



Full wwPDB EM Validation Report ⓘ

May 20, 2026 – 08:00 am BST

PDB ID : 9FY3 / pdb_00009fy3
EMDB ID : EMD-50858
Title : Structure of CliM-stalled *Bacillus subtilis* 70S ribosome with tRNA-Tyr in the A-site
Authors : Gersteuer, F.; Wilson, D.N.
Deposited on : 2024-07-02
Resolution : 2.80 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:

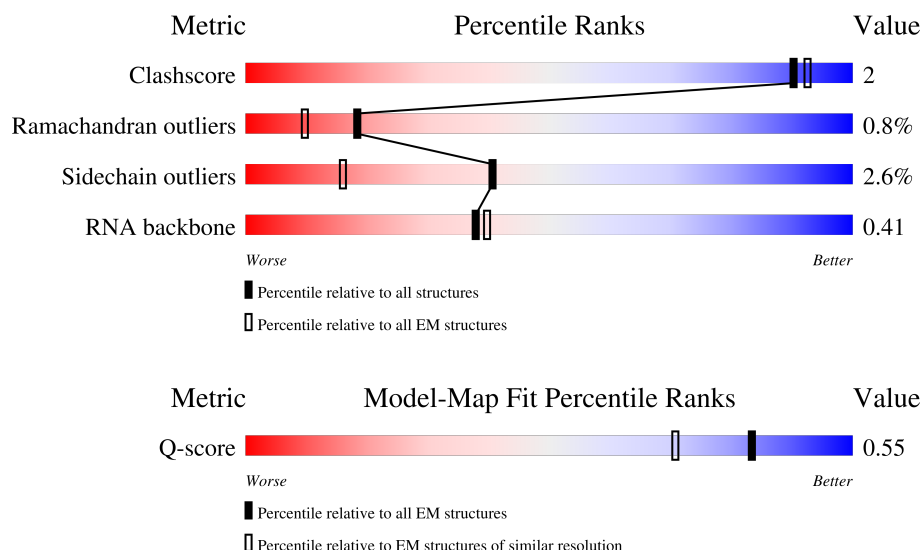
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.80 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.



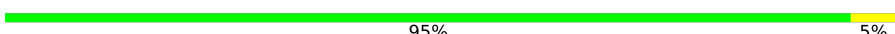
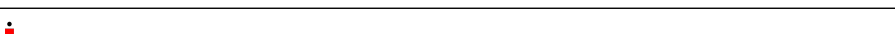
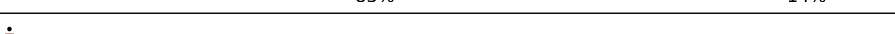
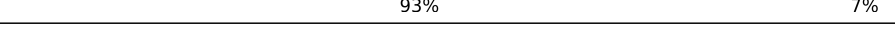
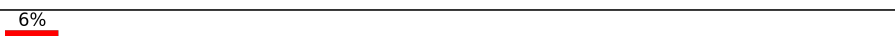
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	0	59	
2	1	49	
3	2	44	

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Mol	Chain	Length	Quality of chain
4	3	66	
5	4	37	
6	5	38	
7	6	66	
8	B	112	
9	C	277	
10	D	209	
11	E	207	
12	F	179	
13	G	179	
14	J	145	
15	K	122	
16	L	146	
17	M	144	
18	N	120	
19	O	120	
20	P	115	
21	Q	119	
22	R	102	
23	S	113	
24	T	95	
25	U	103	
26	X	62	
27	Y	66	
28	Z	59	

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Mol	Chain	Length	Quality of chain
29	c	218	
30	e	166	
31	f	95	
32	g	156	
33	h	132	
34	i	130	
35	j	102	
36	k	131	
37	l	138	
38	m	121	
39	n	61	
40	o	89	
41	p	90	
42	q	87	
43	r	79	
44	t	88	
45	v	76	
46	A	2928	
47	b	246	
48	s	92	
49	7	9	
50	9	85	
51	a	1554	
52	W	94	
53	d	200	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 139157 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	54	Total	C	N	O	S	0	0
			425	262	86	71	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	11	VAL	MET	conflict	UNP O34687

- Molecule 2 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	48	Total	C	N	O	S	0	0
			403	245	81	74	3		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	44	Total	C	N	O	S	0	0
			368	222	89	55	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 6 is a protein called Nascent Chain CliM.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	38	Total	C	N	O	S	0	0
			346	232	56	57	1		

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	46	Total	C	N	O	S	0	0
			356	222	63	66	5		

- Molecule 8 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 9 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	273	Total	C	N	O	S	0	0
			2093	1301	412	374	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	216	VAL	ILE	conflict	UNP P42919

- Molecule 10 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	207	Total	C	N	O	S	0	0
			1575	988	290	292	5		

- Molecule 11 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	206	Total	C	N	O	S	0	0
			1567	983	290	292	2		

- Molecule 12 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	178	Total	C	N	O	S	0	0
			1405	893	245	260	7		

- Molecule 13 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 14 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	144	Total	C	N	O	S	0	0
			1142	720	211	206	5		

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	122	Total	C	N	O	S	0	0
			921	571	173	173	4		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	146	Total	C	N	O	S	0	0
			1082	671	207	202	2		

- Molecule 17 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	119	Total	C	N	O	S	0	0
			954	583	186	181	4		

- Molecule 19 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	120	Total	C	N	O	S	0	0
			913	564	176	172	1		

- Molecule 20 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	114	Total	C	N	O	S	0	0
			933	593	184	156			

- Molecule 21 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	118	Total	C	N	O	S	0	0
			950	597	191	158	4		

- Molecule 22 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	101	Total	C	N	O	S	0	0
			789	503	139	146	1		

- Molecule 23 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	110	Total	C	N	O	S	0	0
			850	530	165	151	4		

- Molecule 24 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	91	Total	C	N	O	S	0	0
			733	458	135	137	3		

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	102	Total	C	N	O	S	0	0
			770	482	143	141	4		

- Molecule 26 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	61	Total	C	N	O	S	0	0
			467	288	98	79	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	33	VAL	LEU	conflict	UNP P37807

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	66	Total	C	N	O	S	0	0
			540	334	104	100	2		

- Molecule 28 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	58	Total	C	N	O	S	0	0
			456	281	89	85	1		

- Molecule 29 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	204	Total	C	N	O	S	0	0
			1608	1004	302	299	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	148	ILE	VAL	conflict	UNP P21465

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	164	Total	C	N	O	S	0	0
			1219	767	225	225	2		

- Molecule 31 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	93	Total	C	N	O	S	0	0
			765	482	136	145	2		

- Molecule 32 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	151	Total	C	N	O	S	0	0
			1199	751	225	217	6		

- Molecule 33 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	130	Total	C	N	O	S	0	0
			1030	650	190	187	3		

- Molecule 34 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	128	Total	C	N	O	S	0	0
			997	618	198	180	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	72	PHE	LEU	conflict	UNP P21470

- Molecule 35 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	97	Total	C	N	O	S	0	0
			779	491	143	143	2		

- Molecule 36 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	115	Total	C	N	O	S	0	0
			847	520	166	159	2		

- Molecule 37 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	134	Total	C	N	O	S	0	0
			1036	642	208	184	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	2	ALA	PRO	conflict	UNP P21472

- Molecule 38 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	118	Total	C	N	O	0	0
			943	579	194	170		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	33	ILE	VAL	conflict	UNP P20282

- Molecule 39 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	60	Total	C	N	O	S	0	0
			498	317	98	78	5		

- Molecule 40 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	87	Total	C	N	O	S	0	0
			730	448	149	132	1		

- Molecule 41 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	87	Total	C	N	O	S	0	0
			691	439	127	123	2		

- Molecule 42 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	84	Total	C	N	O	S	0	0
			693	438	128	125	2		

- Molecule 43 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	65	Total	C	N	O	S	0	0
			522	334	97	89	2		

- Molecule 44 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	86	Total	C	N	O	S	0	0
			658	402	134	121	1		

- Molecule 45 is a RNA chain called P-site tRNA-Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	v	76	Total	C	N	O	P	0	0
			1622	723	290	533	76		

- Molecule 46 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	A	2724	Total	C	N	O	P	0	0
			58523	26110	10840	18851	2722		

- Molecule 47 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	b	195	Total	C	N	O	S	0	0
			1564	996	277	285	6		

- Molecule 48 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	83	Total	C	N	O	S	0	0
			668	429	122	115	2		

- Molecule 49 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	9	Total	C	N	O	P	0	0
			189	85	30	65	9		

- Molecule 50 is a RNA chain called A-site tRNA-Tyr.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	9	74	Total	C	N	O	P	0	0
			1581	705	288	514	74		

- Molecule 51 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	a	1533	Total	C	N	O	P	0	0
			32891	14667	6034	10657	1533		

- Molecule 52 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	W	83	Total	C	N	O	0	0
			639	395	125	119		

- Molecule 53 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	d	199	Total	C	N	O	S	0	0
			1604	1013	298	291	2		

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	0	1	Total	Zn	0
			1	1	
54	4	1	Total	Zn	0
			1	1	
54	6	1	Total	Zn	0
			1	1	
54	n	1	Total	Zn	0
			1	1	

3 Residue-property plots [i](#)

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: Large ribosomal subunit protein bL32

Chain 0:  71% 17% • 8%

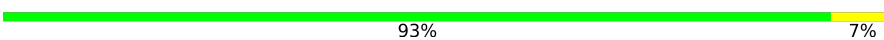


- Molecule 2: 50S ribosomal protein L33 1

Chain 1:  82% 14% • •



- Molecule 3: 50S ribosomal protein L34

Chain 2:  93% 7%



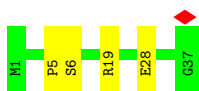
- Molecule 4: 50S ribosomal protein L35

Chain 3:  88% 9% •

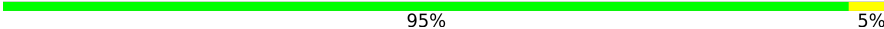


- Molecule 5: 50S ribosomal protein L36

Chain 4:  89% 11%



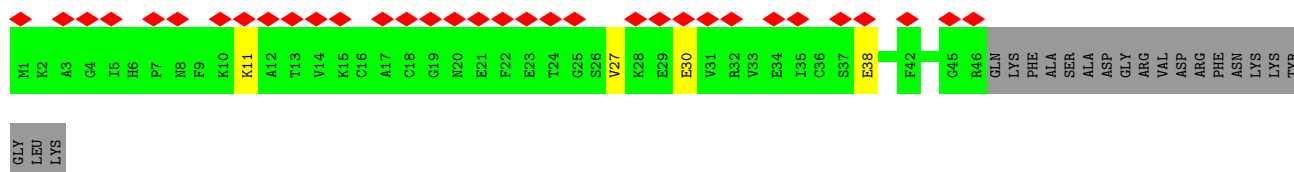
- Molecule 6: Nascent Chain CliM

Chain 5:  95% 5%



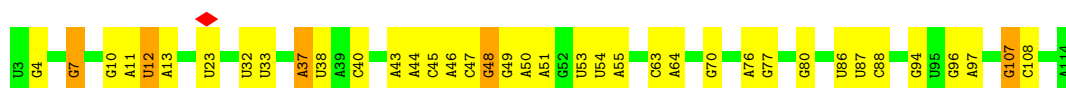
- Molecule 7: 50S ribosomal protein L31

Chain 6:  50% 64% 6% 30%



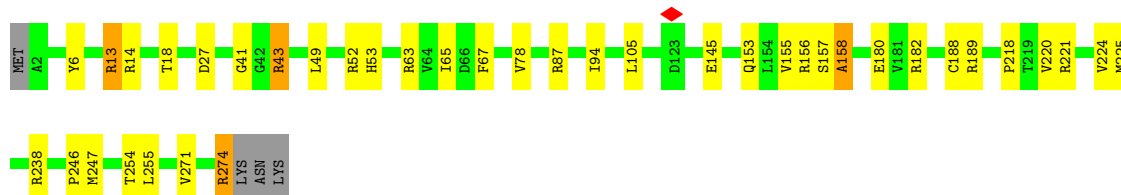
- Molecule 8: 5S rRNA

Chain B:  66% 29%



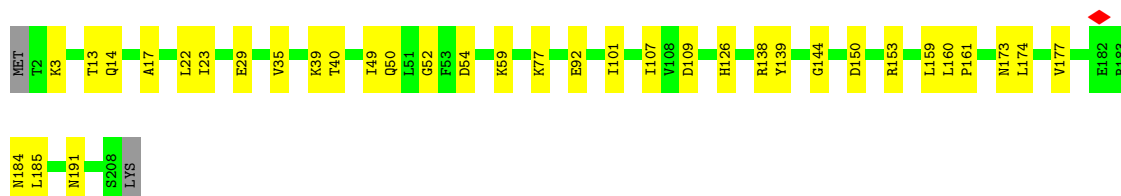
- Molecule 9: Large ribosomal subunit protein uL2

Chain C:  84% 13%



- Molecule 10: 50S ribosomal protein L3

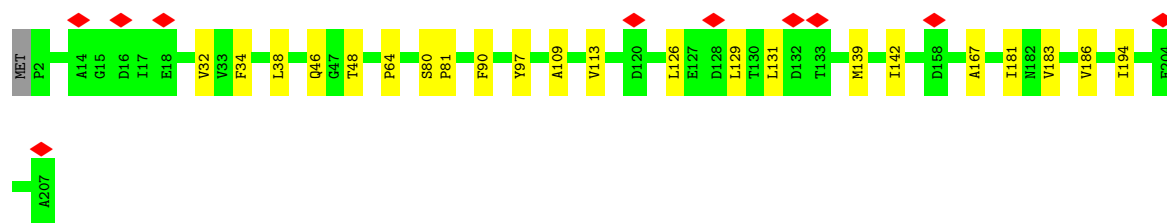
Chain D:  82% 17%



- Molecule 11: 50S ribosomal protein L4

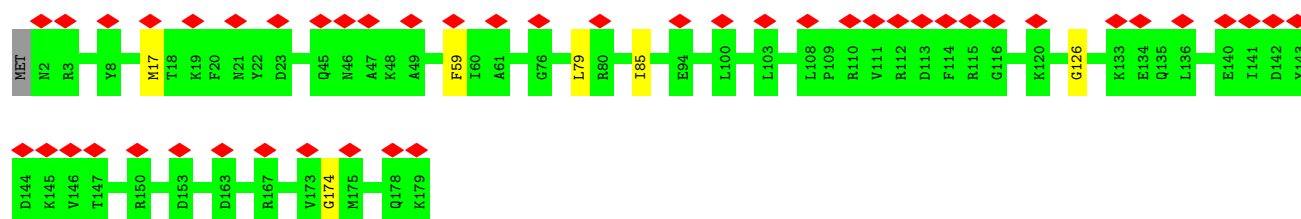
Chain E:  5% 89% 11%





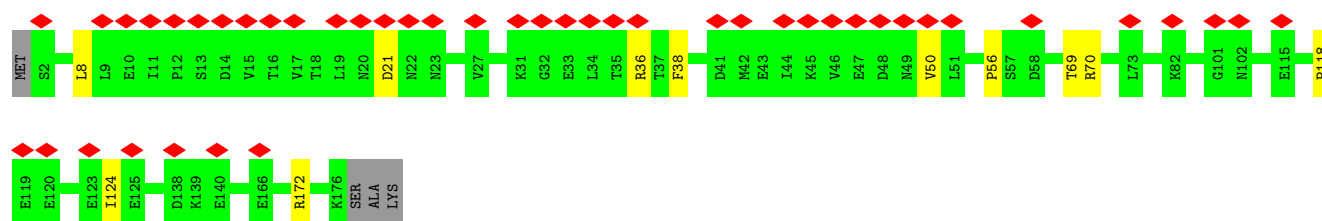
- Molecule 12: 50S ribosomal protein L5

Chain F: 26% 96%



- Molecule 13: Large ribosomal subunit protein uL6

Chain G: 25% 92% 6%



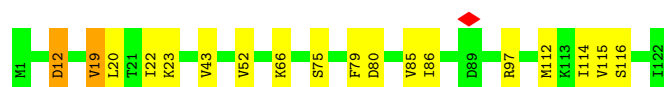
- Molecule 14: 50S ribosomal protein L13

Chain J: 83% 14%



- Molecule 15: 50S ribosomal protein L14

Chain K: 85% 13%

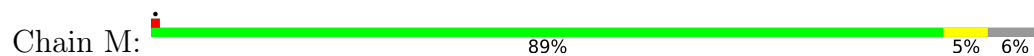


- Molecule 16: 50S ribosomal protein L15

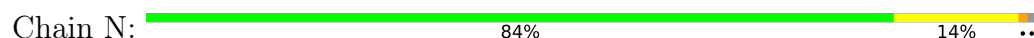
Chain L: 93% 7%



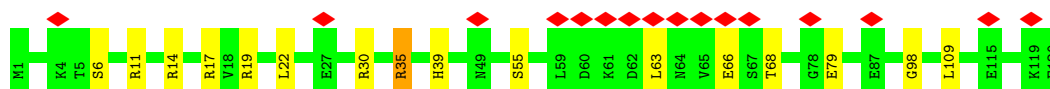
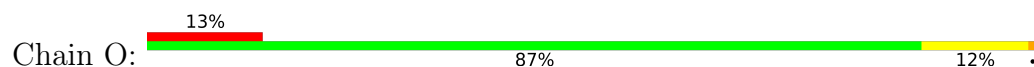
- Molecule 17: 50S ribosomal protein L16



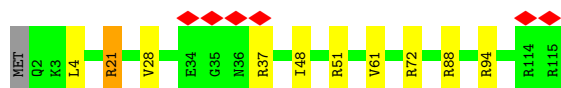
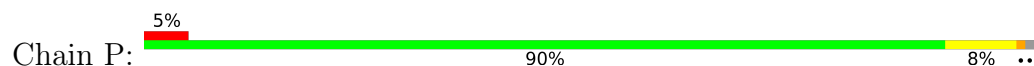
- Molecule 18: 50S ribosomal protein L17



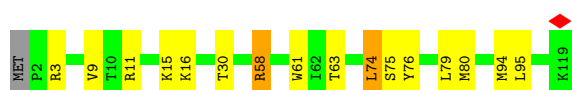
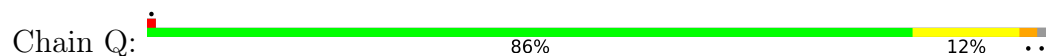
- Molecule 19: 50S ribosomal protein L18



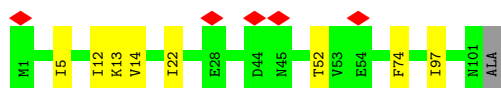
- Molecule 20: 50S ribosomal protein L19



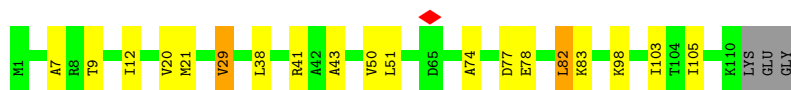
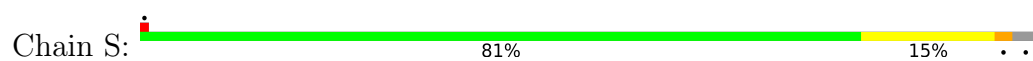
- Molecule 21: Large ribosomal subunit protein bL20



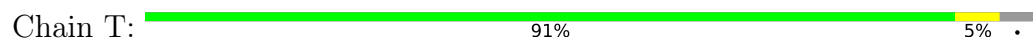
- Molecule 22: 50S ribosomal protein L21



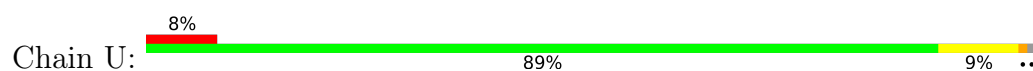
- Molecule 23: 50S ribosomal protein L22



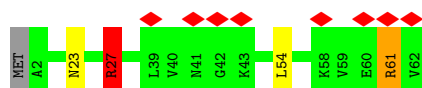
- Molecule 24: Large ribosomal subunit protein uL23



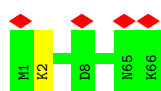
- Molecule 25: 50S ribosomal protein L24



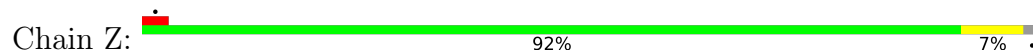
- Molecule 26: Large ribosomal subunit protein bL28



