276	C
33	a	1277	C
33	a	1278	C
33	a	1279	A
33	a	1280	U
33	a	1282	A
33	a	1283	A
33	a	1286	C
33	a	1287	G

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Mol	Chain	Res	Type
33	a	1291	G
33	a	1292	U
33	a	1293	A
33	a	1294	G
33	a	1295	U
33	a	1296	C
33	a	1297	C
33	a	1298	G
33	a	1299	G
33	a	1300	A
33	a	1301	U
33	a	1303	G
33	a	1304	C
33	a	1305	A
33	a	1307	U
33	a	1308	C
33	a	1309	U
33	a	1310	G
33	a	1311	C
33	a	1313	A
33	a	1314	C
33	a	1315	U
33	a	1316	C
33	a	1317	G
33	a	1318	A
33	a	1319	C
33	a	1320	U
33	a	1321	G
33	a	1323	G
33	a	1324	U
33	a	1326	A
33	a	1330	C
33	a	1331	G
33	a	1332	G
33	a	1333	A
33	a	1334	A
33	a	1336	C
33	a	1337	G
33	a	1338	C
33	a	1339	U
33	a	1340	A
33	a	1341	G

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Mol	Chain	Res	Type
33	a	1342	U
33	a	1344	A
33	a	1345	U
33	a	1346	C
33	a	1347	G
33	a	1348	U
33	a	1350	A
33	a	1351	A
33	a	1352	U
33	a	1353	C
33	a	1354	A
33	a	1355	G
33	a	1356	A
33	a	1357	A
33	a	1358	U
33	a	1359	G
33	a	1361	C
33	a	1362	A
33	a	1363	C
33	a	1364	G
33	a	1365	G
33	a	1366	U
33	a	1368	A
33	a	1370	U
33	a	1371	A
33	a	1372	C
33	a	1373	G
33	a	1374	U
33	a	1375	U
33	a	1378	C
33	a	1379	G
33	a	1380	G
33	a	1384	U
33	a	1388	A
33	a	1389	C
33	a	1391	C
33	a	1394	C
33	a	1395	G
33	a	1401	C
33	a	1413	G
33	a	1421	C
33	a	1422	U

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Mol	Chain	Res	Type
33	a	1423	C
33	a	1428	A
33	a	1432	G
33	a	1435	A
33	a	1440	A
33	a	1441	A
33	a	1444	G
33	a	1445	C
33	a	1446	A
33	a	1447	A
33	a	1448	G
33	a	1454	C
33	a	1455	G
33	a	1458	U
33	a	1469	G
33	a	1481	G
33	a	1485	G
33	a	1487	A
33	a	1488	G
33	a	1491	G
33	a	1493	A
33	a	1497	A
33	a	1500	U
33	a	1501	A
33	a	1503	C
33	a	1507	A
33	a	1511	G
33	a	1513	A
33	a	1514	C
33	a	1518	C
33	a	1519	G
33	a	1522	U
33	a	1523	G
33	a	1524	G
33	a	1525	A
33	a	1526	U

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	62	U
1	A	63	A

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Mol	Chain	Res	Type
1	A	81	G
1	A	114	U
1	A	159	G
1	A	227	A
1	A	314	A
1	A	399	G
1	A	434	A
1	A	444	A
1	A	503	G
1	A	540	U
1	A	551	G
1	A	920	C
1	A	953	U
1	A	1016	U
1	A	1065	C
1	A	1070	C
1	A	1088	A
1	A	1166	G
1	A	1169	A
1	A	1213	A
1	A	1431	A
1	A	1441	U
1	A	1496	A
1	A	1642	A
1	A	1893	G
1	A	2228	A
1	A	2274	A
1	A	2317	G
1	A	2389	U
1	A	2408	G
1	A	2536	G
1	A	2703	C
1	A	2731	G
1	A	2743	U
2	B	25	A
2	B	34	A
2	B	51	G
2	B	66	A

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

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](#)

There are no ligands in this entry.

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
33	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	1376:C	O3'	1377:C	P	3.50

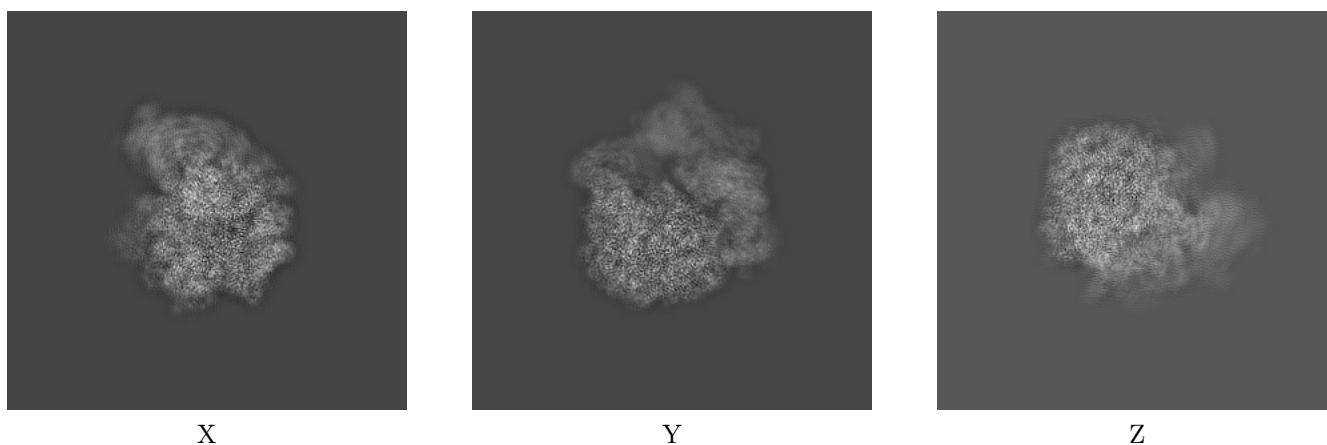
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10284. 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](#)