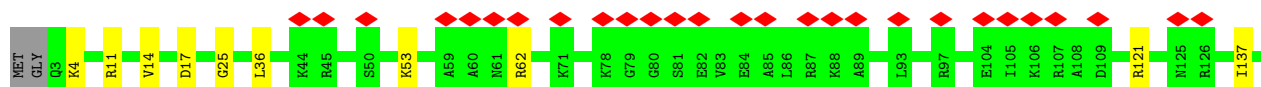
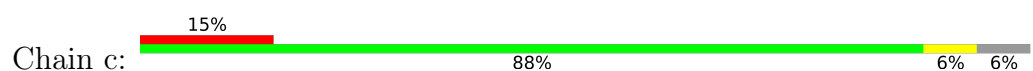
- Molecule 27: 50S ribosomal protein L29

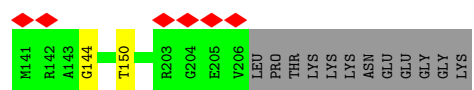


- Molecule 28: Large ribosomal subunit protein uL30



- Molecule 29: Small ribosomal subunit protein uS3

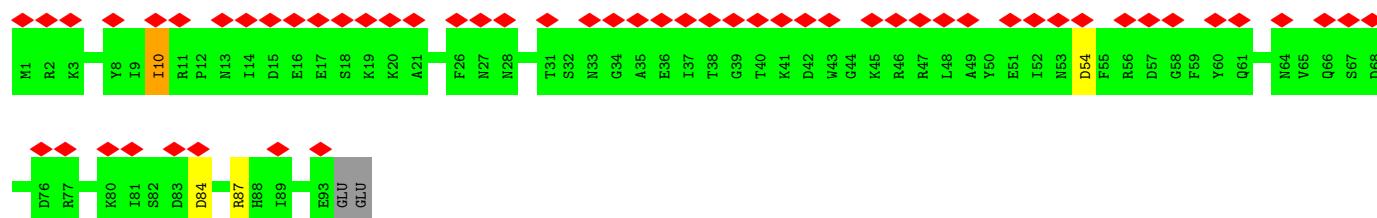




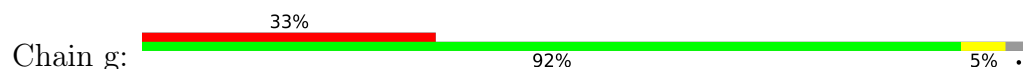
- Molecule 30: 30S ribosomal protein S5



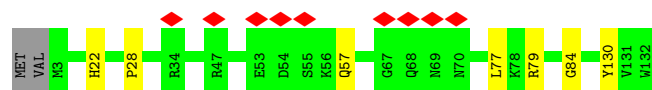
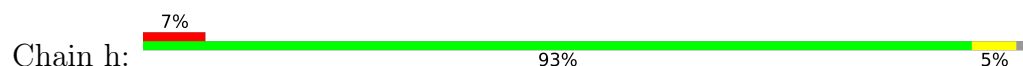
- Molecule 31: 30S ribosomal protein S6



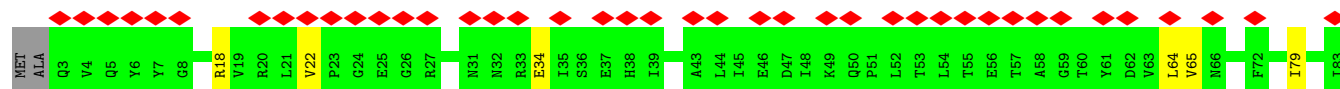
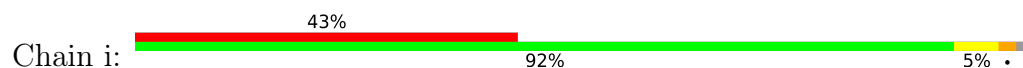
- Molecule 32: Small ribosomal subunit protein uS7

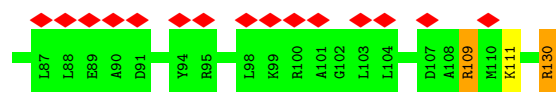


- Molecule 33: 30S ribosomal protein S8

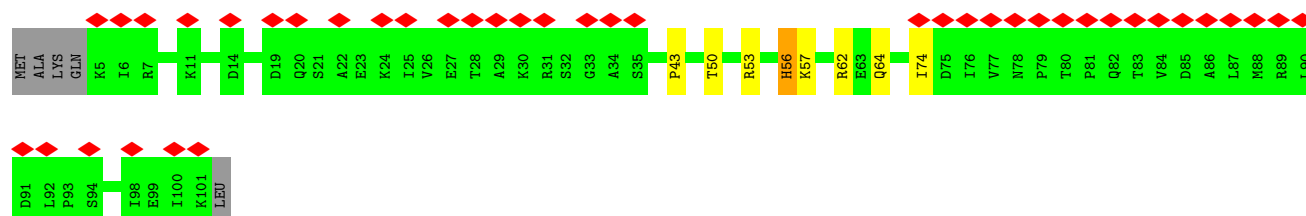
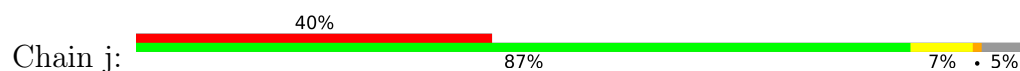


- Molecule 34: Small ribosomal subunit protein uS9

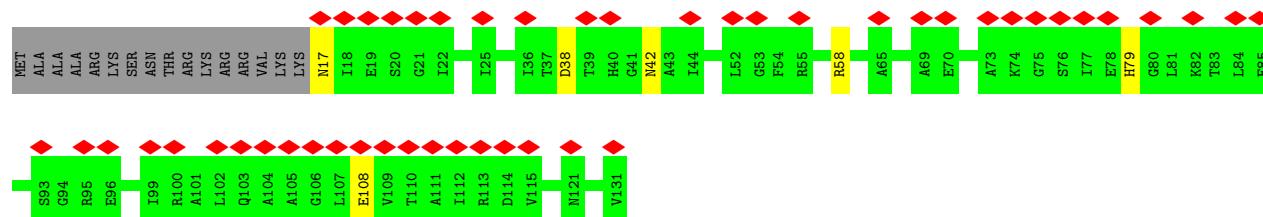
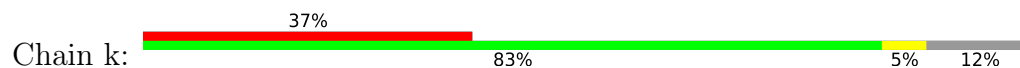




- Molecule 35: 30S ribosomal protein S10



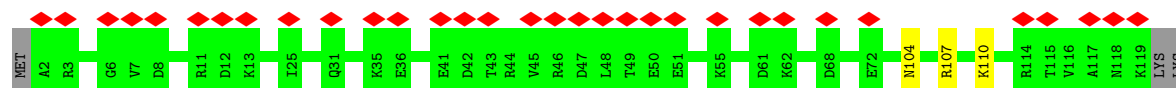
- Molecule 36: 30S ribosomal protein S11



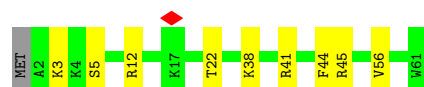
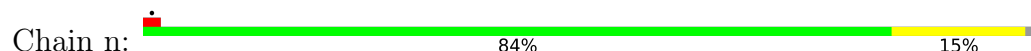
- Molecule 37: Small ribosomal subunit protein uS12



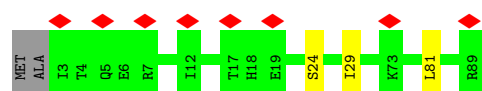
- Molecule 38: Small ribosomal subunit protein uS13



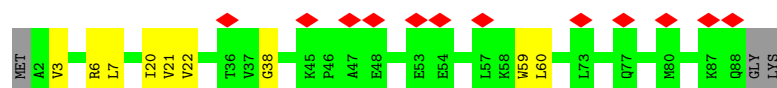
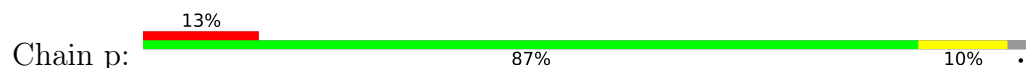
- Molecule 39: 30S ribosomal protein S14



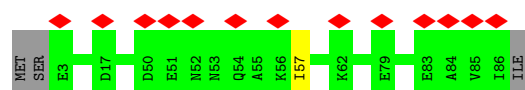
- Molecule 40: 30S ribosomal protein S15



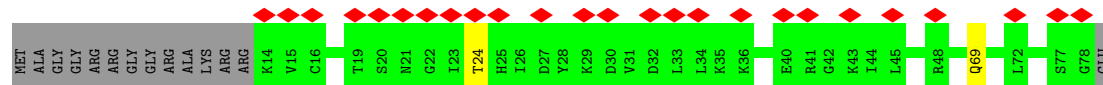
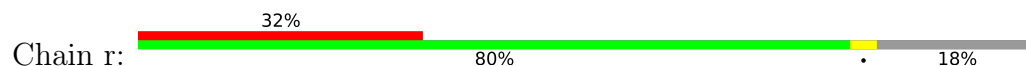
- Molecule 41: 30S ribosomal protein S16



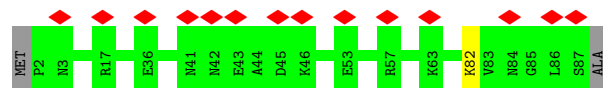
- Molecule 42: 30S ribosomal protein S17



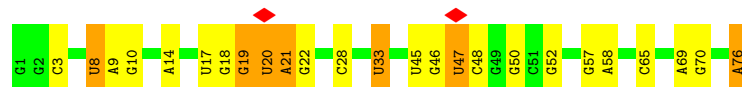
- Molecule 43: 30S ribosomal protein S18



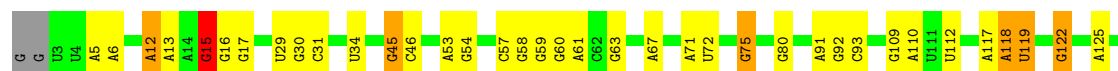
- Molecule 44: 30S ribosomal protein S20

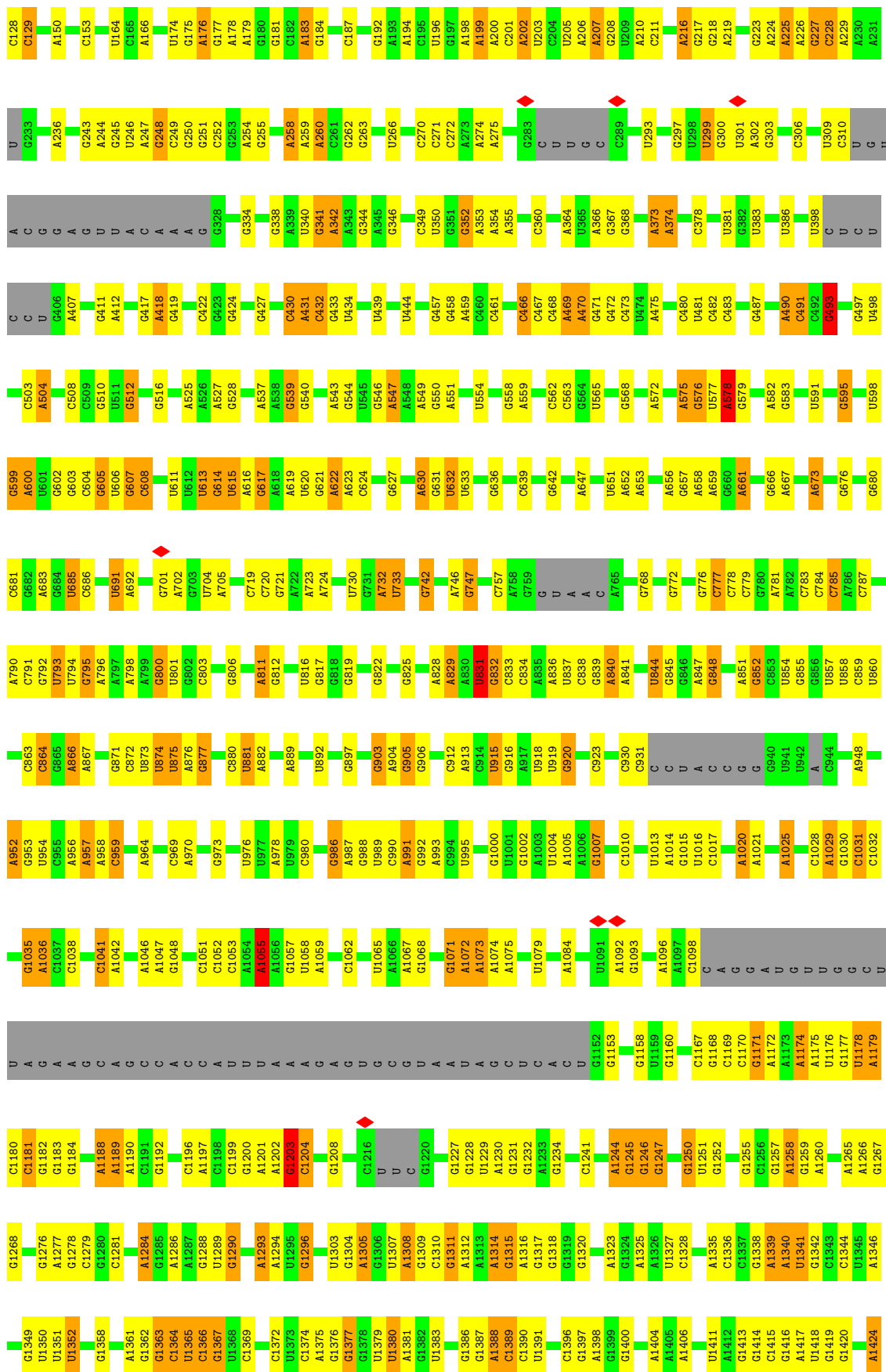


- Molecule 45: P-site tRNA-Phe

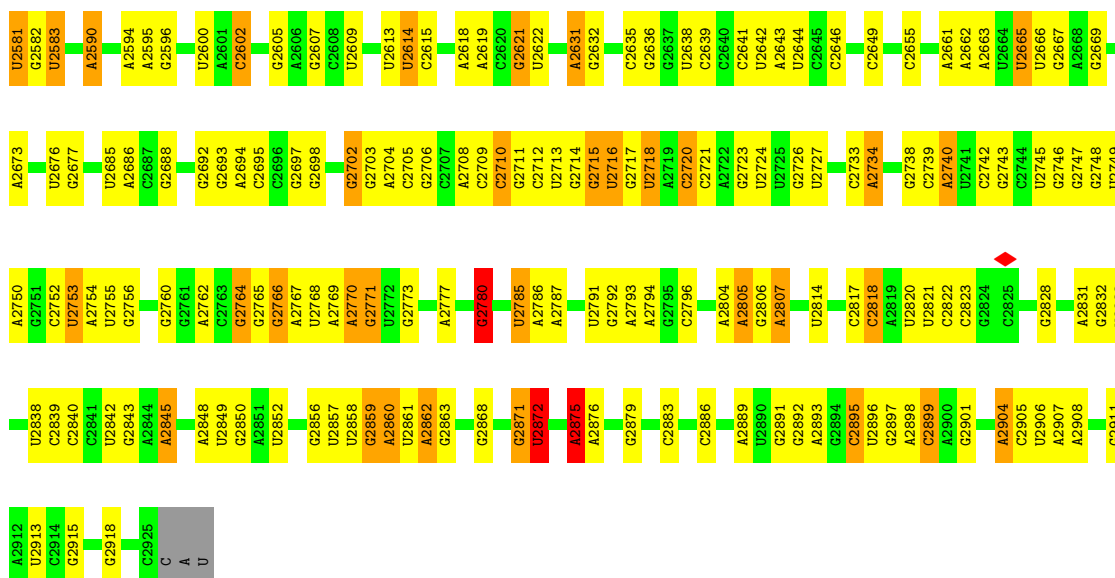


- Molecule 46: 23S rRNA

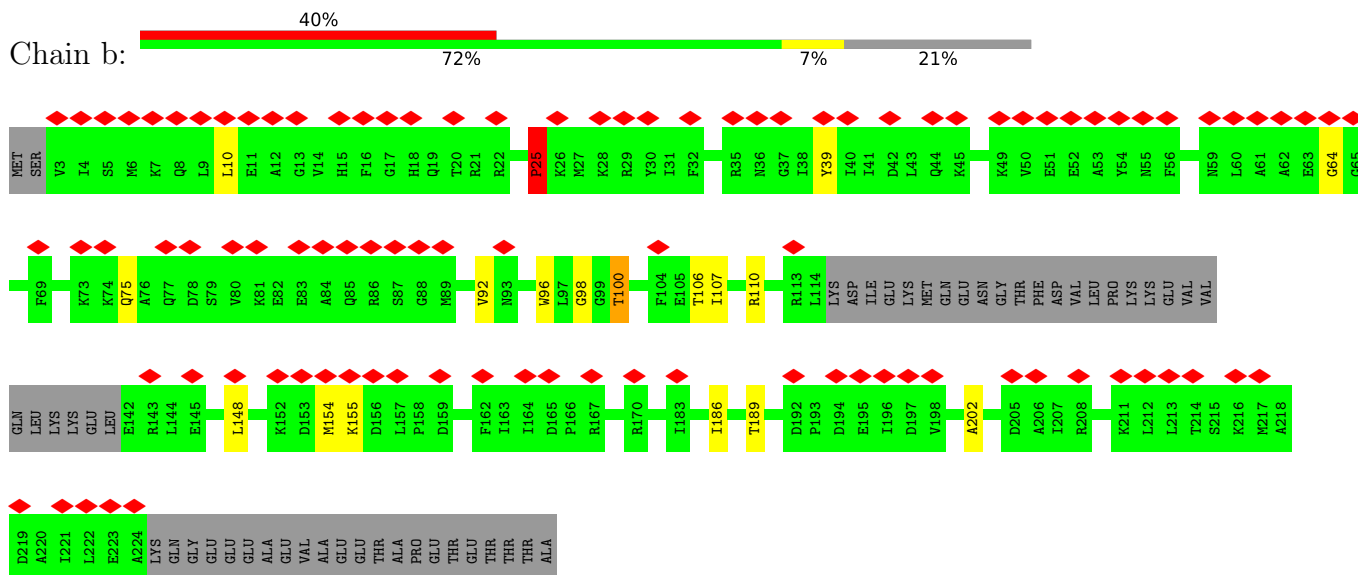




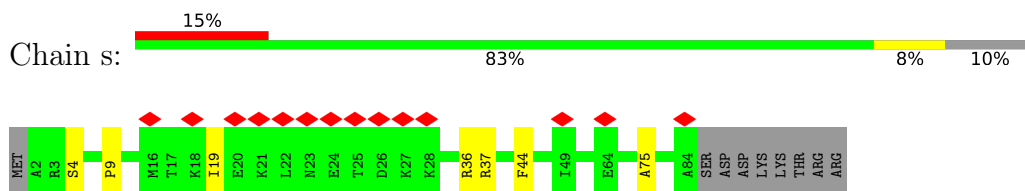
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G2510	C2350	C2351	U2274	C	A	A2052	G1974	A1876	U1807	U1713	U1529	U1530	U1436
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U2573	U2414	U2413	U2342	C	A	U2120	C2040	U1948	G1863	U1797	G1693	A	C1514
C2574	U2415	U2414	U2343	C	A	U2121	C2041	U1949	G1864	U1798	G1694	U	U1513
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C2578	U2419	U2418	U2347	C	A	U2125	C2045	U1953	G1868	U1802	G1698	U	U1513
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• Molecule 47: 30S ribosomal protein S2



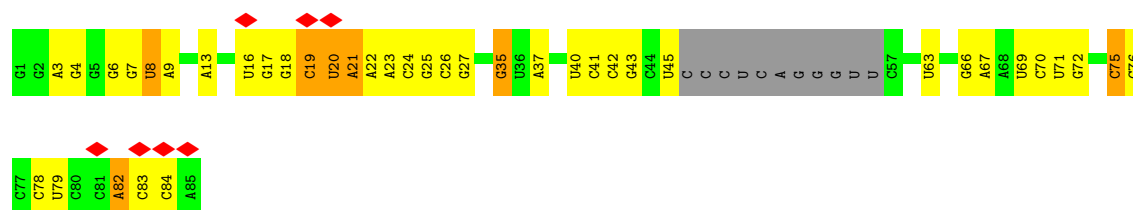
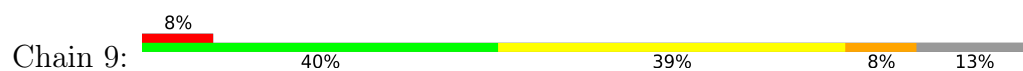
• Molecule 48: 30S ribosomal protein S19



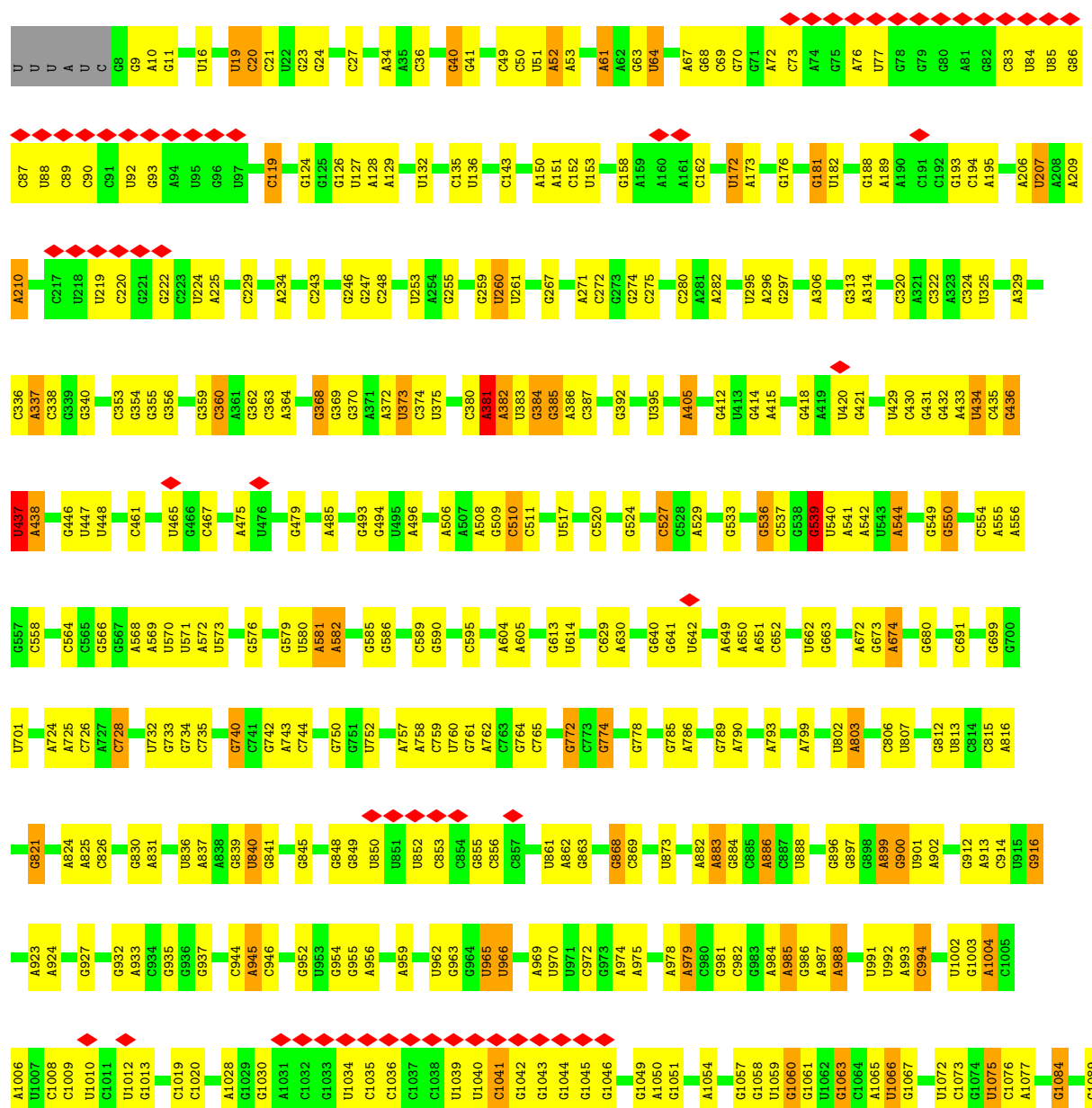
• Molecule 49: mRNA

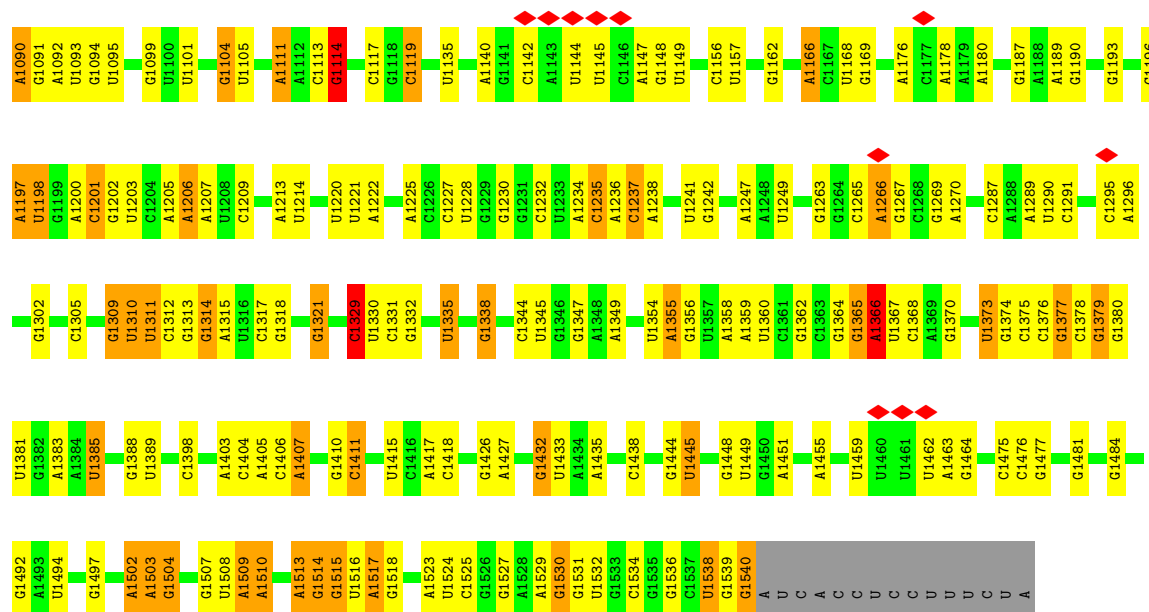


- Molecule 50: A-site tRNA-Tyr

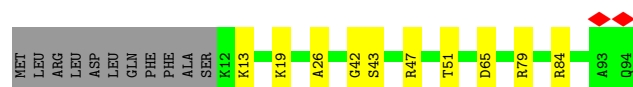
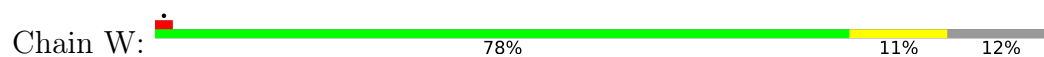


- Molecule 51: 16S rRNA

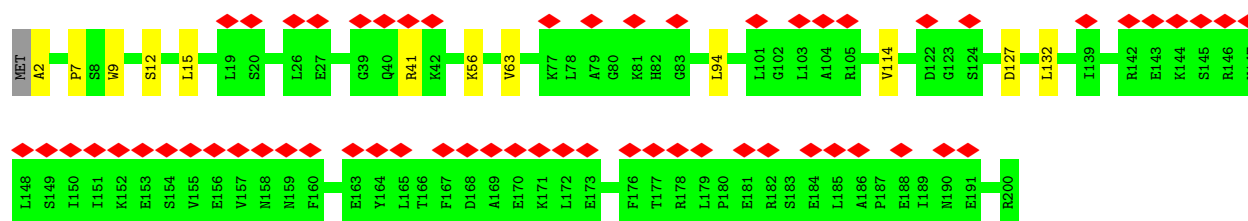




- Molecule 52: Large ribosomal subunit protein bL27



- Molecule 53: 30S ribosomal protein S4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47146	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.14	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	319.104, 319.104, 319.104	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83100003, 0.83100003, 0.83100003	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0	0.67	0/432	1.24	1/574 (0.2%)
2	1	0.50	0/408	1.03	0/541
3	2	0.72	0/371	1.17	0/483
4	3	0.68	0/519	1.16	0/680
5	4	0.57	0/300	1.17	1/393 (0.3%)
6	5	0.50	0/356	1.11	1/481 (0.2%)
7	6	0.54	0/363	1.01	0/485
8	B	0.62	0/2675	1.13	16/4170 (0.4%)
9	C	0.65	1/2130 (0.0%)	1.13	3/2858 (0.1%)
10	D	0.64	0/1597	1.21	4/2140 (0.2%)
11	E	0.56	0/1586	1.09	4/2139 (0.2%)
12	F	0.50	0/1424	1.05	0/1910
13	G	0.52	0/1360	1.02	0/1832
14	J	0.62	0/1165	1.17	1/1566 (0.1%)
15	K	0.60	0/928	1.16	1/1245 (0.1%)
16	L	0.55	0/1094	1.10	0/1457
17	M	0.56	0/1099	1.09	0/1468
18	N	0.61	0/961	1.22	3/1284 (0.2%)
19	O	0.53	0/922	1.01	0/1236
20	P	0.57	0/946	1.09	1/1264 (0.1%)
21	Q	0.68	0/962	1.17	0/1277
22	R	0.54	0/800	0.98	1/1073 (0.1%)
23	S	0.64	0/859	1.19	3/1156 (0.3%)
24	T	0.52	0/739	1.12	2/985 (0.2%)
25	U	0.54	0/780	1.01	1/1043 (0.1%)
26	X	0.57	0/471	1.17	1/626 (0.2%)
27	Y	0.46	0/541	1.05	0/718
28	Z	0.50	0/458	1.04	1/613 (0.2%)
29	c	0.51	0/1630	1.04	0/2193
30	e	0.53	0/1231	1.06	1/1655 (0.1%)
31	f	0.52	0/776	1.08	0/1043
32	g	0.51	0/1215	1.10	0/1629

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.53	0/1042	1.03	0/1397
34	i	0.53	0/1011	1.06	1/1356 (0.1%)
35	j	0.55	0/791	1.06	1/1066 (0.1%)
36	k	0.56	0/861	0.97	0/1164
37	l	0.52	0/1052	1.00	0/1413
38	m	0.53	0/949	1.09	0/1268
39	n	0.53	0/508	1.05	1/672 (0.1%)
40	o	0.48	0/738	1.11	0/985
41	p	0.49	0/704	1.09	0/945
42	q	0.49	0/701	0.96	0/936
43	r	0.49	0/530	1.11	0/710
44	t	0.50	0/661	1.25	0/882
45	v	0.66	0/1812	1.16	12/2823 (0.4%)
46	A	0.63	0/65501	1.36	937/102165 (0.9%)
47	b	0.50	0/1586	1.13	1/2130 (0.0%)
48	s	0.52	0/685	1.05	0/920
49	7	0.70	0/210	1.31	3/324 (0.9%)
50	9	0.66	0/1766	1.08	13/2749 (0.5%)
51	a	0.62	0/36826	1.16	261/57450 (0.5%)
52	W	0.56	0/647	1.10	1/858 (0.1%)
53	d	0.51	0/1635	1.09	1/2196 (0.0%)
All	All	0.61	1/151314 (0.0%)	1.24	1278/226626 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	3
3	2	0	2
9	C	0	7
10	D	0	1
13	G	0	1
14	J	0	3
16	L	0	3
17	M	0	1
18	N	0	1
19	O	0	4
20	P	0	3
21	Q	0	2
23	S	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	U	0	2
26	X	0	1
29	c	0	2
31	f	0	1
33	h	0	1
34	i	0	2
35	j	0	2
36	k	0	1
38	m	0	1
39	n	0	3
46	A	0	3
52	W	0	2
All	All	0	53

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	53	HIS	CG-CD2	-6.17	1.29	1.35