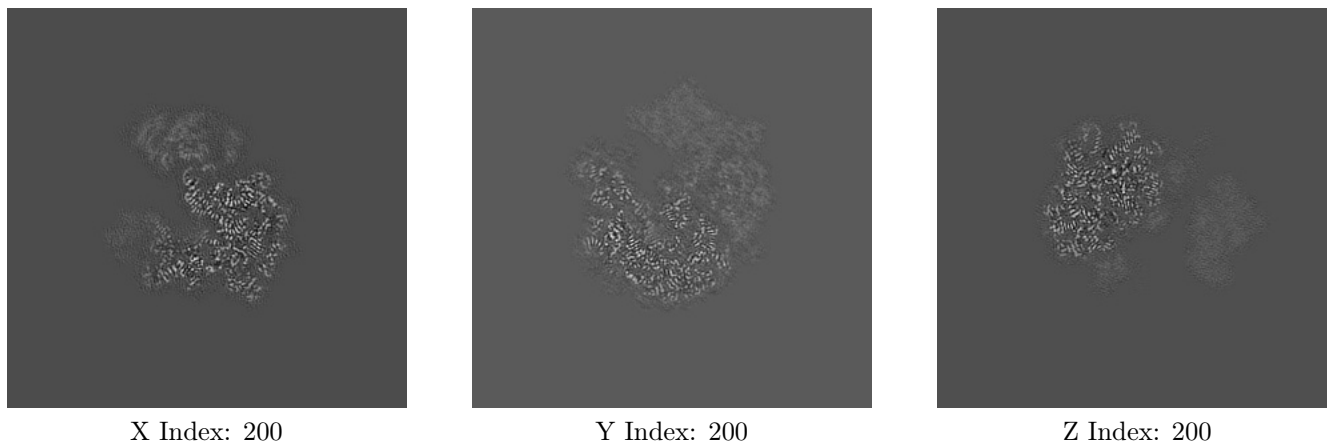
6.1.1 Primary map



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

6.2 Central slices [i](#)

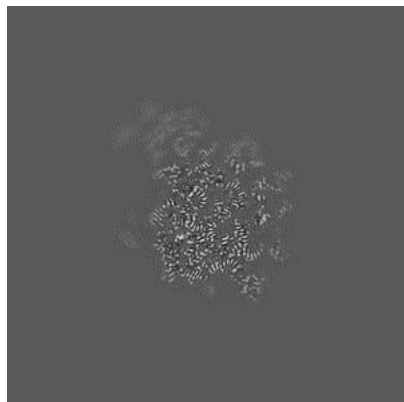
6.2.1 Primary map



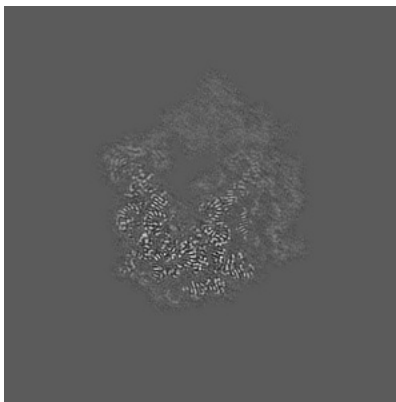
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

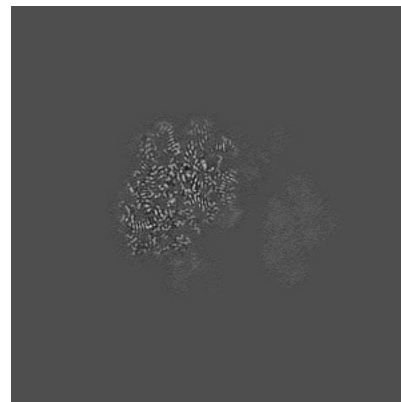
6.3.1 Primary map



X Index: 153



Y Index: 187



Z Index: 198

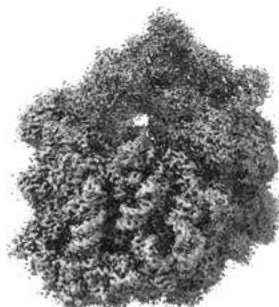
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

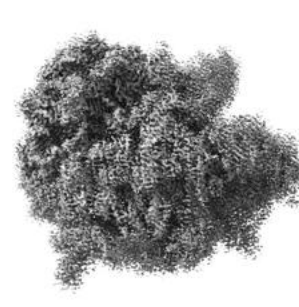
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0491. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