All (1278) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	732	A	O3'-P-O5'	-18.68	75.98	104.00
46	A	1375	A	O3'-P-O5'	-15.29	81.06	104.00
46	A	2904	A	C2'-C3'-O3'	15.28	132.42	109.50
46	A	621	G	O3'-P-O5'	-13.96	83.05	104.00
46	A	373	A	O3'-P-O5'	-13.93	83.11	104.00
51	a	372	A	O3'-P-O5'	-13.69	83.46	104.00
51	a	963	G	O3'-P-O5'	-13.48	83.78	104.00
46	A	2025	C	O3'-P-O5'	-13.08	84.37	104.00
46	A	2805	A	C2'-C3'-O3'	13.08	129.12	109.50
51	a	1207	A	O3'-P-O5'	-12.97	84.55	104.00
46	A	2754	A	O3'-P-O5'	-12.94	84.60	104.00
46	A	1863	U	O3'-P-O5'	-12.86	84.72	104.00
46	A	2415	U	O3'-P-O5'	-12.22	85.67	104.00
46	A	1004	U	O3'-P-O5'	-12.17	85.74	104.00
51	a	1502	A	O3'-P-O5'	-12.02	85.97	104.00
46	A	747	G	O3'-P-O5'	-11.95	86.07	104.00
46	A	1998	A	O3'-P-O5'	-11.85	86.23	104.00
46	A	1657	C	O3'-P-O5'	-11.79	86.32	104.00
46	A	1770	C	O3'-P-O5'	-11.79	86.32	104.00
46	A	1893	U	O3'-P-O5'	-11.79	86.32	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	857	U	O3'-P-O5'	-11.70	86.45	104.00
51	a	1063	G	O3'-P-O5'	-11.70	86.45	104.00
46	A	872	C	O3'-P-O5'	-11.57	86.64	104.00
51	a	555	A	O3'-P-O5'	-11.36	86.96	104.00
51	a	1514	G	O3'-P-O5'	-11.35	86.98	104.00
46	A	2748	G	O3'-P-O5'	-11.27	87.09	104.00
46	A	207	A	O3'-P-O5'	-11.27	87.10	104.00
46	A	2662	A	O3'-P-O5'	-11.06	87.40	104.00
46	A	129	C	O3'-P-O5'	-11.01	87.49	104.00
46	A	1188	A	O3'-P-O5'	-10.99	87.51	104.00
46	A	2665	U	O3'-P-O5'	-10.94	87.59	104.00
51	a	581	A	O3'-P-O5'	-10.87	87.69	104.00
46	A	2710	C	O3'-P-O5'	-10.74	87.90	104.00
51	a	437	U	C2'-C3'-O3'	10.67	125.51	109.50
51	a	734	G	O3'-P-O5'	-10.54	88.19	104.00
46	A	1363	G	O3'-P-O5'	-10.44	88.35	104.00
46	A	1819	C	O3'-P-O5'	-10.43	88.36	104.00
46	A	2382	G	O3'-P-O5'	-10.41	88.39	104.00
46	A	2057	U	O3'-P-O5'	-10.33	88.51	104.00
46	A	1339	A	C4'-C3'-O3'	10.31	124.86	109.40
46	A	2613	U	O3'-P-O5'	-10.30	88.55	104.00
46	A	1286	A	O3'-P-O5'	-10.30	88.55	104.00
51	a	510	C	O3'-P-O5'	-10.30	88.55	104.00
46	A	201	C	O3'-P-O5'	-10.29	88.56	104.00
46	A	354	A	O3'-P-O5'	-10.25	88.62	104.00
46	A	1398	A	O3'-P-O5'	-10.15	88.77	104.00
46	A	1713	A	O3'-P-O5'	-10.07	88.90	104.00
46	A	2872	U	C4'-C3'-O3'	-9.99	98.02	113.00
46	A	2424	C	O3'-P-O5'	-9.98	89.03	104.00
51	a	884	G	O3'-P-O5'	-9.94	89.09	104.00
51	a	261	U	O3'-P-O5'	-9.90	89.15	104.00
46	A	2713	U	O3'-P-O5'	-9.82	89.27	104.00
46	A	2457	G	O3'-P-O5'	-9.75	89.38	104.00
46	A	2644	U	O3'-P-O5'	-9.74	89.38	104.00
46	A	2764	G	O3'-P-O5'	-9.73	89.41	104.00
46	A	1374	C	O3'-P-O5'	-9.71	89.44	104.00
46	A	2084	C	O3'-P-O5'	-9.70	89.45	104.00
51	a	923	A	O3'-P-O5'	-9.68	89.48	104.00
51	a	1091	G	O3'-P-O5'	-9.66	89.51	104.00
46	A	1177	G	O3'-P-O5'	-9.60	89.61	104.00
46	A	851	A	O3'-P-O5'	-9.59	89.61	104.00
46	A	2705	C	O3'-P-O5'	-9.58	89.63	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	559	A	O3'-P-O5'	-9.52	89.72	104.00
46	A	1289	U	O3'-P-O5'	-9.50	89.75	104.00
46	A	1709	A	O3'-P-O5'	-9.45	89.83	104.00
46	A	2052	A	O3'-P-O5'	-9.42	89.86	104.00
46	A	16	G	O3'-P-O5'	-9.41	89.89	104.00
46	A	1655	A	O3'-P-O5'	-9.40	89.90	104.00
51	a	899	A	O3'-P-O5'	-9.38	89.93	104.00
46	A	2580	C	O3'-P-O5'	-9.37	89.94	104.00
46	A	1816	A	C2'-C3'-O3'	-9.33	99.71	113.70
46	A	225	A	O3'-P-O5'	-9.31	90.04	104.00
46	A	1807	U	O3'-P-O5'	-9.30	90.05	104.00
46	A	2493	C	O3'-P-O5'	-9.30	90.05	104.00
46	A	1351	U	O3'-P-O5'	-9.29	90.07	104.00
46	A	1340	A	O3'-P-O5'	-9.28	90.08	104.00
46	A	2631	A	O3'-P-O5'	9.21	117.82	104.00
51	a	965	U	C2'-C3'-O3'	9.18	127.47	113.70
46	A	623	A	O3'-P-O5'	-9.17	90.24	104.00
46	A	205	U	O3'-P-O5'	-9.16	90.25	104.00
46	A	746	A	O3'-P-O5'	-9.15	90.27	104.00
46	A	223	G	O3'-P-O5'	-9.15	90.28	104.00
51	a	785	G	O3'-P-O5'	-9.09	90.37	104.00
46	A	2416	U	O3'-P-O5'	-9.08	90.38	104.00
46	A	497	G	O3'-P-O5'	-9.07	90.39	104.00
51	a	582	A	O3'-P-O5'	-9.06	90.41	104.00
46	A	260	A	O3'-P-O5'	-9.04	90.44	104.00
46	A	2308	G	O3'-P-O5'	-9.03	90.45	104.00
51	a	992	U	O3'-P-O5'	-9.02	90.47	104.00
46	A	2394	G	O3'-P-O5'	-9.00	90.50	104.00
46	A	1690	G	O3'-P-O5'	-8.96	90.55	104.00
46	A	2746	G	C1'-C2'-O2'	8.95	121.82	108.40
46	A	651	U	O3'-P-O5'	8.94	117.41	104.00
46	A	490	A	O3'-P-O5'	-8.93	90.61	104.00
46	A	2639	C	O3'-P-O5'	-8.92	90.62	104.00
46	A	1335	A	O3'-P-O5'	-8.92	90.62	104.00
46	A	61	A	O3'-P-O5'	-8.89	90.66	104.00
46	A	1257	G	O3'-P-O5'	-8.89	90.67	104.00
46	A	2753	U	C3'-C2'-O2'	8.88	124.01	110.70
46	A	2831	A	O3'-P-O5'	-8.86	90.71	104.00
51	a	1057	G	O3'-P-O5'	-8.86	90.71	104.00
46	A	525	A	O3'-P-O5'	-8.86	90.72	104.00
46	A	1759	U	C4'-C3'-O3'	8.83	122.64	109.40
46	A	2643	A	O3'-P-O5'	-8.83	90.76	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	2543	U	O3'-P-O5'	-8.82	90.76	104.00
46	A	383	U	O3'-P-O5'	-8.81	90.78	104.00
46	A	2078	A	O3'-P-O5'	-8.79	90.82	104.00
46	A	1204	C	O3'-P-O5'	-8.76	90.86	104.00
46	A	2020	U	C2'-C3'-O3'	-8.74	100.59	113.70
46	A	2760	G	O3'-P-O5'	-8.74	90.90	104.00
46	A	2755	U	O3'-P-O5'	-8.72	90.91	104.00
51	a	206	A	O3'-P-O5'	-8.71	90.93	104.00
46	A	2704	A	O3'-P-O5'	-8.71	90.94	104.00
51	a	1356	G	O3'-P-O5'	-8.70	90.94	104.00
45	v	47	U	C2'-C3'-O3'	8.70	122.55	109.50
46	A	2519	G	O3'-P-O5'	-8.67	90.99	104.00
46	A	2904	A	C4'-C3'-O3'	-8.67	96.39	109.40
51	a	789	G	O3'-P-O5'	-8.66	91.01	104.00
46	A	1678	G	O3'-P-O5'	-8.65	91.03	104.00
46	A	2526	A	O3'-P-O5'	-8.65	91.03	104.00
46	A	54	G	O3'-P-O5'	-8.64	91.04	104.00
46	A	2032	A	O3'-P-O5'	-8.62	91.07	104.00
46	A	1515	C	O3'-P-O5'	-8.61	91.09	104.00
46	A	297	G	O3'-P-O5'	-8.57	91.15	104.00
46	A	1526	G	O3'-P-O5'	-8.55	91.17	104.00
46	A	1606	A	O3'-P-O5'	-8.54	91.19	104.00
46	A	2581	U	O3'-P-O5'	-8.54	91.20	104.00
46	A	1178	U	O3'-P-O5'	-8.53	91.20	104.00
46	A	656	A	O3'-P-O5'	-8.50	91.25	104.00
46	A	2054	C	O3'-P-O5'	-8.50	91.25	104.00
46	A	1542	A	C4'-C3'-O3'	8.50	125.75	113.00
46	A	1279	C	O3'-P-O5'	-8.47	91.29	104.00
51	a	641	G	C2'-C3'-O3'	8.46	122.19	109.50
51	a	359	G	O3'-P-O5'	-8.46	91.31	104.00
46	A	2468	A	C4'-C3'-O3'	8.46	122.08	109.40
26	X	27	ARG	CB-CA-C	-8.45	95.83	110.45
46	A	2753	U	C2'-C3'-O3'	8.45	126.38	113.70
51	a	1403	A	O3'-P-O5'	-8.45	91.32	104.00
46	A	196	U	O3'-P-O5'	-8.44	91.34	104.00
46	A	539	G	O3'-P-O5'	-8.39	91.42	104.00
51	a	988	A	O3'-P-O5'	-8.38	91.43	104.00
51	a	405	A	O3'-P-O5'	-8.38	91.43	104.00
46	A	1771	C	O3'-P-O5'	-8.37	91.44	104.00
46	A	2109	G	O3'-P-O5'	-8.36	91.46	104.00
46	A	2570	A	O3'-P-O5'	-8.36	91.46	104.00
46	A	432	C	O3'-P-O5'	-8.36	91.46	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	1338	G	C2'-C3'-O3'	-8.36	101.16	113.70
46	A	1787	G	O3'-P-O5'	-8.36	91.47	104.00
46	A	575	A	O3'-P-O5'	-8.35	91.47	104.00
46	A	2594	A	O3'-P-O5'	-8.32	91.51	104.00
46	A	1662	C	C1'-C2'-O2'	-8.31	99.33	111.80
46	A	2340	A	O3'-P-O5'	-8.31	91.53	104.00
46	A	202	A	O3'-P-O5'	-8.30	91.54	104.00
46	A	2458	G	O3'-P-O5'	-8.30	91.54	104.00
46	A	2530	C	O3'-P-O5'	-8.30	91.55	104.00
46	A	572	A	C4'-C3'-O3'	-8.30	100.55	113.00
46	A	444	U	O3'-P-O5'	-8.29	91.56	104.00
46	A	836	A	O3'-P-O5'	-8.29	91.56	104.00
46	A	1682	C	O3'-P-O5'	-8.29	91.57	104.00
46	A	2015	G	O3'-P-O5'	-8.27	91.60	104.00
46	A	1276	G	O3'-P-O5'	-8.25	91.62	104.00
46	A	840	A	O3'-P-O5'	-8.24	91.64	104.00
46	A	249	C	O3'-P-O5'	-8.24	91.64	104.00
46	A	1841	G	O3'-P-O5'	-8.22	91.67	104.00
46	A	2518	G	O3'-P-O5'	-8.21	91.68	104.00
46	A	2753	U	C4'-C3'-O3'	-8.21	100.68	113.00
46	A	2605	G	O3'-P-O5'	-8.21	91.69	104.00
46	A	2306	G	C4'-C3'-O3'	-8.21	100.69	113.00
46	A	831	U	O3'-P-O5'	-8.18	91.73	104.00
51	a	1090	A	O3'-P-O5'	-8.18	91.73	104.00
46	A	2665	U	C4'-C3'-O3'	-8.16	100.76	113.00
46	A	2418	G	C4'-C3'-O3'	-8.16	100.77	113.00
46	A	2522	U	O3'-P-O5'	-8.14	91.78	104.00
46	A	1340	A	C2'-C3'-O3'	8.13	121.70	109.50
46	A	1200	G	C4'-C3'-O3'	-8.13	100.81	113.00
50	9	71	U	O3'-P-O5'	-8.13	91.81	104.00
46	A	1750	G	O3'-P-O5'	-8.12	91.83	104.00
46	A	1316	A	O3'-P-O5'	-8.11	91.83	104.00
51	a	1427	A	O3'-P-O5'	-8.08	91.88	104.00
46	A	919	U	O3'-P-O5'	-8.08	91.88	104.00
46	A	1939	G	O3'-P-O5'	-8.08	91.88	104.00
46	A	723	A	O3'-P-O5'	-8.07	91.89	104.00
51	a	135	C	O3'-P-O5'	-8.06	91.90	104.00
46	A	2669	G	O3'-P-O5'	-8.06	91.91	104.00
46	A	1978	G	O3'-P-O5'	-8.06	91.91	104.00
46	A	2275	G	O3'-P-O5'	-8.05	91.93	104.00
8	B	48	G	C2'-C3'-O3'	8.04	125.77	113.70
46	A	2087	A	C2'-C3'-O3'	-8.04	101.64	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	1911	C	O3'-P-O5'	-8.03	91.96	104.00
46	A	2745	U	O3'-P-O5'	-8.02	91.98	104.00
46	A	2875	A	C1'-C2'-O2'	8.02	120.42	108.40
46	A	1417	A	C2'-C3'-O3'	8.01	121.51	109.50
51	a	1407	A	O3'-P-O5'	-7.99	92.01	104.00
46	A	2037	C	O3'-P-O5'	-7.97	92.04	104.00
46	A	2548	U	O3'-P-O5'	-7.97	92.05	104.00
46	A	1010	C	O3'-P-O5'	-7.94	92.09	104.00
46	A	1036	A	O3'-P-O5'	-7.94	92.08	104.00
46	A	1516	A	O3'-P-O5'	-7.94	92.10	104.00
46	A	1997	G	O3'-P-O5'	-7.93	92.11	104.00
46	A	2402	A	O3'-P-O5'	-7.93	92.11	104.00
51	a	127	U	O3'-P-O5'	-7.93	92.11	104.00
46	A	274	A	O3'-P-O5'	-7.91	92.14	104.00
46	A	1480	A	O3'-P-O5'	-7.90	92.14	104.00
46	A	1181	C	C4'-C3'-O3'	-7.90	101.15	113.00
46	A	1406	A	O3'-P-O5'	-7.87	92.20	104.00
51	a	1510	A	O3'-P-O5'	-7.87	92.20	104.00
51	a	436	G	C4'-C3'-O3'	7.87	121.20	109.40
46	A	546	G	O3'-P-O5'	-7.86	92.21	104.00
46	A	1501	U	C2'-C3'-O3'	7.86	121.29	109.50
46	A	828	A	C4'-C3'-O3'	-7.86	101.22	113.00
51	a	1502	A	C4'-C3'-O3'	7.86	121.18	109.40
46	A	1369	C	O3'-P-O5'	-7.83	92.25	104.00
46	A	2550	C	O3'-P-O5'	-7.83	92.26	104.00
46	A	2290	C	O3'-P-O5'	-7.82	92.26	104.00
46	A	2551	U	O3'-P-O5'	-7.82	92.26	104.00
46	A	2527	C	O3'-P-O5'	-7.82	92.27	104.00
46	A	1776	A	O3'-P-O5'	-7.80	92.30	104.00
51	a	735	C	O3'-P-O5'	-7.77	92.35	104.00
46	A	2089	A	C2'-C3'-O3'	7.77	121.15	109.50
46	A	1318	G	O3'-P-O5'	-7.77	92.35	104.00
18	N	23	ASP	CA-CB-CG	7.76	120.36	112.60
46	A	991	A	C2'-C3'-O3'	7.75	121.13	109.50
46	A	1310	C	O3'-P-O5'	-7.72	92.41	104.00
51	a	1198	U	O3'-P-O5'	-7.72	92.42	104.00
46	A	2414	C	O3'-P-O5'	-7.69	92.47	104.00
46	A	2569	C	C2'-C3'-O3'	7.68	125.22	113.70
46	A	1955	U	O3'-P-O5'	-7.66	92.51	104.00
51	a	793	A	O3'-P-O5'	-7.66	92.51	104.00
46	A	1281	C	O3'-P-O5'	-7.66	92.51	104.00
51	a	1365	G	O3'-P-O5'	-7.66	92.51	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	2615	C	O3'-P-O5'	-7.64	92.54	104.00
46	A	2542	A	O3'-P-O5'	-7.63	92.55	104.00
46	A	1367	G	O3'-P-O5'	-7.61	92.58	104.00
46	A	2310	C	C1'-C2'-O2'	-7.61	96.98	108.40
46	A	2347	G	O3'-P-O5'	-7.60	92.59	104.00
51	a	1368	C	O3'-P-O5'	-7.60	92.60	104.00
46	A	2332	G	O3'-P-O5'	-7.60	92.60	104.00
46	A	889	A	O3'-P-O5'	-7.60	92.60	104.00
46	A	819	G	O3'-P-O5'	-7.60	92.60	104.00
23	S	83	LYS	CB-CA-C	7.58	122.26	109.75
51	a	1104	G	O3'-P-O5'	-7.58	92.64	104.00
46	A	1717	C	O3'-P-O5'	-7.57	92.64	104.00
46	A	918	U	O3'-P-O5'	-7.57	92.65	104.00
46	A	733	U	C1'-C2'-O2'	-7.55	100.47	111.80
46	A	873	U	C2'-C3'-O3'	-7.55	102.37	113.70
51	a	544	A	O3'-P-O5'	-7.55	92.67	104.00
50	9	75	C	C2'-C3'-O3'	7.55	125.03	113.70
46	A	2092	C	O3'-P-O5'	-7.55	92.67	104.00
46	A	1229	U	O3'-P-O5'	-7.54	92.69	104.00
46	A	1414	G	O3'-P-O5'	-7.53	92.71	104.00
46	A	2871	G	O3'-P-O5'	-7.52	92.71	104.00
46	A	360	C	O3'-P-O5'	-7.51	92.74	104.00
46	A	263	G	O3'-P-O5'	-7.51	92.74	104.00
46	A	1958	G	O3'-P-O5'	-7.50	92.75	104.00
49	7	408	U	O3'-P-O5'	-7.49	92.77	104.00
46	A	1432	A	O3'-P-O5'	-7.48	92.78	104.00
46	A	1031	C	O3'-P-O5'	-7.47	92.79	104.00
51	a	415	A	O3'-P-O5'	-7.47	92.80	104.00
46	A	1959	G	O3'-P-O5'	-7.47	92.80	104.00
46	A	2302	A	O3'-P-O5'	-7.46	92.81	104.00
46	A	2693	G	O3'-P-O5'	-7.46	92.81	104.00
46	A	1704	U	O3'-P-O5'	-7.45	92.82	104.00
46	A	806	G	O3'-P-O5'	-7.45	92.83	104.00
46	A	2868	G	O3'-P-O5'	-7.44	92.84	104.00
51	a	1404	C	O3'-P-O5'	-7.44	92.84	104.00
51	a	260	U	O3'-P-O5'	-7.43	92.85	104.00
46	A	493	G	O3'-P-O5'	-7.43	92.85	104.00
46	A	2461	A	O3'-P-O5'	-7.43	92.86	104.00
46	A	1930	A	O3'-P-O5'	-7.41	92.89	104.00
51	a	1117	C	O3'-P-O5'	-7.41	92.89	104.00
46	A	2590	A	O3'-P-O5'	-7.39	92.92	104.00
46	A	1252	G	O3'-P-O5'	-7.38	92.93	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	a	1058	G	O3'-P-O5'	-7.38	92.93	104.00
51	a	1230	G	C2'-C3'-O3'	-7.37	102.64	113.70
46	A	1362	G	O3'-P-O5'	-7.36	92.95	104.00
51	a	1206	A	O3'-P-O5'	-7.36	92.96	104.00
46	A	110	A	O3'-P-O5'	-7.35	92.97	104.00
46	A	2433	C	C2'-C3'-O3'	-7.34	102.69	113.70
45	v	70	G	O3'-P-O5'	-7.34	92.99	104.00
46	A	1817	C	O3'-P-O5'	-7.34	92.99	104.00
46	A	2636	G	O3'-P-O5'	-7.33	93.01	104.00
46	A	2895	C	C2'-C3'-O3'	-7.33	102.71	113.70
46	A	352	G	O3'-P-O5'	-7.29	93.06	104.00
46	A	1227	G	C1'-C2'-O2'	7.29	119.33	108.40
46	A	2468	A	P-O3'-C3'	7.29	131.13	120.20
46	A	2301	U	O3'-P-O5'	-7.28	93.08	104.00
51	a	582	A	C4'-C3'-O3'	-7.28	102.08	113.00
46	A	746	A	C4'-C3'-O3'	-7.28	102.09	113.00
46	A	2510	G	C4'-C3'-O3'	-7.27	102.09	113.00
46	A	2476	G	C4'-C3'-O3'	-7.27	98.50	109.40
46	A	1481	G	O3'-P-O5'	-7.26	93.11	104.00
46	A	1007	G	O3'-P-O5'	-7.24	93.14	104.00
46	A	1197	A	O3'-P-O5'	-7.22	93.16	104.00
46	A	2582	G	C1'-C2'-O2'	7.22	119.22	108.40
51	a	1370	G	O3'-P-O5'	-7.21	93.18	104.00
46	A	2123	A	O3'-P-O5'	-7.20	93.20	104.00
46	A	801	U	O3'-P-O5'	-7.19	93.21	104.00
46	A	613	U	C4'-C3'-O3'	-7.19	102.21	113.00
46	A	867	A	C4'-C3'-O3'	-7.18	102.22	113.00
46	A	2317	A	O3'-P-O5'	-7.17	93.25	104.00
46	A	603	G	O3'-P-O5'	-7.17	93.25	104.00
51	a	1410	G	O3'-P-O5'	-7.16	93.26	104.00
46	A	1949	C	O3'-P-O5'	-7.15	93.28	104.00
46	A	607	G	O3'-P-O5'	-7.15	93.28	104.00
46	A	2476	G	O3'-P-O5'	-7.14	93.28	104.00
46	A	2655	C	O3'-P-O5'	-7.14	93.30	104.00
46	A	915	U	O3'-P-O5'	-7.13	93.31	104.00
46	A	1892	C	O3'-P-O5'	-7.12	93.32	104.00
51	a	436	G	O3'-P-O5'	-7.12	93.32	104.00
46	A	2404	G	O3'-P-O5'	-7.11	93.33	104.00
51	a	322	C	O3'-P-O5'	-7.10	93.34	104.00
46	A	2711	G	O3'-P-O5'	-7.10	93.35	104.00
46	A	1389	C	O3'-P-O5'	-7.09	93.37	104.00
46	A	2456	C	C2'-C3'-O3'	-7.08	103.07	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	798	A	O3'-P-O5'	-7.08	93.39	104.00
46	A	776	G	C4'-C3'-O3'	-7.07	102.39	113.00
46	A	2856	G	O3'-P-O5'	-7.07	93.39	104.00
46	A	1267	G	O3'-P-O5'	-7.07	93.39	104.00
46	A	1375	A	C4'-C3'-O3'	-7.05	102.42	113.00
51	a	1209	C	C1'-C2'-O2'	-7.05	101.22	111.80
46	A	2915	G	C1'-C2'-O2'	7.05	118.97	108.40
46	A	1184	G	C2'-C3'-O3'	-7.05	103.13	113.70
51	a	446	G	O3'-P-O5'	-7.04	93.44	104.00
46	A	1002	G	C4'-C3'-O3'	-7.04	102.44	113.00
46	A	2641	C	C4'-C3'-O3'	-7.02	102.47	113.00
46	A	1829	C	C1'-C2'-O2'	-7.01	101.28	111.80
46	A	2553	G	O3'-P-O5'	-7.01	93.48	104.00
46	A	857	U	C4'-C3'-O3'	-7.01	102.48	113.00
46	A	1190	A	O3'-P-O5'	-7.01	93.49	104.00
46	A	953	G	O3'-P-O5'	-7.00	93.50	104.00
46	A	1631	A	C4'-C3'-O3'	7.00	119.91	109.40
51	a	517	U	O3'-P-O5'	-7.00	93.50	104.00
46	A	2506	C	O3'-P-O5'	-7.00	93.51	104.00
46	A	547	A	O3'-P-O5'	-6.98	93.53	104.00
46	A	2392	U	O3'-P-O5'	-6.98	93.53	104.00
46	A	2264	G	O3'-P-O5'	-6.98	93.54	104.00
46	A	2530	C	C1'-C2'-O2'	-6.98	97.94	108.40
46	A	431	A	C4'-C3'-O3'	-6.97	102.55	113.00
51	a	1524	U	O3'-P-O5'	-6.96	93.55	104.00
46	A	2362	A	O3'-P-O5'	-6.96	93.56	104.00
46	A	540	G	O3'-P-O5'	-6.95	93.58	104.00
46	A	2569	C	C4'-C3'-C2'	-6.94	95.66	102.60
46	A	1884	G	O3'-P-O5'	-6.94	93.59	104.00
46	A	2804	A	O3'-P-O5'	-6.93	93.60	104.00
46	A	1777	G	O3'-P-O5'	-6.93	93.61	104.00
46	A	627	G	O3'-P-O5'	-6.92	93.61	104.00
46	A	1387	G	O3'-P-O5'	-6.92	93.62	104.00
46	A	2796	C	O3'-P-O5'	-6.89	93.66	104.00
46	A	2760	G	C4'-C3'-O3'	-6.89	102.66	113.00
46	A	174	U	O3'-P-O5'	-6.89	93.66	104.00
46	A	2756	G	C4'-C3'-C2'	-6.89	95.71	102.60
51	a	821	G	O3'-P-O5'	-6.88	93.68	104.00
46	A	2036	U	O3'-P-O5'	-6.88	93.68	104.00
46	A	178	A	O3'-P-O5'	-6.87	93.70	104.00
46	A	880	C	C4'-C3'-O3'	-6.86	102.70	113.00
51	a	802	U	O3'-P-O5'	-6.86	93.70	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	a	1330	U	C2'-C3'-O3'	-6.86	103.41	113.70
51	a	566	G	O3'-P-O5'	-6.85	93.72	104.00
46	A	1945	A	C4'-C3'-O3'	6.85	119.68	109.40
46	A	208	G	O3'-P-O5'	-6.85	93.73	104.00
46	A	176	A	O3'-P-O5'	-6.85	93.73	104.00
23	S	78	GLU	CB-CG-CD	6.83	124.22	112.60
46	A	1842	C	O3'-P-O5'	-6.83	93.75	104.00
46	A	2271	G	O3'-P-O5'	-6.83	93.75	104.00
46	A	2267	G	O3'-P-O5'	-6.83	93.76	104.00
46	A	604	C	C2'-C3'-O3'	6.82	123.93	113.70
46	A	800	G	O3'-P-O5'	-6.82	93.77	104.00
46	A	1255	G	O3'-P-O5'	-6.82	93.77	104.00
46	A	1369	C	C3'-C2'-O2'	6.82	120.93	110.70
46	A	2720	C	C1'-C2'-O2'	6.82	118.63	108.40
46	A	303	G	O3'-P-O5'	-6.81	93.78	104.00
46	A	1498	U	O3'-P-O5'	-6.81	93.78	104.00
51	a	1415	U	O3'-P-O5'	-6.81	93.78	104.00
46	A	211	C	O3'-P-O5'	-6.81	93.78	104.00
51	a	1092	A	O3'-P-O5'	-6.81	93.79	104.00
51	a	229	C	O3'-P-O5'	-6.80	93.79	104.00
51	a	1411	C	C3'-C2'-O2'	6.80	120.90	110.70
8	B	70	G	O3'-P-O5'	-6.79	93.81	104.00
46	A	2753	U	O3'-P-O5'	-6.79	93.82	104.00
46	A	2042	A	C1'-C2'-O2'	6.79	118.58	108.40
51	a	395	U	O3'-P-O5'	-6.78	93.83	104.00
46	A	2746	G	O3'-P-O5'	-6.78	93.84	104.00
46	A	466	C	C3'-C2'-O2'	6.77	120.85	110.70
46	A	504	A	O3'-P-O5'	-6.77	93.85	104.00
46	A	2473	G	O3'-P-O5'	-6.76	93.86	104.00
46	A	613	U	O3'-P-O5'	-6.75	93.88	104.00
46	A	2078	A	C4'-C3'-O3'	-6.75	102.88	113.00
51	a	119	C	O3'-P-O5'	-6.74	93.89	104.00
46	A	2121	U	C2'-C3'-O3'	6.74	119.61	109.50
46	A	1613	C	O3'-P-O5'	-6.74	93.90	104.00
46	A	2035	C	C4'-C3'-O3'	-6.74	102.90	113.00
46	A	112	U	O3'-P-O5'	-6.73	93.90	104.00
46	A	2458	G	C4'-C3'-O3'	-6.73	102.91	113.00
51	a	799	A	O3'-P-O5'	-6.73	93.91	104.00
46	A	527	A	O3'-P-O5'	-6.72	93.92	104.00
51	a	1517	A	O3'-P-O5'	-6.72	93.93	104.00
51	a	1538	U	C2'-C3'-O3'	6.71	119.57	109.50
49	7	405	G	O3'-P-O5'	-6.71	93.93	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	217	G	O3'-P-O5'	-6.71	93.94	104.00
46	A	1035	G	O3'-P-O5'	-6.70	93.94	104.00
46	A	192	G	C4'-C3'-O3'	-6.70	102.95	113.00
46	A	993	A	C4'-C3'-O3'	-6.70	102.95	113.00
51	a	1364	G	O3'-P-O5'	-6.70	93.95	104.00
46	A	1294	A	C4'-C3'-O3'	-6.70	102.95	113.00
51	a	914	C	O3'-P-O5'	-6.70	93.96	104.00
51	a	1477	G	O3'-P-O5'	-6.68	93.98	104.00
45	v	33	U	O3'-P-O5'	-6.68	93.98	104.00
51	a	825	A	C4'-C3'-O3'	-6.68	102.99	113.00
46	A	2065	C	C2'-C3'-O3'	-6.67	103.69	113.70
46	A	970	A	O3'-P-O5'	-6.66	94.01	104.00
46	A	1171	G	C4'-C3'-O3'	-6.66	103.01	113.00
46	A	200	A	C3'-C2'-O2'	6.65	120.67	110.70
8	B	80	G	O3'-P-O5'	-6.64	94.03	104.00
46	A	2508	U	O3'-P-O5'	-6.64	94.03	104.00
51	a	381	A	O3'-P-O5'	-6.64	94.05	104.00
46	A	470	A	O3'-P-O5'	-6.63	94.05	104.00
46	A	187	C	O3'-P-O5'	-6.63	94.05	104.00
46	A	1189	A	C3'-C2'-O2'	-6.63	104.65	114.60
46	A	1567	U	O3'-P-O5'	-6.63	94.05	104.00
46	A	2677	G	O3'-P-O5'	-6.63	94.06	104.00
46	A	1352	U	O3'-P-O5'	-6.62	94.07	104.00
46	A	1296	G	C2'-C3'-O3'	-6.62	103.77	113.70
46	A	1342	G	O3'-P-O5'	-6.61	94.08	104.00
51	a	320	C	O3'-P-O5'	-6.61	94.08	104.00
46	A	1482	G	O3'-P-O5'	-6.61	94.09	104.00
46	A	1443	C	O3'-P-O5'	-6.60	94.09	104.00
46	A	2805	A	O3'-P-O5'	6.60	113.90	104.00
46	A	2279	G	C2'-C3'-O3'	6.60	119.40	109.50
46	A	2661	A	O3'-P-O5'	-6.60	94.10	104.00
46	A	2832	G	O3'-P-O5'	-6.60	94.10	104.00
51	a	1484	G	O3'-P-O5'	-6.60	94.11	104.00
46	A	563	C	C4'-C3'-O3'	-6.59	103.11	113.00
46	A	2635	C	O3'-P-O5'	-6.59	94.12	104.00
46	A	1176	U	C1'-C2'-O2'	-6.59	101.92	111.80
51	a	1503	A	C2'-C3'-O3'	6.58	119.38	109.50
51	a	1091	G	C2'-C3'-O3'	6.58	123.57	113.70
46	A	2495	C	C4'-C3'-O3'	-6.58	103.13	113.00
46	A	817	G	O3'-P-O5'	-6.58	94.13	104.00
46	A	2713	U	C4'-C3'-O3'	-6.58	103.13	113.00
46	A	2721	C	C1'-C2'-O2'	6.58	118.26	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	a	509	G	O3'-P-O5'	-6.57	94.14	104.00
46	A	721	G	C1'-C2'-O2'	6.56	118.24	108.40
51	a	1338	G	O3'-P-O5'	-6.56	94.16	104.00
46	A	2283	C	O3'-P-O5'	-6.55	94.17	104.00
46	A	681	C	O3'-P-O5'	-6.55	94.17	104.00
46	A	1990	C	O3'-P-O5'	-6.55	94.17	104.00
46	A	875	U	O3'-P-O5'	-6.55	94.18	104.00
46	A	2253	G	O3'-P-O5'	-6.55	94.18	104.00
46	A	2310	C	C3'-C2'-O2'	6.54	120.52	110.70
9	C	218	PRO	CB-CA-C	-6.54	103.02	111.39
46	A	349	C	O3'-P-O5'	-6.54	94.19	104.00
46	A	2908	A	C4'-C3'-C2'	-6.54	96.06	102.60
11	E	81	PRO	CB-CA-C	-6.53	101.27	112.64
46	A	772	G	O3'-P-O5'	-6.53	94.20	104.00
46	A	1241	C	O3'-P-O5'	-6.53	94.21	104.00
51	a	994	C	O3'-P-O5'	-6.53	94.21	104.00
46	A	2524	G	C4'-C3'-O3'	-6.52	103.22	113.00
46	A	2415	U	C4'-C3'-O3'	-6.52	103.22	113.00
46	A	600	A	C4'-C3'-O3'	-6.52	103.22	113.00
46	A	386	U	O3'-P-O5'	-6.51	94.23	104.00
46	A	475	A	O3'-P-O5'	-6.50	94.24	104.00
46	A	2412	G	O3'-P-O5'	-6.50	94.25	104.00
46	A	1415	C	O3'-P-O5'	-6.50	94.26	104.00
46	A	1417	A	O3'-P-O5'	-6.50	94.26	104.00
51	a	1508	U	O3'-P-O5'	-6.50	94.26	104.00
51	a	1365	G	C4'-C3'-O3'	-6.49	103.26	113.00
46	A	1659	A	O3'-P-O5'	-6.49	94.27	104.00
46	A	1600	G	O3'-P-O5'	-6.48	94.28	104.00
51	a	701	U	O3'-P-O5'	-6.48	94.28	104.00
51	a	418	G	O3'-P-O5'	-6.47	94.29	104.00
46	A	2478	U	O3'-P-O5'	-6.46	94.31	104.00
46	A	860	U	C2'-C3'-O3'	-6.45	104.03	113.70
51	a	296	A	O3'-P-O5'	-6.45	94.33	104.00
46	A	2016	G	O3'-P-O5'	-6.44	94.33	104.00
51	a	433	A	O3'-P-O5'	-6.44	94.33	104.00
46	A	1829	C	O3'-P-O5'	6.44	113.66	104.00
51	a	954	G	O3'-P-O5'	-6.43	94.35	104.00
46	A	2901	G	O3'-P-O5'	-6.43	94.36	104.00
46	A	2034	A	O3'-P-O5'	6.42	113.64	104.00
50	9	35	G	O3'-P-O5'	-6.42	94.37	104.00
51	a	882	A	O3'-P-O5'	-6.42	94.38	104.00
51	a	1089	G	C4'-C3'-O3'	-6.41	103.38	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	920	G	O3'-P-O5'	-6.41	94.38	104.00
46	A	1619	A	O3'-P-O5'	-6.41	94.38	104.00
51	a	806	C	O3'-P-O5'	-6.41	94.38	104.00
46	A	685	U	C4'-C3'-O3'	-6.40	103.40	113.00
46	A	2715	G	C4'-C3'-C2'	-6.40	96.20	102.60
46	A	1025	A	C4'-C3'-C2'	-6.39	96.21	102.60
51	a	210	A	O3'-P-O5'	-6.39	94.41	104.00
51	a	1377	G	O3'-P-O5'	-6.39	94.41	104.00
46	A	1525	G	C2'-C3'-O3'	6.39	123.28	113.70
46	A	2264	G	C3'-C2'-O2'	6.38	120.28	110.70
46	A	342	A	C4'-C3'-O3'	-6.38	103.43	113.00
46	A	434	U	C2'-C3'-O3'	6.38	119.06	109.50
51	a	434	U	O3'-P-O5'	-6.37	94.44	104.00
46	A	2411	G	C1'-C2'-O2'	6.37	121.35	111.80
46	A	2570	A	C1'-C2'-O2'	6.37	117.95	108.40
46	A	2791	U	O3'-P-O5'	-6.36	94.46	104.00
51	a	124	G	O3'-P-O5'	-6.35	94.48	104.00
51	a	1536	G	O3'-P-O5'	-6.35	94.48	104.00
46	A	1268	G	O3'-P-O5'	-6.35	94.48	104.00
46	A	2845	A	O3'-P-O5'	-6.34	94.48	104.00
51	a	883	A	C2'-C3'-O3'	6.34	119.01	109.50
46	A	2899	C	O3'-P-O5'	-6.34	94.49	104.00
51	a	36	C	O3'-P-O5'	-6.34	94.49	104.00
51	a	1335	U	O3'-P-O5'	-6.34	94.49	104.00
46	A	2436	A	O3'-P-O5'	-6.33	94.50	104.00
46	A	498	U	C1'-O4'-C4'	-6.33	103.57	109.90
46	A	2702	G	O3'-P-O5'	-6.33	94.51	104.00
46	A	1616	G	C4'-C3'-O3'	-6.32	103.51	113.00
46	A	2863	G	C3'-C2'-O2'	6.32	120.18	110.70
46	A	2649	C	O3'-P-O5'	-6.32	94.52	104.00
46	A	1013	U	O3'-P-O5'	-6.32	94.53	104.00
51	a	966	U	O3'-P-O5'	-6.32	94.53	104.00
51	a	529	A	O3'-P-O5'	-6.31	94.53	104.00
46	A	642	G	C3'-C2'-O2'	6.31	120.17	110.70
46	A	852	G	O3'-P-O5'	-6.31	94.53	104.00
46	A	730	U	O3'-P-O5'	-6.31	94.54	104.00
46	A	2770	A	O3'-P-O5'	-6.30	94.54	104.00
46	A	1167	C	O3'-P-O5'	-6.30	94.55	104.00
51	a	982	C	C4'-C3'-O3'	-6.30	103.55	113.00
46	A	2225	C	O3'-P-O5'	-6.30	94.55	104.00
46	A	611	U	O3'-P-O5'	-6.30	94.55	104.00
8	B	107	G	C4'-C3'-O3'	6.30	118.84	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	j	43	PRO	N-CA-C	6.29	121.11	111.11
51	a	207	U	O3'-P-O5'	-6.29	94.56	104.00
46	A	1516	A	C4'-C3'-O3'	-6.29	103.57	113.00
51	a	511	C	O3'-P-O5'	-6.29	94.57	104.00
51	a	386	A	O3'-P-O5'	-6.28	94.58	104.00
51	a	1481	G	O3'-P-O5'	-6.28	94.58	104.00
46	A	2307	A	C4'-C3'-O3'	-6.28	103.58	113.00
10	D	150	ASP	CA-CB-CG	6.28	118.88	112.60
46	A	15	G	O3'-P-O5'	-6.28	94.58	104.00
46	A	1250	G	C4'-C3'-O3'	6.28	118.82	109.40
51	a	64	U	O3'-P-O5'	-6.28	94.58	104.00
46	A	128	C	C4'-C3'-O3'	-6.27	103.59	113.00
46	A	1751	U	O3'-P-O5'	-6.27	94.59	104.00
51	a	901	U	O3'-P-O5'	-6.27	94.60	104.00
51	a	172	U	O3'-P-O5'	-6.27	94.60	104.00
46	A	2770	A	C3'-C2'-O2'	6.27	120.10	110.70
51	a	295	U	O3'-P-O5'	-6.27	94.60	104.00
51	a	558	C	C4'-C3'-O3'	-6.26	103.60	113.00
46	A	299	U	O3'-P-O5'	-6.25	94.62	104.00
46	A	1782	G	C3'-C2'-O2'	6.25	120.08	110.70
46	A	2377	U	C1'-C2'-O2'	6.25	117.78	108.40
46	A	1073	A	O3'-P-O5'	-6.25	94.63	104.00
46	A	1779	G	O3'-P-O5'	-6.25	94.63	104.00
46	A	2438	G	O3'-P-O5'	-6.25	94.63	104.00
51	a	765	C	O3'-P-O5'	-6.25	94.63	104.00
46	A	1305	A	O3'-P-O5'	-6.24	94.64	104.00
46	A	2334	U	O3'-P-O5'	-6.24	94.64	104.00
51	a	385	G	O3'-P-O5'	-6.24	94.64	104.00
46	A	1995	A	O3'-P-O5'	-6.24	94.64	104.00
46	A	2452	U	O3'-P-O5'	-6.24	94.64	104.00
46	A	1771	C	C4'-C3'-O3'	-6.23	103.65	113.00
46	A	2023	C	O3'-P-O5'	-6.23	94.65	104.00
46	A	673	A	O3'-P-O5'	-6.23	94.65	104.00
46	A	1681	U	C4'-C3'-O3'	-6.23	103.65	113.00
46	A	1007	G	C1'-C2'-O2'	-6.23	102.46	111.80
51	a	1417	A	O3'-P-O5'	-6.23	94.66	104.00
46	A	467	C	C1'-C2'-O2'	-6.22	99.06	108.40
46	A	198	A	C4'-C3'-O3'	-6.22	103.67	113.00
46	A	1361	A	C1'-C2'-O2'	6.22	117.73	108.40
51	a	558	C	O3'-P-O5'	-6.22	94.67	104.00
46	A	227	G	C3'-C2'-O2'	6.22	120.03	110.70
51	a	1201	C	O3'-P-O5'	-6.22	94.67	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	125	A	C4'-C3'-O3'	-6.22	103.67	113.00
46	A	844	U	C3'-C2'-O2'	6.21	120.02	110.70
46	A	1981	A	O3'-P-O5'	-6.21	94.68	104.00
46	A	831	U	C2'-C3'-O3'	-6.21	104.39	113.70
46	A	1543	U	O3'-P-O5'	-6.21	94.69	104.00
46	A	1974	G	O3'-P-O5'	-6.21	94.69	104.00
51	a	836	U	O3'-P-O5'	-6.21	94.69	104.00
46	A	864	C	O3'-P-O5'	-6.20	94.70	104.00
45	v	19	G	O3'-P-O5'	-6.20	94.71	104.00
46	A	373	A	C2'-C3'-O3'	6.20	118.79	109.50
46	A	2859	G	O3'-P-O5'	-6.20	94.71	104.00
51	a	1332	G	O3'-P-O5'	-6.20	94.71	104.00
46	A	1246	G	O4'-C4'-C3'	-6.19	97.81	104.00
46	A	12	A	O3'-P-O5'	-6.18	94.72	104.00
46	A	210	A	O3'-P-O5'	-6.18	94.72	104.00
46	A	562	C	C3'-C2'-O2'	6.18	119.98	110.70
46	A	956	A	C4'-C3'-O3'	-6.18	103.73	113.00
51	a	982	C	O3'-P-O5'	-6.18	94.72	104.00
46	A	1201	A	O3'-P-O5'	-6.17	94.74	104.00
46	A	2578	G	O3'-P-O5'	-6.17	94.74	104.00
46	A	2454	A	O3'-P-O5'	-6.17	94.74	104.00
46	A	467	C	C3'-C2'-O2'	6.16	119.95	110.70
46	A	1231	G	C4'-C3'-C2'	-6.16	96.44	102.60
46	A	1814	A	O3'-P-O5'	-6.16	94.76	104.00
46	A	218	G	O3'-P-O5'	-6.15	94.78	104.00
46	A	1005	A	O3'-P-O5'	-6.15	94.77	104.00
46	A	1448	U	O3'-P-O5'	-6.15	94.78	104.00
1	0	18	THR	CB-CA-C	-6.15	100.23	110.68
46	A	1649	C	C4'-C3'-O3'	-6.14	103.79	113.00
46	A	510	G	C1'-C2'-O2'	6.14	117.61	108.40
46	A	2708	A	O3'-P-O5'	-6.14	94.79	104.00
46	A	2843	G	C3'-C2'-O2'	6.14	119.91	110.70
46	A	254	A	C4'-C3'-O3'	-6.14	103.79	113.00
46	A	457	G	C2'-C3'-O3'	-6.13	104.50	113.70
51	a	652	C	O3'-P-O5'	-6.13	94.81	104.00
51	a	572	A	O3'-P-O5'	-6.12	94.81	104.00
51	a	1075	U	O3'-P-O5'	-6.12	94.82	104.00
51	a	1515	G	O3'-P-O5'	-6.12	94.82	104.00
46	A	2496	C	C4'-C3'-O3'	-6.12	103.82	113.00
46	A	205	U	C4'-C3'-O3'	-6.12	103.83	113.00
46	A	1055	A	O3'-P-O5'	-6.12	94.83	104.00
51	a	831	A	O3'-P-O5'	-6.12	94.83	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	1530	G	C2'-C3'-O3'	6.11	122.87	113.70
46	A	2649	C	C3'-C2'-O2'	6.11	119.86	110.70
51	a	1200	A	O3'-P-O5'	-6.10	94.84	104.00
46	A	2716	U	O3'-P-O5'	-6.10	94.84	104.00
51	a	740	G	O3'-P-O5'	-6.10	94.85	104.00
46	A	1865	C	O3'-P-O5'	-6.10	94.85	104.00
51	a	1329	C	O3'-P-O5'	-6.10	94.85	104.00
46	A	2842	U	C3'-C2'-O2'	6.09	119.84	110.70
46	A	2762	A	O3'-P-O5'	-6.09	94.86	104.00
46	A	2863	G	O3'-P-O5'	-6.09	94.87	104.00
46	A	1854	G	O3'-P-O5'	-6.08	94.87	104.00
51	a	1101	U	O3'-P-O5'	-6.08	94.87	104.00
46	A	1339	A	P-O3'-C3'	6.08	129.32	120.20
51	a	1492	G	O3'-P-O5'	-6.08	94.88	104.00
50	9	75	C	C4'-C3'-O3'	-6.08	103.88	113.00
46	A	2913	U	O3'-P-O5'	-6.07	94.89	104.00
46	A	2614	U	O3'-P-O5'	-6.07	94.90	104.00
46	A	1960	U	O3'-P-O5'	-6.07	94.90	104.00
46	A	2715	G	O3'-P-O5'	-6.07	94.90	104.00
51	a	1525	C	O3'-P-O5'	-6.07	94.90	104.00
50	9	21	A	C4'-C3'-O3'	6.06	118.49	109.40
46	A	2091	A	C2'-C3'-O3'	6.06	118.59	109.50
51	a	1376	C	O3'-P-O5'	-6.06	94.91	104.00
46	A	1508	C	O3'-P-O5'	-6.06	94.91	104.00
45	v	45	U	O3'-P-O5'	-6.06	94.92	104.00
46	A	1376	G	O3'-P-O5'	-6.06	94.92	104.00
46	A	2311	G	O3'-P-O5'	-6.05	94.92	104.00
46	A	540	G	C4'-C3'-O3'	-6.05	103.92	113.00
51	a	816	A	O3'-P-O5'	-6.05	94.93	104.00
46	A	1810	G	O3'-P-O5'	-6.04	94.93	104.00
51	a	181	G	O3'-P-O5'	-6.04	94.94	104.00
51	a	356	G	O3'-P-O5'	-6.04	94.94	104.00
46	A	53	A	O3'-P-O5'	-6.03	94.95	104.00
46	A	848	G	O3'-P-O5'	-6.03	94.95	104.00
46	A	1486	G	O3'-P-O5'	-6.03	94.96	104.00
46	A	2435	C	O3'-P-O5'	-6.03	94.96	104.00
51	a	873	U	O3'-P-O5'	-6.03	94.96	104.00
46	A	980	C	O3'-P-O5'	-6.02	94.97	104.00
46	A	1169	C	O3'-P-O5'	-6.02	94.97	104.00
46	A	1328	C	C3'-C2'-O2'	6.02	119.73	110.70
8	B	12	U	C2'-C3'-O3'	6.02	118.52	109.50
46	A	2282	G	O3'-P-O5'	-6.01	94.98	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	1749	G	O3'-P-O5'	-6.01	94.99	104.00
51	a	803	A	C1'-C2'-O2'	6.01	117.41	108.40
46	A	1307	U	C3'-C2'-O2'	6.01	119.71	110.70
46	A	1614	A	O3'-P-O5'	-6.01	94.99	104.00
46	A	2621	G	O3'-P-O5'	-6.00	94.99	104.00
46	A	1436	U	O3'-P-O5'	-6.00	95.00	104.00
46	A	2708	A	C1'-C2'-O2'	6.00	117.40	108.40
46	A	266	U	O3'-P-O5'	-6.00	95.00	104.00
46	A	341	G	O3'-P-O5'	-6.00	95.00	104.00
51	a	1313	G	O3'-P-O5'	-6.00	95.00	104.00
46	A	2306	G	O3'-P-O5'	-6.00	95.00	104.00
46	A	825	G	C4'-C3'-O3'	-5.99	104.01	113.00
46	A	2849	U	C4'-C3'-O3'	-5.99	104.01	113.00
46	A	1183	G	C4'-C3'-C2'	-5.99	96.61	102.60
46	A	430	C	O4'-C4'-C3'	-5.99	98.02	104.00
46	A	986	G	C2'-C3'-O3'	-5.98	104.72	113.70
46	A	1284	A	O3'-P-O5'	-5.98	95.03	104.00
46	A	2618	A	O3'-P-O5'	-5.98	95.03	104.00
46	A	59	G	O3'-P-O5'	-5.98	95.04	104.00
51	a	1309	G	O3'-P-O5'	-5.97	95.04	104.00
46	A	2290	C	C4'-C3'-O3'	-5.97	104.05	113.00
45	v	50	G	O3'-P-O5'	-5.97	95.05	104.00
51	a	900	G	O3'-P-O5'	-5.97	95.05	104.00
46	A	2103	U	C3'-C2'-O2'	5.97	119.65	110.70
46	A	2475	G	O3'-P-O5'	-5.96	95.06	104.00
45	v	21	A	O3'-P-O5'	-5.96	95.07	104.00
46	A	338	G	O3'-P-O5'	-5.96	95.06	104.00
51	a	360	C	O3'-P-O5'	-5.96	95.07	104.00
46	A	1969	U	O3'-P-O5'	-5.95	95.07	104.00
46	A	667	A	O3'-P-O5'	-5.95	95.08	104.00
46	A	2583	U	O3'-P-O5'	-5.95	95.08	104.00
46	A	1234	G	O3'-P-O5'	-5.95	95.08	104.00
46	A	544	G	O3'-P-O5'	-5.94	95.08	104.00
51	a	1196	G	O3'-P-O5'	-5.94	95.09	104.00
45	v	20	U	C2'-C3'-O3'	5.94	118.41	109.50
51	a	965	U	C4'-C3'-C2'	-5.94	96.66	102.60
46	A	1277	A	O3'-P-O5'	-5.94	95.09	104.00
51	a	1197	A	O3'-P-O5'	-5.94	95.09	104.00
51	a	595	C	O3'-P-O5'	-5.93	95.10	104.00
45	v	76	A	C1'-O4'-C4'	-5.93	103.77	109.70
46	A	208	G	C3'-C2'-C1'	-5.93	95.57	101.50
46	A	2302	A	C4'-C3'-O3'	-5.92	104.11	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	1790	U	C4'-C3'-O3'	-5.92	104.12	113.00
46	A	2229	C	O3'-P-O5'	-5.92	95.12	104.00
51	a	580	U	O3'-P-O5'	-5.92	95.12	104.00
46	A	364	A	O3'-P-O5'	-5.91	95.13	104.00
8	B	76	A	O3'-P-O5'	-5.91	95.14	104.00
51	a	913	A	O3'-P-O5'	-5.91	95.14	104.00
51	a	807	U	O3'-P-O5'	-5.90	95.14	104.00
51	a	1448	G	O3'-P-O5'	-5.90	95.15	104.00
11	E	90	PHE	CB-CA-C	-5.90	103.52	111.89
46	A	2481	C	O3'-P-O5'	-5.90	95.15	104.00
51	a	812	G	O3'-P-O5'	-5.90	95.15	104.00
46	A	2875	A	O3'-P-O5'	-5.89	95.16	104.00
51	a	370	G	O3'-P-O5'	-5.89	95.16	104.00
46	A	1366	C	O3'-P-O5'	-5.89	95.17	104.00
51	a	1119	C	C4'-C3'-C2'	-5.89	96.71	102.60
46	A	1075	A	C2'-C3'-O3'	-5.88	104.87	113.70
51	a	1209	C	O3'-P-O5'	-5.88	95.17	104.00
46	A	1854	G	C1'-C2'-O2'	5.88	117.22	108.40
39	n	45	ARG	CB-CA-C	-5.88	101.41	110.81
51	a	1266	A	C2'-C3'-O3'	5.87	118.31	109.50
46	A	2740	A	C4'-C3'-O3'	-5.87	104.20	113.00
46	A	2821	U	O3'-P-O5'	-5.87	95.20	104.00
46	A	543	A	O3'-P-O5'	-5.86	95.22	104.00
46	A	1365	U	O3'-P-O5'	-5.85	95.22	104.00
46	A	874	U	C2'-C3'-O3'	-5.85	104.93	113.70
51	a	387	C	C3'-C2'-O2'	5.85	119.47	110.70
46	A	1258	A	O3'-P-O5'	-5.84	95.23	104.00
46	A	2688	G	O3'-P-O5'	-5.84	95.24	104.00
46	A	2372	U	C4'-C3'-O3'	-5.83	104.25	113.00
46	A	1259	G	C4'-C3'-O3'	-5.83	104.26	113.00
51	a	1374	G	C1'-C2'-O2'	5.82	117.13	108.40
46	A	565	U	O3'-P-O5'	-5.81	95.28	104.00
46	A	1072	A	C4'-C3'-O3'	5.81	118.12	109.40
51	a	896	G	O3'-P-O5'	-5.81	95.28	104.00
51	a	1148	G	C2'-C3'-O3'	5.81	118.22	109.50
51	a	136	U	O3'-P-O5'	-5.80	95.29	104.00
51	a	927	G	O3'-P-O5'	-5.80	95.29	104.00
46	A	418	A	O3'-P-O5'	-5.80	95.30	104.00
46	A	903	G	C3'-C2'-O2'	5.80	119.40	110.70
46	A	2342	C	O3'-P-O5'	-5.80	95.30	104.00
46	A	1201	A	C3'-C2'-O2'	5.80	119.40	110.70
46	A	2780	G	O3'-P-O5'	-5.80	95.30	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	2662	A	C3'-C2'-O2'	5.79	119.39	110.70
51	a	19	U	O3'-P-O5'	-5.79	95.31	104.00
51	a	539	G	O4'-C1'-C2'	-5.79	100.01	105.80
46	A	194	A	O3'-P-O5'	-5.79	95.32	104.00
51	a	888	U	O3'-P-O5'	-5.79	95.32	104.00
46	A	216	A	O3'-P-O5'	-5.79	95.32	104.00
46	A	1426	A	O3'-P-O5'	-5.79	95.32	104.00
46	A	1062	C	O3'-P-O5'	-5.78	95.33	104.00
51	a	848	G	C2'-C3'-O3'	5.78	122.37	113.70
46	A	1682	C	C1'-C2'-O2'	5.78	117.07	108.40
46	A	598	U	C4'-C3'-O3'	-5.77	104.35	113.00
46	A	2569	C	P-O5'-C5'	-5.76	112.25	120.90
51	a	1310	U	O3'-P-O5'	5.76	112.65	104.00
46	A	1988	G	C4'-C3'-O3'	-5.76	104.36	113.00
46	A	243	G	C1'-C2'-O2'	5.76	117.04	108.40
9	C	254	THR	CB-CA-C	5.76	119.94	111.65
46	A	1290	G	O5'-P-OP1	5.76	125.27	108.00
51	a	1041	C	C2'-C3'-O3'	5.76	118.13	109.50
46	A	1941	A	O3'-P-O5'	-5.75	95.37	104.00
46	A	792	G	C4'-C3'-O3'	-5.75	104.38	113.00
46	A	58	G	O3'-P-O5'	-5.75	95.38	104.00
46	A	1447	C	O3'-P-O5'	-5.75	95.38	104.00
46	A	1615	A	C2'-C3'-O3'	-5.75	100.88	109.50
46	A	2352	G	O3'-P-O5'	-5.74	95.39	104.00
51	a	935	G	C3'-C2'-O2'	5.74	119.31	110.70
46	A	1655	A	C2'-C3'-O3'	5.73	118.10	109.50
46	A	1289	U	C4'-C3'-O3'	-5.73	104.41	113.00
51	a	728	C	O3'-P-O5'	-5.73	95.41	104.00
46	A	1255	G	C1'-C2'-O2'	5.72	116.99	108.40
46	A	1690	G	C2'-C3'-O3'	-5.72	105.12	113.70
46	A	2004	G	O3'-P-O5'	-5.72	95.42	104.00
46	A	1293	A	C2'-C3'-O3'	5.72	118.08	109.50
51	a	640	G	O3'-P-O5'	-5.72	95.42	104.00
46	A	2419	U	C4'-C3'-O3'	-5.71	104.44	113.00
46	A	432	C	C2'-C3'-O3'	-5.71	105.14	113.70
46	A	2814	U	C3'-C2'-O2'	5.71	119.26	110.70
50	9	21	A	O3'-P-O5'	5.71	112.56	104.00
46	A	2296	A	N9-C1'-C2'	5.71	120.56	112.00
46	A	1400	G	O3'-P-O5'	-5.70	95.45	104.00
51	a	40	G	O3'-P-O5'	-5.70	95.45	104.00
46	A	306	C	O3'-P-O5'	-5.69	95.46	104.00
46	A	615	U	C1'-C2'-O2'	-5.69	103.26	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	2417	A	C4'-C3'-O3'	-5.69	104.46	113.00
46	A	254	A	C3'-C2'-O2'	5.69	119.24	110.70
46	A	473	C	O3'-P-O5'	-5.68	95.47	104.00
46	A	787	C	O3'-P-O5'	-5.68	95.48	104.00
51	a	23	G	O3'-P-O5'	-5.68	95.47	104.00
51	a	564	C	O3'-P-O5'	-5.68	95.48	104.00
46	A	1259	G	O3'-P-O5'	-5.68	95.48	104.00
46	A	2325	U	C2'-C3'-O3'	5.68	118.02	109.50
46	A	1179	A	C1'-O4'-C4'	-5.68	104.02	109.70
51	a	752	U	O3'-P-O5'	-5.68	95.49	104.00
46	A	1617	A	O3'-P-O5'	-5.67	95.49	104.00
46	A	228	C	O3'-P-O5'	-5.67	95.50	104.00
51	a	1504	G	O3'-P-O5'	-5.67	95.50	104.00
46	A	1052	C	C1'-C2'-O2'	5.67	116.90	108.40
46	A	1534	A	O3'-P-O5'	-5.67	95.50	104.00
46	A	1651	G	O3'-P-O5'	-5.67	95.50	104.00
46	A	2860	A	O3'-P-O5'	-5.66	95.51	104.00
46	A	1178	U	C2'-C3'-O3'	5.66	117.99	109.50
46	A	959	C	O3'-P-O5'	5.66	112.49	104.00
45	v	3	C	O3'-P-O5'	-5.66	95.52	104.00
46	A	661	A	C1'-C2'-O2'	5.66	116.89	108.40
46	A	1364	C	C1'-C2'-O2'	-5.65	103.32	111.80
46	A	2097	U	C2'-C3'-O3'	-5.65	105.22	113.70
46	A	2539	C	C4'-C3'-O3'	-5.65	104.53	113.00
46	A	2052	A	C4'-C3'-O3'	-5.65	104.53	113.00
46	A	483	C	O3'-P-O5'	-5.64	95.53	104.00
46	A	630	A	C4'-C3'-O3'	-5.64	104.53	113.00
46	A	995	U	O3'-P-O5'	-5.64	95.53	104.00
46	A	583	G	C4'-C3'-O3'	-5.64	104.54	113.00
51	a	1509	A	O3'-P-O5'	-5.64	95.54	104.00
46	A	1883	A	O3'-P-O5'	-5.64	95.54	104.00
46	A	1989	A	O3'-P-O5'	-5.64	95.54	104.00
46	A	2402	A	C4'-C3'-O3'	-5.64	104.54	113.00
51	a	385	G	C4'-C3'-O3'	-5.64	104.54	113.00
46	A	1799	G	O3'-P-O5'	-5.64	95.54	104.00
46	A	2715	G	C4'-C3'-O3'	-5.64	104.55	113.00
51	a	246	G	O3'-P-O5'	-5.63	95.55	104.00
46	A	620	U	O3'-P-O5'	-5.63	95.55	104.00
46	A	636	G	O3'-P-O5'	-5.63	95.55	104.00
46	A	1789	A	O3'-P-O5'	-5.63	95.55	104.00
46	A	768	G	O3'-P-O5'	-5.63	95.56	104.00
46	A	1065	U	C4'-C3'-O3'	-5.63	104.56	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	U	73	PRO	N-CA-CB	-5.63	99.04	102.81
46	A	367	G	O3'-P-O5'	-5.63	95.56	104.00
46	A	439	U	O3'-P-O5'	-5.63	95.56	104.00
46	A	834	C	O5'-P-OP1	5.63	124.88	108.00
46	A	224	A	O3'-P-O5'	-5.62	95.57	104.00
46	A	614	G	C4'-C3'-O3'	-5.62	104.57	113.00
46	A	803	C	O3'-P-O5'	-5.62	95.58	104.00
46	A	1202	A	C3'-C2'-O2'	-5.62	106.17	114.60
46	A	1317	G	C3'-C2'-O2'	5.61	119.12	110.70
46	A	461	C	O3'-P-O5'	-5.61	95.58	104.00
46	A	897	G	O3'-P-O5'	-5.61	95.58	104.00
46	A	72	U	C1'-C2'-O2'	5.61	120.21	111.80
46	A	1668	G	O3'-P-O5'	-5.61	95.59	104.00
51	a	963	G	C4'-C3'-O3'	-5.61	104.59	113.00
46	A	427	G	C1'-C2'-O2'	5.60	116.80	108.40
46	A	381	U	O3'-P-O5'	-5.60	95.60	104.00
46	A	969	C	O3'-P-O5'	-5.60	95.60	104.00
49	7	409	U	O3'-P-O5'	-5.59	95.61	104.00
46	A	599	G	O3'-P-O5'	-5.59	95.61	104.00
46	A	2850	G	O3'-P-O5'	5.59	112.38	104.00
51	a	369	G	O3'-P-O5'	-5.59	95.62	104.00
46	A	228	C	C3'-C2'-O2'	5.58	119.08	110.70
46	A	811	A	C1'-C2'-O2'	-5.58	103.42	111.80
46	A	1987	C	O3'-P-O5'	-5.58	95.63	104.00
46	A	986	G	C4'-C3'-C2'	-5.58	97.02	102.60
51	a	672	A	O3'-P-O5'	-5.58	95.63	104.00
51	a	969	A	O3'-P-O5'	-5.58	95.63	104.00
46	A	2353	U	C4'-C3'-O3'	-5.58	104.63	113.00
46	A	1031	C	C4'-C3'-O3'	-5.58	104.64	113.00
50	9	40	U	O3'-P-O5'	-5.58	95.64	104.00
51	a	1433	U	O3'-P-O5'	-5.57	95.64	104.00
46	A	863	C	C3'-C2'-O2'	5.57	119.05	110.70
46	A	1872	C	O3'-P-O5'	-5.56	95.66	104.00
51	a	1207	A	C4'-C3'-O3'	-5.56	104.66	113.00
46	A	263	G	C4'-C3'-O3'	-5.56	104.66	113.00
46	A	624	C	C1'-C2'-O2'	-5.56	100.06	108.40