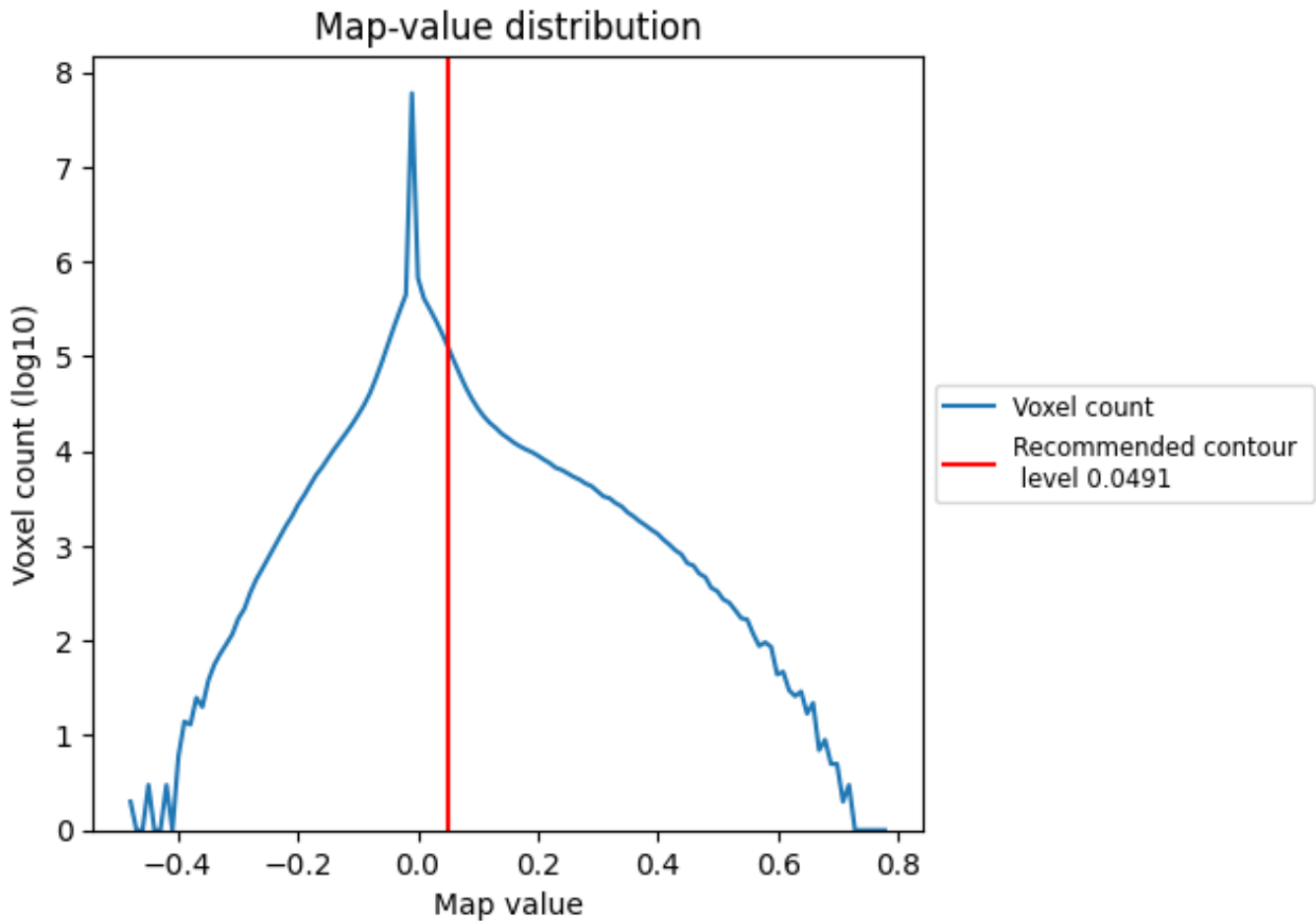
6.5 Mask visualisation

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

7 Map analysis [i](#)

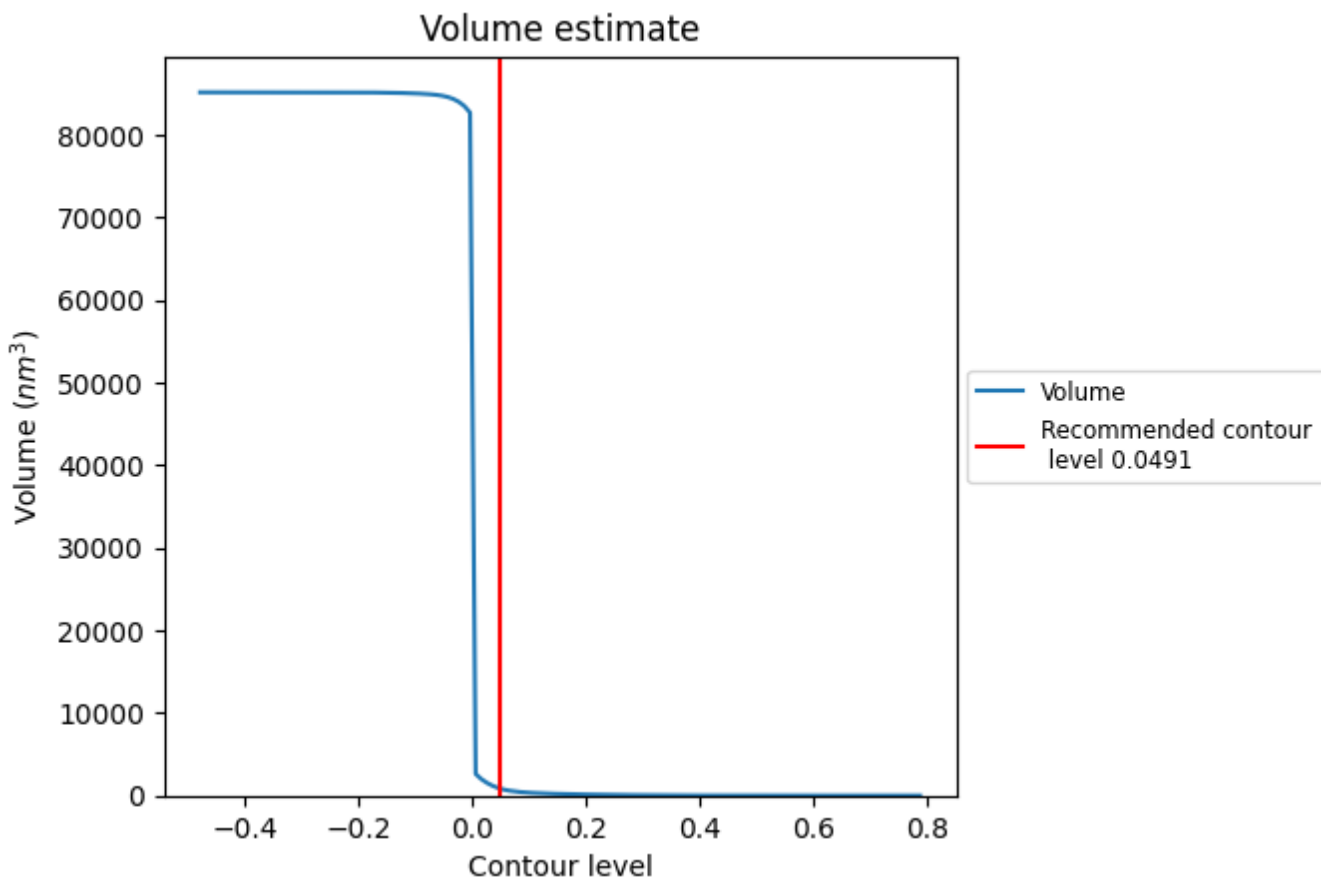
This section contains the results of statistical analysis of the map.