46	A	724	A	C4'-C3'-O3'	-5.56	104.67	113.00
46	A	851	A	C4'-C3'-O3'	-5.56	104.66	113.00
46	A	1208	G	C4'-C3'-C2'	-5.56	97.04	102.60
46	A	1341	U	O3'-P-O5'	-5.56	95.66	104.00
46	A	1929	A	C1'-C2'-O2'	-5.56	103.46	111.80
46	A	2908	A	O3'-P-O5'	-5.56	95.66	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	125	A	O3'-P-O5'	-5.55	95.67	104.00
46	A	378	C	O3'-P-O5'	-5.55	95.67	104.00
46	A	1174	A	O3'-P-O5'	-5.55	95.67	104.00
46	A	2062	A	C4'-C3'-O3'	5.55	117.73	109.40
46	A	2308	G	C4'-C3'-C2'	-5.55	97.05	102.60
46	A	1046	A	C4'-C3'-O3'	-5.55	104.68	113.00
46	A	2703	G	O3'-P-O5'	-5.54	95.69	104.00
46	A	2720	C	C2'-C3'-O3'	-5.54	105.39	113.70
51	a	1389	U	O3'-P-O5'	-5.54	95.70	104.00
46	A	2545	G	O3'-P-O5'	-5.53	95.70	104.00
46	A	2532	A	O3'-P-O5'	5.53	112.30	104.00
46	A	2662	A	C4'-C3'-O3'	-5.53	104.71	113.00
46	A	1615	A	O3'-P-O5'	-5.52	95.72	104.00
46	A	2531	G	C4'-C3'-O3'	-5.52	104.72	113.00
46	A	1644	C	O3'-P-O5'	-5.52	95.72	104.00
51	a	1237	C	O3'-P-O5'	-5.52	95.72	104.00
46	A	2676	U	O3'-P-O5'	-5.51	95.73	104.00
46	A	2056	G	O3'-P-O5'	-5.51	95.73	104.00
9	C	27	ASP	CA-CB-CG	5.51	118.11	112.60
46	A	2895	C	O3'-P-O5'	5.50	112.25	104.00
51	a	1373	U	O3'-P-O5'	-5.50	95.75	104.00
15	K	12	ASP	CA-CB-CG	5.50	118.10	112.60
46	A	2383	A	C4'-C3'-O3'	-5.50	104.75	113.00
46	A	2029	G	C1'-C2'-O2'	5.50	116.64	108.40
46	A	2734	A	O3'-P-O5'	-5.50	95.76	104.00
46	A	1179	A	O3'-P-O5'	-5.49	95.76	104.00
46	A	2276	A	O3'-P-O5'	-5.49	95.76	104.00
51	a	573	U	O3'-P-O5'	-5.49	95.76	104.00
51	a	1418	C	C3'-C2'-O2'	5.49	118.94	110.70
10	D	50	GLN	CB-CA-C	-5.49	100.69	109.75
46	A	1267	G	C3'-C2'-O2'	5.49	118.93	110.70
46	A	2862	A	C3'-C2'-O2'	5.48	118.92	110.70
46	A	881	U	O3'-P-O5'	-5.48	95.78	104.00
46	A	1203	G	O5'-P-OP1	-5.48	91.56	108.00
46	A	2528	C	O3'-P-O5'	-5.48	95.78	104.00
46	A	595	G	O3'-P-O5'	-5.48	95.78	104.00
46	A	2749	U	C1'-C2'-O2'	5.48	116.62	108.40
46	A	2817	C	C2'-C3'-O3'	-5.48	105.48	113.70
51	a	436	G	C1'-O4'-C4'	-5.48	104.22	109.70
46	A	1873	U	O3'-P-O5'	-5.48	95.79	104.00
51	a	774	G	O3'-P-O5'	-5.48	95.79	104.00
46	A	1427	G	O3'-P-O5'	-5.47	95.79	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	250	G	C4'-C3'-C2'	-5.47	97.13	102.60
46	A	2727	U	C4'-C3'-O3'	-5.47	104.79	113.00
51	a	916	G	O3'-P-O5'	-5.47	95.79	104.00
46	A	2333	G	O3'-P-O5'	-5.47	95.80	104.00
46	A	2842	U	O3'-P-O5'	-5.47	95.80	104.00
46	A	1320	G	O3'-P-O5'	-5.46	95.80	104.00
46	A	1742	G	C2'-C3'-O3'	5.46	121.90	113.70
51	a	282	A	O3'-P-O5'	-5.46	95.80	104.00
24	T	29	GLU	CB-CA-C	5.46	118.42	109.90
46	A	1925	A	O3'-P-O5'	-5.46	95.81	104.00
46	A	2499	G	O3'-P-O5'	-5.46	95.81	104.00
46	A	1308	A	C4'-C3'-C2'	-5.46	97.14	102.60
46	A	1480	A	O4'-C4'-C3'	-5.46	98.54	104.00
46	A	2899	C	C2'-C3'-O3'	5.46	121.88	113.70
46	A	1719	G	O3'-P-O5'	-5.45	95.82	104.00
46	A	2407	A	C2'-C3'-O3'	-5.45	105.52	113.70
46	A	2609	U	C4'-C3'-O3'	-5.45	104.83	113.00
51	a	20	C	O3'-P-O5'	-5.45	95.83	104.00
46	A	1651	G	C2'-C3'-O3'	-5.45	105.53	113.70
20	P	21	ARG	CB-CA-C	-5.45	102.91	110.37
46	A	1246	G	C4'-C3'-C2'	-5.45	97.15	102.60
46	A	2609	U	O3'-P-O5'	-5.44	95.84	104.00
50	9	67	A	O3'-P-O5'	-5.44	95.84	104.00
46	A	1475	G	O3'-P-O5'	-5.44	95.84	104.00
46	A	2249	G	O3'-P-O5'	-5.43	95.85	104.00
46	A	2673	A	C3'-C2'-O2'	5.43	118.85	110.70
51	a	760	U	O3'-P-O5'	-5.43	95.85	104.00
46	A	378	C	C4'-C3'-O3'	-5.43	104.86	113.00
46	A	719	C	O3'-P-O5'	-5.43	95.86	104.00
46	A	1913	A	O3'-P-O5'	-5.42	95.86	104.00
46	A	639	C	C3'-C2'-O2'	5.42	118.83	110.70
46	A	431	A	C1'-C2'-O2'	5.42	116.53	108.40
46	A	2273	U	C2'-C3'-O3'	-5.42	105.57	113.70
51	a	20	C	C4'-C3'-O3'	-5.42	104.87	113.00
51	a	962	U	O3'-P-O5'	-5.42	95.87	104.00
46	A	1424	A	O4'-C1'-C2'	-5.42	100.38	105.80
46	A	676	G	C4'-C3'-O3'	-5.41	104.88	113.00
46	A	1380	U	C2'-C3'-O3'	5.41	117.61	109.50
46	A	1543	U	C4'-C3'-O3'	5.41	117.52	109.40
46	A	1665	G	O3'-P-O5'	-5.41	95.88	104.00
46	A	2822	C	O3'-P-O5'	-5.41	95.89	104.00
51	a	1385	U	O3'-P-O5'	-5.41	95.89	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	1170	C	O3'-P-O5'	-5.41	95.89	104.00
53	d	127	ASP	CA-CB-CG	5.41	118.01	112.60
46	A	2602	C	O3'-P-O5'	5.40	112.11	104.00
46	A	2506	C	C4'-C3'-O3'	-5.40	104.90	113.00
46	A	199	A	C1'-C2'-O2'	-5.40	103.70	111.80
46	A	871	G	C3'-C2'-O2'	5.40	118.80	110.70
46	A	1016	U	O3'-P-O5'	-5.40	95.90	104.00
46	A	1398	A	C4'-C3'-O3'	-5.40	104.90	113.00
23	S	77	ASP	CB-CA-C	5.40	118.70	109.80
46	A	153	C	O3'-P-O5'	-5.39	95.91	104.00
46	A	1852	G	O3'-P-O5'	-5.39	95.91	104.00
51	a	1404	C	C4'-C3'-O3'	-5.39	104.91	113.00
46	A	1247	G	O3'-P-O5'	-5.39	95.91	104.00
46	A	2915	G	C3'-C2'-O2'	-5.39	102.61	110.70
46	A	617	G	O3'-P-O5'	-5.39	95.92	104.00
46	A	874	U	C1'-C2'-O2'	-5.39	100.31	108.40
46	A	1744	G	O3'-P-O5'	-5.39	95.92	104.00
46	A	1038	C	C4'-C3'-O3'	-5.39	104.92	113.00
46	A	1607	C	O3'-P-O5'	-5.39	95.92	104.00
51	a	193	G	O3'-P-O5'	-5.39	95.92	104.00
46	A	831	U	P-O5'-C5'	-5.38	112.82	120.90
51	a	1445	U	O3'-P-O5'	-5.38	95.92	104.00
46	A	582	A	C4'-C3'-O3'	-5.38	104.93	113.00
46	A	572	A	N9-C1'-C2'	5.38	120.07	112.00
46	A	877	G	O3'-P-O5'	-5.38	95.93	104.00
46	A	72	U	O3'-P-O5'	-5.37	95.94	104.00
50	9	82	A	O3'-P-O5'	-5.37	95.94	104.00
51	a	572	A	C4'-C3'-O3'	-5.37	104.94	113.00
51	a	759	C	O3'-P-O5'	-5.37	95.94	104.00
46	A	245	G	O3'-P-O5'	5.37	112.06	104.00
46	A	1653	A	C2'-C3'-O3'	5.37	117.56	109.50
46	A	2358	A	O3'-P-O5'	-5.37	95.94	104.00
50	9	25	G	O3'-P-O5'	-5.37	95.94	104.00
28	Z	18	ASP	CA-CB-CG	5.37	117.97	112.60
46	A	2484	G	C4'-C3'-O3'	-5.37	104.95	113.00
46	A	119	U	O3'-P-O5'	-5.36	95.95	104.00
46	A	1244	A	O3'-P-O5'	-5.36	95.96	104.00
51	a	972	C	O3'-P-O5'	-5.36	95.96	104.00
46	A	122	G	C4'-C3'-C2'	-5.36	97.24	102.60
46	A	838	C	C3'-C2'-C1'	-5.36	96.14	101.50
46	A	1777	G	C4'-C3'-O3'	-5.36	104.97	113.00
46	A	1057	G	C1'-C2'-O2'	5.35	119.83	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	2440	A	O3'-P-O5'	-5.35	95.97	104.00
46	A	512	G	N9-C1'-C2'	5.35	120.03	112.00
46	A	1228	G	C4'-C3'-O3'	-5.35	104.97	113.00
46	A	109	G	O3'-P-O5'	-5.35	95.97	104.00
46	A	424	G	O3'-P-O5'	-5.35	95.97	104.00
46	A	1265	A	O3'-P-O5'	-5.35	95.97	104.00
46	A	1949	C	C3'-C2'-O2'	5.35	118.72	110.70
46	A	1041	C	C3'-C2'-C1'	-5.35	96.15	101.50
46	A	2494	C	O3'-P-O5'	-5.35	95.98	104.00
51	a	27	C	O3'-P-O5'	-5.35	95.98	104.00
51	a	243	C	O3'-P-O5'	-5.35	95.98	104.00
51	a	1540	G	C1'-C2'-O2'	5.35	116.42	108.40
46	A	1565	U	C4'-C3'-O3'	-5.35	104.98	113.00
46	A	1800	C	C2'-C3'-O3'	5.35	121.72	113.70
46	A	785	C	C2'-C3'-O3'	-5.34	105.68	113.70
46	A	1848	A	C1'-C2'-O2'	-5.34	103.78	111.80
46	A	1904	G	C4'-C3'-O3'	-5.34	104.98	113.00
46	A	923	C	O3'-P-O5'	-5.34	95.99	104.00
10	D	109	ASP	CA-CB-CG	5.34	117.94	112.60
46	A	1388	A	P-O5'-C5'	-5.34	112.89	120.90
46	A	2639	C	C4'-C3'-O3'	-5.34	101.40	109.40
22	R	74	PHE	CA-CB-CG	-5.33	108.47	113.80
46	A	2572	G	C4'-C3'-O3'	-5.33	105.00	113.00
8	B	46	A	C2'-C3'-O3'	5.33	121.70	113.70
10	D	39	LYS	CB-CA-C	5.33	118.54	109.80
46	A	781	A	O3'-P-O5'	-5.33	96.00	104.00
46	A	1800	C	C4'-C3'-C2'	-5.33	97.27	102.60
51	a	1214	U	O3'-P-O5'	-5.33	96.01	104.00
46	A	854	U	C4'-C3'-C2'	-5.33	97.28	102.60
46	A	30	G	C2'-C3'-O3'	-5.32	105.72	113.70
46	A	1363	G	C2'-C3'-O3'	5.32	117.48	109.50
46	A	1724	A	C4'-C3'-O3'	-5.32	105.02	113.00
46	A	1867	C	C1'-C2'-O2'	-5.32	103.82	111.80
46	A	2590	A	C4'-C3'-C2'	-5.32	97.28	102.60
46	A	192	G	C2'-C3'-O3'	5.32	121.68	113.70
51	a	772	G	O3'-P-O5'	-5.32	96.02	104.00
51	a	868	G	O3'-P-O5'	-5.32	96.03	104.00
46	A	1757	G	C1'-O4'-C4'	-5.31	104.39	109.70
46	A	1000	G	O3'-P-O5'	-5.31	96.04	104.00
46	A	1377	G	O3'-P-O5'	-5.31	96.04	104.00
46	A	1413	G	O3'-P-O5'	-5.31	96.04	104.00
46	A	2580	C	C4'-C3'-O3'	-5.30	105.05	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	37	A	C4'-C3'-C2'	-5.30	97.30	102.60
46	A	206	A	C2'-C3'-O3'	5.30	121.65	113.70
46	A	472	G	O3'-P-O5'	-5.30	96.05	104.00
46	A	2063	U	C4'-C3'-O3'	-5.30	105.05	113.00
46	A	491	C	C4'-C3'-C2'	-5.30	97.30	102.60
51	a	368	G	O3'-P-O5'	-5.29	96.06	104.00
50	9	63	U	O3'-P-O5'	-5.29	96.07	104.00
18	N	23	ASP	CB-CA-C	5.29	120.41	110.63
46	A	1615	A	C1'-C2'-O2'	-5.29	103.87	111.80
46	A	1616	G	O3'-P-O5'	-5.29	96.07	104.00
46	A	2286	U	O3'-P-O5'	-5.28	96.07	104.00
46	A	2631	A	C4'-C3'-O3'	5.28	117.33	109.40
51	a	837	A	O3'-P-O5'	-5.28	96.08	104.00
46	A	1673	G	C3'-C2'-O2'	5.28	118.62	110.70
51	a	129	A	O3'-P-O5'	-5.28	96.08	104.00
51	a	1410	G	C1'-C2'-O2'	5.28	116.32	108.40
46	A	816	U	C4'-C3'-O3'	-5.28	105.09	113.00
46	A	1945	A	C1'-C2'-O2'	5.27	119.71	111.80
46	A	2374	G	OP1-P-O3'	5.27	123.82	108.00
46	A	1841	G	C4'-C3'-O3'	-5.27	105.09	113.00
46	A	2458	G	OP2-P-O3'	5.27	123.82	108.00
46	A	75	G	O5'-C5'-C4'	-5.27	103.59	111.50
46	A	875	U	C4'-C3'-O3'	-5.27	105.09	113.00
6	5	97	LYS	N-CA-CB	5.27	119.39	110.49
46	A	1846	G	O3'-P-O5'	-5.27	96.10	104.00
51	a	539	G	C2'-C3'-O3'	5.27	117.40	109.50
8	B	47	C	C4'-C3'-O3'	-5.26	105.11	113.00
46	A	2667	G	O3'-P-O5'	-5.26	96.11	104.00
46	A	2619	A	O3'-P-O5'	-5.26	96.11	104.00
46	A	1323	A	O3'-P-O5'	-5.26	96.11	104.00
46	A	2458	G	OP1-P-O3'	-5.26	92.22	108.00
51	a	173	A	O3'-P-O5'	-5.26	96.11	104.00
46	A	1365	U	C1'-C2'-O2'	-5.26	100.52	108.40
51	a	902	A	O3'-P-O5'	-5.26	96.11	104.00
51	a	744	C	O3'-P-O5'	-5.25	96.12	104.00
46	A	208	G	O4'-C1'-C2'	-5.25	100.55	105.80
46	A	246	U	O3'-P-O5'	-5.25	96.12	104.00
46	A	2843	G	O3'-P-O5'	-5.25	96.12	104.00
46	A	1386	G	C4'-C3'-C2'	-5.25	97.35	102.60
46	A	1606	A	C4'-C3'-O3'	5.25	117.28	109.40
46	A	1807	U	C4'-C3'-O3'	-5.25	105.12	113.00
46	A	2714	G	C3'-C2'-O2'	5.25	118.58	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	v	8	U	O3'-P-O5'	-5.25	96.12	104.00
46	A	1709	A	N9-C1'-C2'	5.25	119.87	112.00
46	A	2607	G	C4'-C3'-C2'	-5.25	97.35	102.60
46	A	1358	G	O3'-P-O5'	-5.25	96.13	104.00
51	a	1354	U	O3'-P-O5'	-5.25	96.13	104.00
46	A	122	G	C2'-C3'-O3'	5.24	121.57	113.70
46	A	2060	A	C4'-C3'-O3'	-5.24	101.54	109.40
46	A	1797	A	O3'-P-O5'	-5.24	96.15	104.00
46	A	374	A	C2'-C3'-O3'	5.23	117.35	109.50
46	A	1782	G	C2'-C3'-O3'	5.23	121.55	113.70
51	a	373	U	C1'-O4'-C4'	-5.23	104.67	109.90
46	A	1569	A	C1'-O4'-C4'	-5.23	104.47	109.70
46	A	956	A	O3'-P-O5'	-5.22	96.17	104.00
51	a	1147	A	O3'-P-O5'	-5.22	96.17	104.00
46	A	1071	G	C3'-C2'-O2'	-5.22	106.77	114.60
46	A	1708	U	C3'-C2'-O2'	5.22	118.53	110.70
46	A	1693	C	O3'-P-O5'	-5.22	96.17	104.00
51	a	1503	A	O4'-C4'-C3'	-5.22	100.88	106.10
46	A	2473	G	C1'-C2'-O2'	5.21	116.22	108.40
46	A	2556	C	O3'-P-O5'	5.21	111.82	104.00
46	A	1192	G	O3'-P-O5'	-5.21	96.18	104.00
50	9	41	C	O3'-P-O5'	-5.21	96.18	104.00
51	a	247	G	O3'-P-O5'	-5.21	96.18	104.00
51	a	840	U	O3'-P-O5'	-5.21	96.18	104.00
18	N	22	THR	CA-CB-OG1	-5.21	101.78	109.60
46	A	29	U	C3'-C2'-O2'	5.21	118.52	110.70
46	A	227	G	C4'-C3'-C2'	-5.21	97.39	102.60
11	E	97	TYR	N-CA-CB	-5.21	102.66	110.73
46	A	1390	C	C4'-C3'-C2'	-5.21	97.39	102.60
52	W	51	THR	CB-CA-C	5.20	119.53	112.09
46	A	2717	G	C1'-C2'-O2'	5.20	116.20	108.40
46	A	1694	G	O5'-C5'-C4'	-5.20	103.70	111.50
30	e	41	ASP	CA-CB-CG	5.20	117.80	112.60
46	A	366	A	C4'-C3'-O3'	5.20	117.19	109.40
46	A	1383	U	O3'-P-O5'	-5.20	96.20	104.00
8	B	76	A	C1'-C2'-O2'	5.20	116.19	108.40
46	A	469	A	O3'-P-O5'	-5.20	96.21	104.00
46	A	872	C	OP1-P-O3'	5.19	123.58	108.00
51	a	1232	C	C3'-C2'-O2'	5.19	118.49	110.70
46	A	1824	C	C4'-C3'-O3'	-5.19	105.21	113.00
51	a	1366	A	C1'-C2'-O2'	5.19	116.19	108.40
46	A	2026	A	C4'-C3'-O3'	-5.19	105.22	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	244	A	C4'-C3'-O3'	5.19	117.18	109.40
46	A	1513	U	O3'-P-O5'	-5.18	96.22	104.00
46	A	2079	C	O3'-P-O5'	-5.18	96.22	104.00
51	a	1403	A	C2'-C3'-O3'	5.18	117.27	109.50
5	4	5	PRO	N-CD-CG	-5.18	95.43	103.20
46	A	31	C	C2'-C3'-O3'	-5.18	105.93	113.70
46	A	228	C	C4'-C3'-C2'	-5.18	97.42	102.60
46	A	2374	G	O5'-C5'-C4'	-5.18	103.93	111.70
46	A	1826	C	C4'-C3'-O3'	-5.18	105.24	113.00
46	A	2753	U	C1'-C2'-O2'	-5.18	100.64	108.40
51	a	699	G	O3'-P-O5'	-5.18	96.23	104.00
8	B	37	A	C3'-C2'-O2'	5.17	118.46	110.70
51	a	1066	U	C2'-C3'-O3'	-5.17	105.94	113.70
51	a	21	C	C4'-C3'-O3'	-5.17	105.24	113.00
46	A	1416	G	C4'-C3'-O3'	-5.17	105.24	113.00
46	A	2375	A	C2'-C3'-O3'	5.17	117.26	109.50
46	A	630	A	O3'-P-O5'	-5.17	96.25	104.00
46	A	2375	A	O5'-P-OP1	-5.17	92.50	108.00
46	A	2756	G	C3'-C2'-O2'	5.17	118.45	110.70
47	b	25	PRO	N-CA-C	5.17	123.11	112.47
46	A	2739	C	O3'-P-O5'	-5.16	96.26	104.00
51	a	1162	G	O3'-P-O5'	-5.16	96.26	104.00
46	A	480	C	O3'-P-O5'	-5.16	96.26	104.00
46	A	720	C	O3'-P-O5'	-5.16	96.26	104.00
46	A	605	G	C4'-C3'-O3'	-5.16	105.26	113.00
46	A	1336	C	O3'-P-O5'	-5.16	96.27	104.00
46	A	1721	A	C2'-C3'-O3'	-5.16	105.97	113.70
8	B	96	G	O3'-P-O5'	-5.15	96.27	104.00
46	A	525	A	C4'-C3'-O3'	-5.15	105.27	113.00
46	A	2434	G	OP1-P-O3'	5.15	123.46	108.00
51	a	382	A	O3'-P-O5'	-5.15	96.27	104.00
46	A	2765	G	C1'-C2'-O2'	5.15	116.13	108.40
46	A	2852	U	O3'-P-O5'	-5.15	96.28	104.00
46	A	1424	A	C3'-C2'-C1'	-5.15	96.35	101.50
24	T	75	ARG	CB-CA-C	5.15	118.45	109.65
46	A	512	G	O3'-P-O5'	-5.15	96.28	104.00
46	A	2106	A	C4'-C3'-O3'	-5.15	105.28	113.00
46	A	2459	A	C1'-O4'-C4'	-5.15	104.55	109.70
46	A	5	A	O3'-P-O5'	-5.14	96.28	104.00
51	a	630	A	O3'-P-O5'	-5.14	96.29	104.00
46	A	245	G	C2'-C3'-O3'	5.14	117.21	109.50
51	a	1438	C	C3'-C2'-O2'	5.14	118.41	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	417	G	O3'-P-O5'	-5.14	96.30	104.00
46	A	1966	A	O3'-P-O5'	-5.13	96.30	104.00
46	A	2248	G	O3'-P-O5'	-5.13	96.30	104.00
46	A	2771	G	O4'-C4'-C3'	-5.13	98.87	104.00
46	A	2237	C	O3'-P-O5'	-5.13	96.30	104.00
51	a	1006	A	O3'-P-O5'	-5.13	96.30	104.00
46	A	2121	U	P-O3'-C3'	5.13	127.90	120.20
51	a	1065	A	O3'-P-O5'	-5.13	96.30	104.00
46	A	468	C	O3'-P-O5'	-5.13	96.31	104.00
46	A	1020	A	C2'-C3'-O3'	5.13	117.19	109.50
46	A	1168	G	O3'-P-O5'	-5.13	96.31	104.00
51	a	324	C	O3'-P-O5'	-5.13	96.31	104.00
8	B	77	G	O3'-P-O5'	-5.13	96.31	104.00
46	A	1940	U	O3'-P-O5'	-5.13	96.31	104.00
46	A	2049	A	C4'-C3'-O3'	-5.13	105.31	113.00
50	9	21	A	P-O3'-C3'	5.13	127.89	120.20
45	v	28	C	O3'-P-O5'	-5.12	96.31	104.00
51	a	886	A	O3'-P-O5'	-5.12	96.31	104.00
46	A	989	U	O3'-P-O5'	-5.12	96.31	104.00
46	A	1817	C	C1'-C2'-O2'	-5.12	100.71	108.40
51	a	815	C	O3'-P-O5'	-5.12	96.31	104.00
46	A	2476	G	C2'-C3'-O3'	5.12	117.18	109.50
46	A	2907	A	O3'-P-O5'	-5.12	96.32	104.00
51	a	152	C	O3'-P-O5'	-5.12	96.32	104.00
51	a	1114	G	O3'-P-O5'	-5.12	96.32	104.00
46	A	508	C	O3'-P-O5'	-5.12	96.32	104.00
8	B	46	A	O3'-P-O5'	-5.12	96.32	104.00
46	A	2077	G	C4'-C3'-O3'	-5.12	105.32	113.00
46	A	1694	G	C4'-C3'-O3'	-5.12	105.32	113.00
46	A	1864	G	C4'-C3'-O3'	-5.12	105.32	113.00
51	a	1530	G	C4'-C3'-O3'	-5.11	105.33	113.00
46	A	1801	G	C1'-C2'-O2'	5.11	116.07	108.40
46	A	1831	A	O3'-P-O5'	-5.11	96.33	104.00
46	A	2540	U	C4'-C3'-C2'	-5.11	97.49	102.60
51	a	384	G	O3'-P-O5'	-5.11	96.34	104.00
46	A	1232	G	C4'-C3'-O3'	-5.11	105.34	113.00
46	A	490	A	C2'-C3'-O3'	-5.11	106.04	113.70
46	A	1067	A	O3'-P-O5'	-5.11	96.34	104.00
46	A	2296	A	O4'-C1'-N9	-5.11	100.84	108.50
46	A	2341	U	O3'-P-O5'	-5.10	96.34	104.00
8	B	44	A	O3'-P-O5'	-5.10	96.34	104.00
51	a	991	U	O3'-P-O5'	-5.10	96.35	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	516	G	O3'-P-O5'	-5.10	96.35	104.00
46	A	2030	A	O3'-P-O5'	-5.10	96.35	104.00
51	a	830	G	O3'-P-O5'	-5.10	96.35	104.00
46	A	202	A	C1'-O4'-C4'	-5.09	104.61	109.70
46	A	847	A	O3'-P-O5'	-5.09	96.36	104.00
46	A	2818	C	C1'-O4'-C4'	-5.09	104.81	109.90
46	A	2011	U	O3'-P-O5'	-5.09	96.36	104.00
51	a	16	U	O3'-P-O5'	-5.09	96.36	104.00
46	A	2600	U	C4'-C3'-O3'	-5.09	105.37	113.00
46	A	757	C	O3'-P-O5'	-5.09	96.37	104.00
46	A	2322	C	O3'-P-O5'	-5.09	96.37	104.00
46	A	578	A	O5'-C5'-C4'	-5.09	104.07	111.70
46	A	1794	C	O3'-P-O5'	-5.09	96.37	104.00
46	A	2048	U	C4'-C3'-O3'	-5.09	105.37	113.00
46	A	952	A	C4'-C3'-C2'	-5.08	97.52	102.60
46	A	622	A	O3'-P-O5'	-5.08	96.37	104.00
46	A	632	U	O3'-P-O5'	-5.08	96.38	104.00
46	A	864	C	C4'-C3'-C2'	-5.08	97.52	102.60
46	A	988	G	C3'-C2'-O2'	5.08	118.32	110.70
46	A	2663	A	C4'-C3'-O3'	-5.08	105.38	113.00
46	A	466	C	C2'-C3'-O3'	5.08	121.32	113.70
46	A	1014	A	C3'-C2'-O2'	5.08	118.32	110.70
51	a	1241	U	O3'-P-O5'	-5.08	96.39	104.00
46	A	912	C	O3'-P-O5'	-5.07	96.39	104.00
46	A	2393	C	C3'-C2'-O2'	5.07	118.31	110.70
51	a	126	G	O3'-P-O5'	-5.07	96.39	104.00
46	A	833	C	O3'-P-O5'	-5.07	96.40	104.00
46	A	1683	C	C2'-C3'-O3'	-5.07	106.10	113.70
51	a	1432	G	O3'-P-O5'	-5.07	96.40	104.00
46	A	2316	A	O3'-P-O5'	-5.07	96.40	104.00
46	A	1568	G	C4'-C3'-O3'	-5.06	105.40	113.00
51	a	1426	G	O3'-P-O5'	-5.06	96.40	104.00
46	A	255	G	O3'-P-O5'	-5.06	96.41	104.00
46	A	2376	C	C2'-C3'-O3'	-5.06	106.11	113.70
46	A	2646	C	O3'-P-O5'	-5.06	96.41	104.00
46	A	2090	G	O3'-P-O5'	-5.06	96.41	104.00
46	A	6	A	C1'-C2'-O2'	5.06	115.99	108.40
46	A	194	A	C4'-C3'-C2'	-5.06	97.54	102.60
46	A	57	C	C4'-C3'-O3'	-5.05	105.42	113.00
46	A	199	A	C4'-C3'-O3'	5.05	116.98	109.40
46	A	1840	G	C1'-C2'-O2'	5.05	115.98	108.40
46	A	2738	G	C1'-C2'-O2'	5.05	115.98	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	a	984	A	C2'-C3'-O3'	5.05	117.08	109.50
46	A	1168	G	C1'-C2'-O2'	5.05	115.98	108.40
46	A	72	U	C3'-C2'-C1'	-5.05	96.45	101.50
46	A	691	U	O4'-C1'-C2'	-5.05	102.55	107.60
46	A	2766	G	C4'-C3'-C2'	-5.05	97.55	102.60
51	a	436	G	O4'-C1'-C2'	-5.05	100.75	105.80
46	A	2479	A	C4'-C3'-C2'	-5.05	97.55	102.60
46	A	2614	U	OP1-P-O3'	5.04	123.14	108.00
46	A	1853	G	C1'-C2'-O2'	5.04	115.97	108.40
51	a	735	C	C3'-C2'-O2'	5.04	118.27	110.70
46	A	2478	U	C2'-C3'-O3'	5.04	117.06	109.50
46	A	2420	G	C1'-O4'-C4'	-5.04	104.66	109.70
14	J	2	ARG	CB-CA-C	5.04	119.67	110.10
46	A	621	G	C2'-C3'-O3'	5.04	121.26	113.70
46	A	1659	A	C4'-C3'-O3'	-5.04	105.44	113.00
46	A	2003	C	O3'-P-O5'	-5.04	96.44	104.00
46	A	2322	C	C3'-C2'-O2'	5.04	118.26	110.70
51	a	1077	A	C1'-C2'-O2'	-5.04	104.25	111.80
46	A	1631	A	P-O3'-C3'	5.03	127.75	120.20
51	a	761	G	O3'-P-O5'	-5.03	96.45	104.00
51	a	132	U	O3'-P-O5'	-5.03	96.46	104.00
46	A	608	C	C1'-C2'-O2'	5.03	115.94	108.40
46	A	2807	A	C2'-C3'-O3'	5.03	117.04	109.50
46	A	2697	G	O3'-P-O5'	-5.03	96.46	104.00
46	A	779	C	O3'-P-O5'	-5.02	96.46	104.00
46	A	1836	G	O3'-P-O5'	-5.02	96.46	104.00
46	A	2848	A	O3'-P-O5'	-5.02	96.47	104.00
51	a	1203	U	O3'-P-O5'	-5.02	96.47	104.00
46	A	795	G	C1'-O4'-C4'	-5.02	104.88	109.90
46	A	1196	C	O3'-P-O5'	-5.02	96.47	104.00
46	A	2104	U	C4'-C3'-O3'	-5.02	105.47	113.00
46	A	2662	A	C2'-C3'-O3'	5.02	121.23	113.70
46	A	1779	G	C4'-C3'-O3'	-5.01	105.48	113.00
51	a	337	A	O3'-P-O5'	-5.01	96.48	104.00
46	A	118	A	O3'-P-O5'	-5.01	96.48	104.00
8	B	45	C	C4'-C3'-O3'	-5.01	105.49	113.00
46	A	1746	A	O3'-P-O5'	-5.00	96.49	104.00
11	E	64	PRO	CB-CA-C	-5.00	103.94	112.64
34	i	111	LYS	CB-CA-C	5.00	118.50	110.29
51	a	306	A	O3'-P-O5'	-5.00	96.50	104.00

There are no chirality outliers.

All (53) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	20	PHE	Peptide
1	0	41	ARG	Sidechain
1	0	6	ARG	Sidechain
3	2	12	ARG	Sidechain
3	2	28	ARG	Sidechain
46	A	2296	A	Sidechain
46	A	512	G	Sidechain
46	A	558	G	Sidechain
9	C	13	ARG	Sidechain
9	C	14	ARG	Sidechain
9	C	189	ARG	Sidechain
9	C	238	ARG	Sidechain
9	C	274	ARG	Sidechain
9	C	43	ARG	Sidechain
9	C	52	ARG	Sidechain
10	D	138	ARG	Sidechain
13	G	36	ARG	Sidechain
14	J	2	ARG	Peptide
14	J	38	ARG	Sidechain
14	J	77	ARG	Sidechain
16	L	53	GLY	Peptide
16	L	64	ARG	Peptide
16	L	71	ARG	Sidechain
17	M	18	ARG	Sidechain
18	N	107	ARG	Sidechain
19	O	14	ARG	Sidechain
19	O	17	ARG	Sidechain
19	O	30	ARG	Sidechain
19	O	35	ARG	Sidechain
20	P	21	ARG	Sidechain
20	P	51	ARG	Sidechain
20	P	94	ARG	Sidechain
21	Q	58	ARG	Sidechain
21	Q	74	LEU	Peptide
23	S	41	ARG	Sidechain
25	U	32	ARG	Sidechain
25	U	92	ARG	Sidechain
52	W	47	ARG	Sidechain
52	W	79	ARG	Sidechain
26	X	27	ARG	Sidechain
29	c	11	ARG	Sidechain
29	c	121	ARG	Sidechain