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.

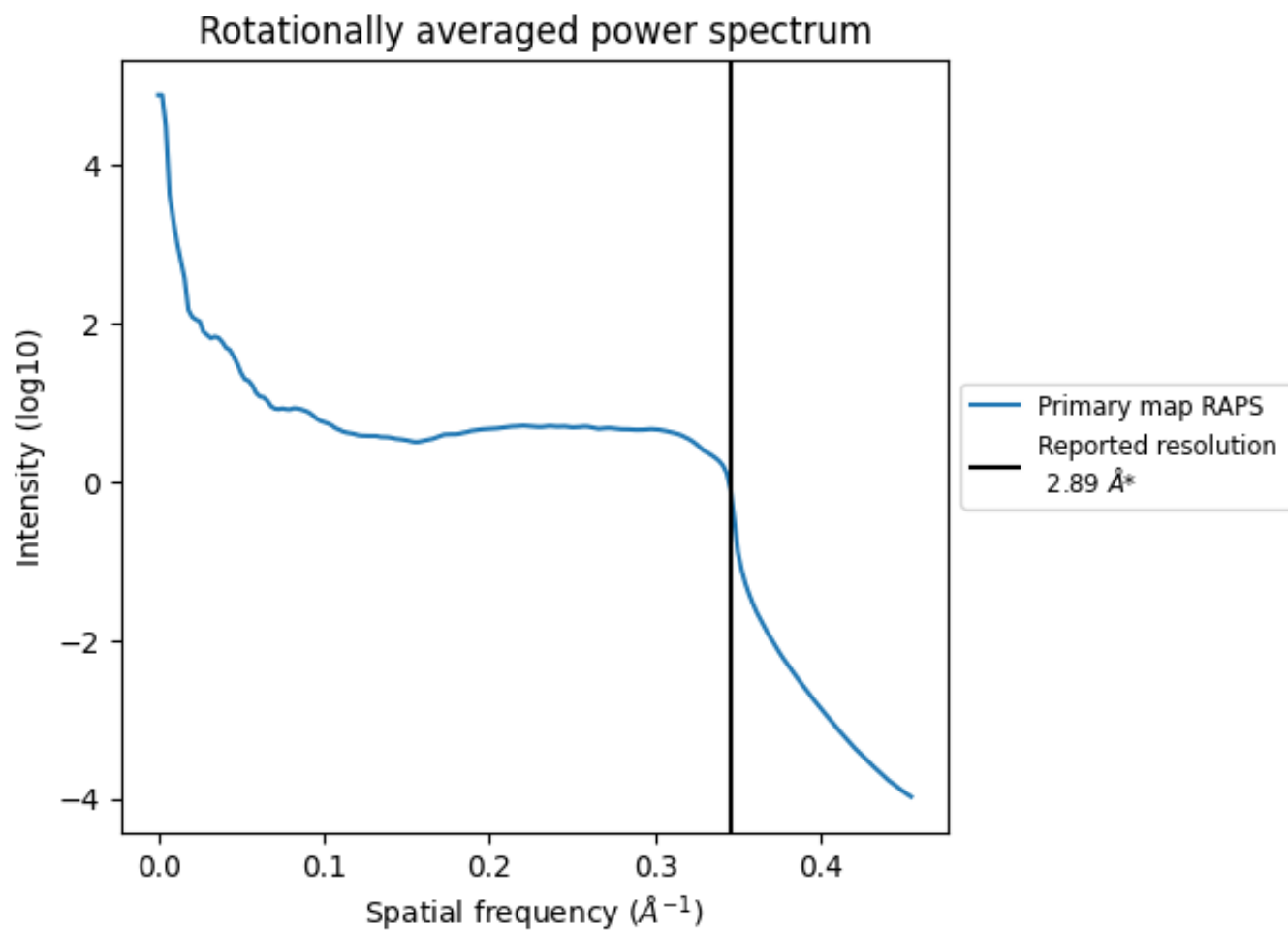
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 861 nm³; this corresponds to an approximate mass of 778 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 0.346 Å⁻¹

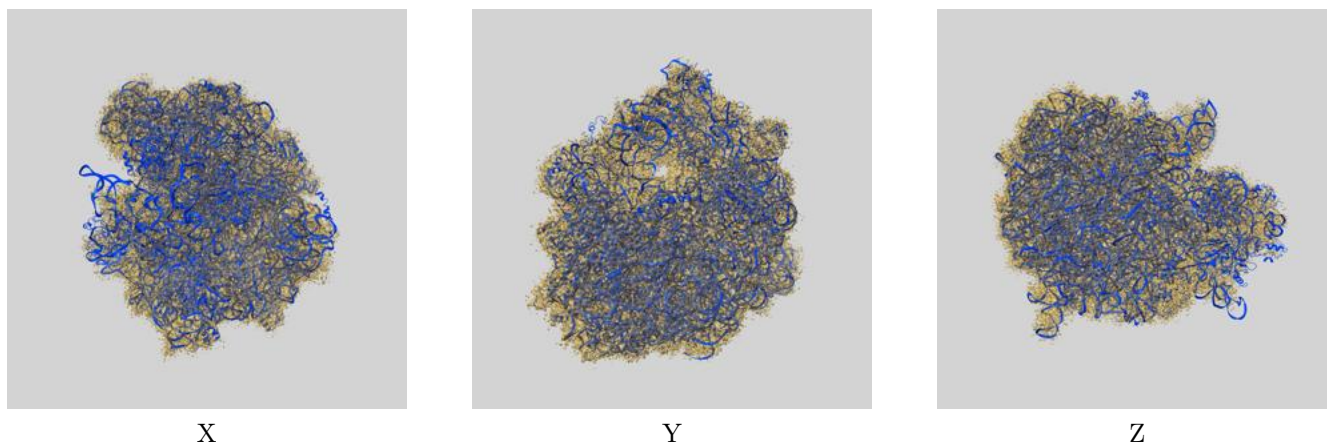
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

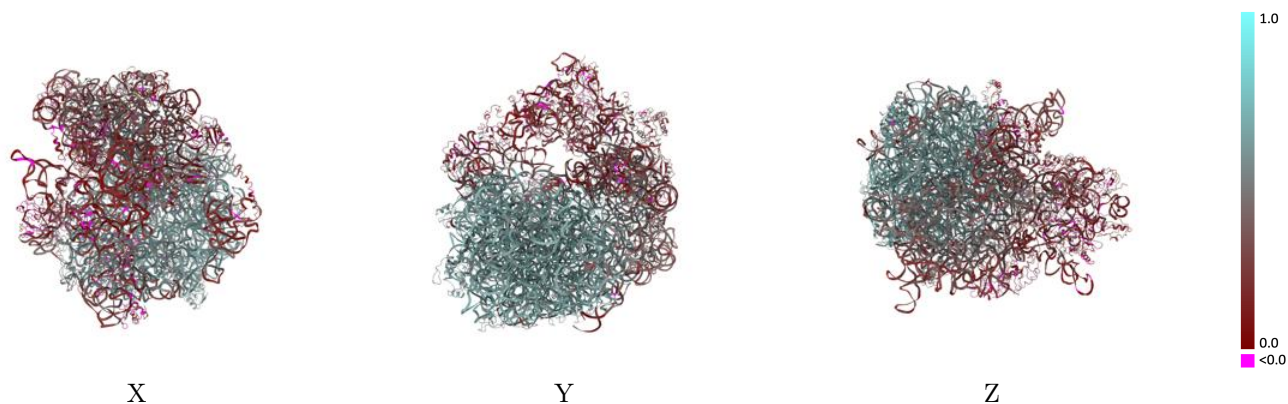
This section contains information regarding the fit between EMDB map EMD-10284 and PDB model 6SPF. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



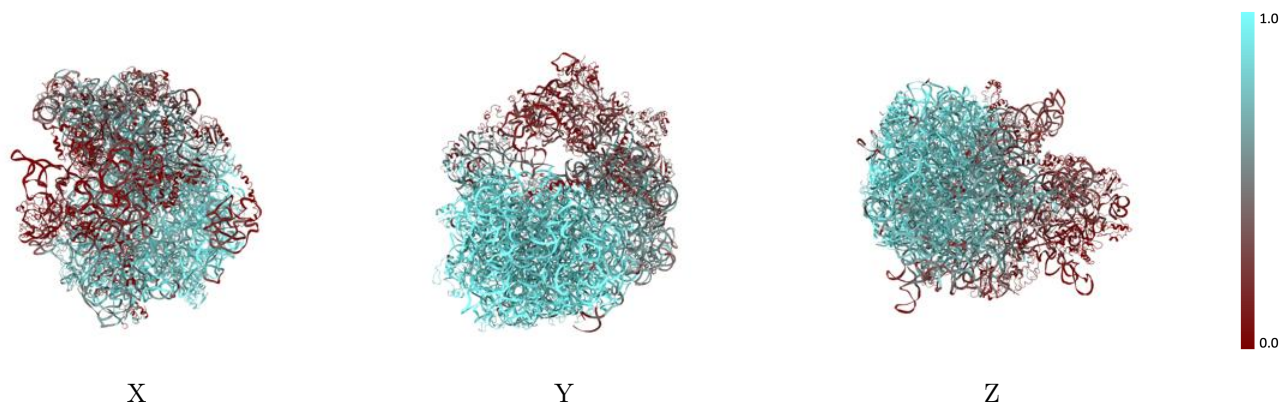
The images above show the 3D surface view of the map at the recommended contour level 0.0491 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



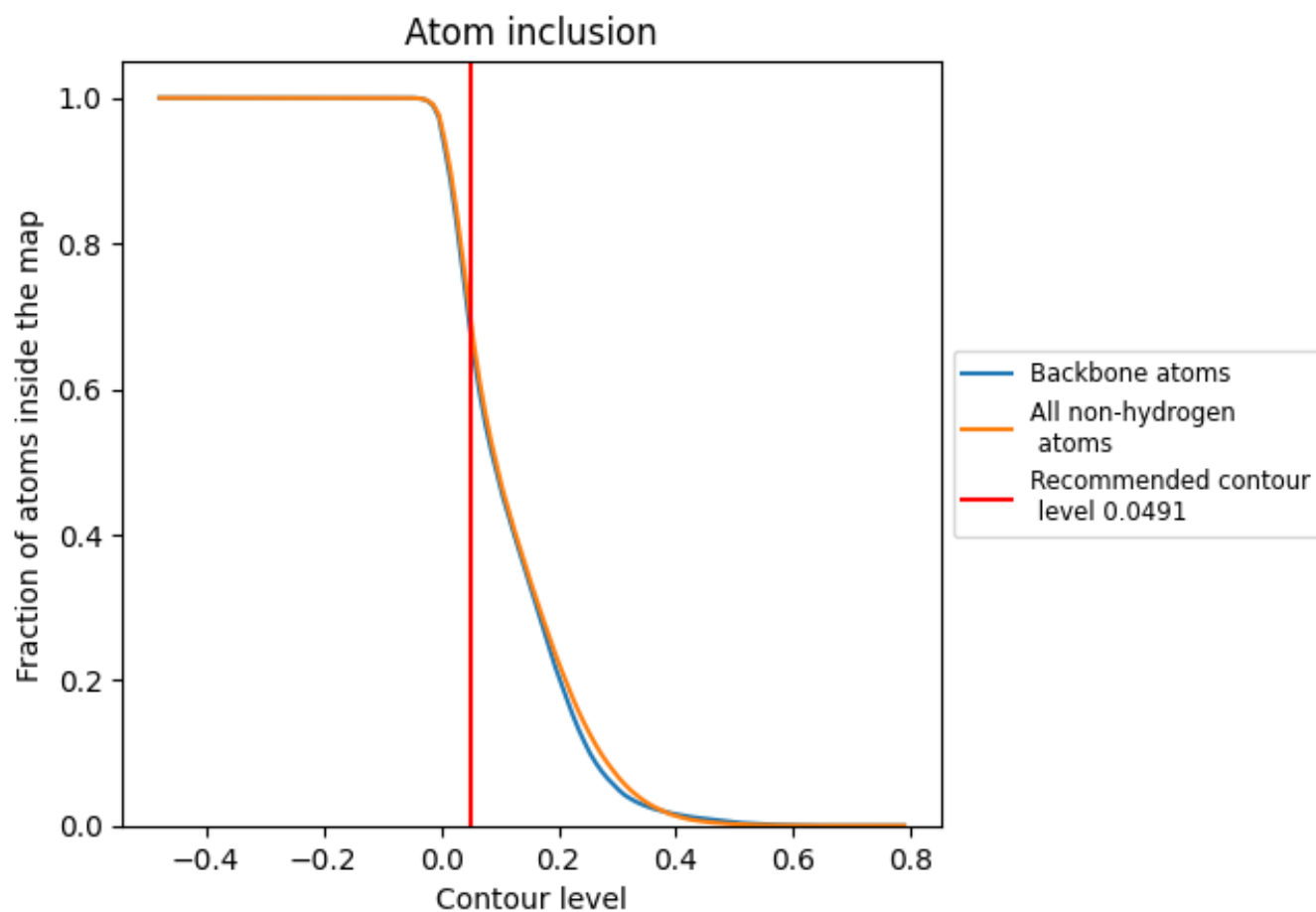
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0491).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 70% 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 (0.0491) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7027	 0.4610
1	 0.0000	 0.1520
2	 0.9356	 0.6140
3	 0.5088	 0.3640
4	 0.9708	 0.6320
5	 0.8909	 0.5960
6	 0.8201	 0.5610
A	 0.8871	 0.5680
B	 0.7483	 0.3920
C	 0.9333	 0.6170
D	 0.9490	 0.6250
E	 0.9199	 0.5960
F	 0.3800	 0.2220
G	 0.3761	 0.3870
H	 0.3081	 0.2770
I	 0.0286	 0.1110
J	 0.9425	 0.6150
K	 0.9064	 0.6100
L	 0.9130	 0.5920
M	 0.8165	 0.5770
N	 0.9535	 0.6200
O	 0.5129	 0.2330
P	 0.8938	 0.5950
Q	 0.9228	 0.6060
R	 0.8799	 0.5620
S	 0.9227	 0.6200
T	 0.8986	 0.5870
U	 0.8310	 0.5470
V	 0.7333	 0.4960
W	 0.8946	 0.5910
X	 0.9101	 0.6020
Y	 0.8865	 0.5720
Z	 0.9307	 0.6070
a	 0.5372	 0.3220
b	 0.2520	 0.2730



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Chain	Atom inclusion	Q-score
c	 0.0564	 0.1670
d	 0.2677	 0.2390
e	 0.2913	 0.3050
f	 0.2169	 0.2100
g	 0.0944	 0.2300
h	 0.3721	 0.3130
i	 0.1352	 0.1730
j	 0.0632	 0.1880
k	 0.1993	 0.2160
l	 0.2991	 0.3490
m	 0.1089	 0.1710
n	 0.0577	 0.1730
o	 0.3765	 0.2550
p	 0.4437	 0.3410
q	 0.4799	 0.3650
r	 0.2209	 0.1440
s	 0.1337	 0.1910
t	 0.5597	 0.3880
u	 0.1232	 0.2450