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Mol	Chain	Res	Type	Group
31	f	87	ARG	Sidechain
33	h	28	PRO	Peptide
34	i	109	ARG	Sidechain
34	i	130	ARG	Sidechain
35	j	53	ARG	Sidechain
35	j	62	ARG	Sidechain
36	k	79	HIS	Peptide
38	m	107	ARG	Sidechain
39	n	12	ARG	Sidechain
39	n	22	THR	Peptide
39	n	41	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	425	0	441	5	0
2	1	403	0	414	4	0
3	2	368	0	410	0	0
4	3	512	0	564	2	0
5	4	297	0	339	2	0
6	5	346	0	345	2	0
7	6	356	0	346	1	0
8	B	2392	0	1213	1	0
9	C	2093	0	2179	16	0
10	D	1575	0	1642	16	0
11	E	1567	0	1652	7	0
12	F	1405	0	1467	2	0
13	G	1342	0	1388	3	0
14	J	1142	0	1182	10	0
15	K	921	0	977	8	0
16	L	1082	0	1132	4	0
17	M	1076	0	1145	3	0
18	N	954	0	983	8	0
19	O	913	0	947	4	0
20	P	933	0	1004	2	0
21	Q	950	0	1018	8	0
22	R	789	0	833	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	S	850	0	911	8	0
24	T	733	0	781	2	0
25	U	770	0	825	2	0
26	X	467	0	512	2	0
27	Y	540	0	581	0	0
28	Z	456	0	491	2	0
29	c	1608	0	1646	1	0
30	e	1219	0	1300	3	0
31	f	765	0	765	1	0
32	g	1199	0	1256	5	0
33	h	1030	0	1086	1	0
34	i	997	0	1033	4	0
35	j	779	0	821	3	0
36	k	847	0	860	2	0
37	l	1036	0	1091	1	0
38	m	943	0	1008	1	0
39	n	498	0	529	2	0
40	o	730	0	759	1	0
41	p	691	0	718	5	0
42	q	693	0	734	0	0
43	r	522	0	558	0	0
44	t	658	0	715	0	0
45	v	1622	0	820	1	0
46	A	58523	0	29464	179	0
47	b	1564	0	1625	5	0
48	s	668	0	682	3	0
49	7	189	0	95	1	0
50	9	1581	0	804	2	0
51	a	32891	0	16559	79	0
52	W	639	0	652	2	0
53	d	1604	0	1638	5	0
54	0	1	0	0	0	0
54	4	1	0	0	0	0
54	6	1	0	0	0	0
54	n	1	0	0	0	0
All	All	139157	0	92940	378	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (378) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:A:1808:U:H5	46:A:1813:A:N7	1.80	0.80
46:A:1709:A:H61	46:A:2025:C:H5	1.32	0.75
46:A:1411:U:HO2'	46:A:2241:A:H8	1.37	0.69
32:g:148:ASN:HD22	36:k:58:ARG:HH22	1.44	0.65
51:a:437:U:H3'	53:d:9:TRP:CD2	2.31	0.64
46:A:2229:C:O2	46:A:2255:C:N4	2.30	0.64
46:A:957:A:H2'	46:A:958:A:C8	2.31	0.64
51:a:1444:G:H2'	51:a:1445:U:C6	2.34	0.62
32:g:10:ARG:NH1	51:a:1385:U:O4	2.36	0.59
14:J:38:ARG:HH11	46:A:1053:C:H5''	1.67	0.59
18:N:59:ARG:HA	18:N:84:PHE:CZ	2.37	0.59
23:S:51:LEU:HA	23:S:105:ILE:HG21	1.84	0.58
47:b:186:ILE:HG23	47:b:202:ALA:HB3	1.84	0.58
46:A:2467:U:O3'	46:A:2468:A:H3'	2.03	0.58
51:a:955:G:C2	51:a:956:A:C8	2.92	0.58
46:A:45:G:H21	46:A:183:A:H61	1.50	0.57
26:X:23:ASN:ND2	46:A:2108:U:O2'	2.33	0.57
46:A:831:U:H5	46:A:840:A:N1	2.02	0.57
6:5:101:VAL:HG21	46:A:793:U:O2'	2.04	0.57
10:D:185:LEU:HD11	20:P:4:LEU:HD11	1.86	0.57
46:A:1681:U:H2'	46:A:1682:C:C6	2.39	0.56
13:G:118:PRO:HG3	13:G:124:ILE:HD12	1.86	0.56
51:a:1113:C:H2'	51:a:1114:G:O4'	2.05	0.56
23:S:29:VAL:HG22	23:S:51:LEU:HD11	1.88	0.56
10:D:14:GLN:NE2	10:D:22:LEU:HD21	2.21	0.56
46:A:1819:C:H2'	46:A:1820:A:C5	2.41	0.56
51:a:1201:C:H2'	51:a:1202:G:O4'	2.04	0.56
46:A:1808:U:C5	46:A:1813:A:N7	2.70	0.55
1:0:11:VAL:HG22	46:A:17:G:H5''	1.87	0.55
48:s:36:ARG:NH2	48:s:75:ALA:O	2.37	0.55
46:A:2715:G:C6	46:A:2716:U:N3	2.74	0.55
51:a:1380:G:C6	51:a:1381:U:C4	2.95	0.55
9:C:6:TYR:CZ	9:C:18:THR:HG21	2.42	0.54
51:a:224:U:H2'	51:a:225:A:C8	2.42	0.54
46:A:576:G:N3	46:A:576:G:H2'	2.22	0.54
46:A:2715:G:C5	46:A:2716:U:C4	2.95	0.54
51:a:1072:U:H2'	51:a:1073:C:C6	2.42	0.54
51:a:52:A:O2'	51:a:368:G:N2	2.40	0.54
46:A:2554:G:O2'	46:A:2771:G:O2'	2.10	0.54
41:p:6:ARG:HB2	51:a:384:G:H5''	1.91	0.53
46:A:1542:A:O2'	46:A:1544:C:N4	2.42	0.53
51:a:674:A:H1'	51:a:742:G:O4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:a:985:A:N1	51:a:1375:C:O2'	2.36	0.53
10:D:139:TYR:OH	10:D:144:GLY:N	2.40	0.53
51:a:778:G:H4'	51:a:1523:A:H4'	1.90	0.53
51:a:1305:C:H4'	51:a:1311:U:O4	2.08	0.53
51:a:1379:G:C2	51:a:1380:G:C8	2.97	0.53
9:C:87:ARG:NH2	46:A:1846:G:OP1	2.41	0.53
46:A:704:U:H2'	46:A:705:A:C8	2.43	0.53
2:1:9:CYS:SG	2:1:12:CYS:SG	3.07	0.53
9:C:78:VAL:HG22	9:C:94:ILE:CD1	2.39	0.53
51:a:1060:G:C2	51:a:1061:G:C8	2.97	0.53
23:S:82:LEU:HB2	23:S:98:LYS:HB2	1.91	0.53
46:A:903:G:H2'	46:A:904:A:C8	2.43	0.53
46:A:2785:U:H5	46:A:2787:A:N7	2.07	0.52
51:a:1084:G:O2'	51:a:1111:A:N1	2.38	0.52
51:a:1411:C:O2	51:a:1510:A:N1	2.42	0.52
46:A:2092:C:O2	46:A:2479:A:N1	2.42	0.52
21:Q:58:ARG:HA	21:Q:61:TRP:CE3	2.45	0.52
35:j:56:HIS:O	35:j:57:LYS:HG2	2.10	0.52
46:A:2686:A:H1'	46:A:2694:A:N6	2.24	0.52
5:4:19:ARG:NE	46:A:2785:U:OP2	2.38	0.52
10:D:17:ALA:HB2	10:D:23:ILE:HD11	1.92	0.52
46:A:1825:U:H2'	46:A:1826:C:C6	2.45	0.52
32:g:10:ARG:NH2	51:a:1355:A:O2'	2.43	0.52
46:A:1047:A:H2'	46:A:1048:G:O4'	2.09	0.52
46:A:2710:C:C5	46:A:2753:U:C5	2.98	0.52
11:E:109:ALA:HB1	11:E:183:VAL:HG21	1.92	0.52
23:S:20:VAL:HG21	23:S:43:ALA:HB3	1.92	0.51
24:T:55:ASN:HD22	46:A:1381:A:H5'	1.75	0.51
46:A:2062:A:H4'	46:A:2063:U:OP1	2.09	0.51
46:A:1379:U:C5	46:A:1648:A:C8	2.98	0.51
29:c:137:ILE:HD11	29:c:150:THR:HG23	1.93	0.51
46:A:2487:U:O2'	46:A:2489:U:O4	2.28	0.51
48:s:36:ARG:HB2	51:a:1329:C:N3	2.26	0.51
46:A:1961:A:H2'	46:A:1962:G:O4'	2.11	0.50
51:a:63:G:H2'	51:a:64:U:O4'	2.12	0.50
46:A:247:A:C2	46:A:258:A:C4	3.00	0.50
47:b:96:TRP:CH2	47:b:100:THR:HG21	2.46	0.50
46:A:1444:C:H2'	46:A:1445:A:C8	2.46	0.50
40:o:29:ILE:HG21	40:o:81:LEU:HD21	1.94	0.50
9:C:220:VAL:HG21	46:A:829:A:C8	2.45	0.50
9:C:105:LEU:HD11	9:C:156:ARG:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:126:HIS:CD2	10:D:159:LEU:HB3	2.47	0.50
46:A:1363:G:C6	46:A:1367:G:C6	3.00	0.50
46:A:1426:A:H2'	46:A:1427:G:O4'	2.11	0.50
33:h:77:LEU:O	33:h:130:TYR:O	2.29	0.49
46:A:1485:A:H2	46:A:1600:G:H21	1.60	0.49
46:A:1755:C:O2'	46:A:2883:C:N3	2.44	0.49
18:N:24:LEU:HD23	18:N:44:VAL:HG21	1.94	0.49
18:N:58:ALA:O	18:N:59:ARG:C	2.55	0.49
31:f:10:ILE:HD13	31:f:84:ASP:HB3	1.94	0.49
51:a:381:A:C2	51:a:382:A:C8	3.00	0.49
46:A:2402:A:H2'	46:A:2403:C:C6	2.47	0.49
9:C:41:GLY:O	9:C:43:ARG:NH2	2.45	0.49
13:G:38:PHE:CD1	13:G:69:THR:HG23	2.48	0.49
1:0:54:ILE:HD12	18:N:102:MET:HE3	1.93	0.49
9:C:65:ILE:HB	9:C:67:PHE:CE2	2.48	0.49
15:K:85:VAL:HG11	15:K:114:ILE:HD12	1.95	0.48
46:A:747:G:O2'	46:A:1677:A:N3	2.42	0.48
46:A:2235:G:C6	46:A:2236:C:C4	3.01	0.48
13:G:8:LEU:HD13	13:G:50:VAL:HG13	1.95	0.48
15:K:75:SER:OG	20:P:72:ARG:NH2	2.46	0.48
1:0:38:LEU:HG	23:S:38:LEU:HD22	1.95	0.48
25:U:64:HIS:CE1	25:U:66:SER:HG	2.31	0.48
46:A:777:C:OP2	46:A:778:C:OP2	2.31	0.48
17:M:119:ARG:NH2	46:A:2497:A:OP1	2.47	0.48
51:a:438:A:H5''	53:d:7:PRO:HA	1.96	0.48
9:C:63:ARG:NH2	46:A:1616:G:OP2	2.47	0.48
46:A:866:A:C4	46:A:1230:A:C2	3.02	0.48
46:A:1327:U:H5	46:A:1365:U:O2	1.97	0.48
51:a:527:C:H2'	51:a:539:G:C8	2.49	0.48
46:A:352:G:H2'	46:A:353:A:C8	2.49	0.48
24:T:11:PRO:HG2	24:T:13:ILE:HD11	1.95	0.48
46:A:790:A:O2'	46:A:1704:U:OP1	2.24	0.48
16:L:21:ARG:HA	46:A:858:U:H2'	1.96	0.47
18:N:40:LEU:HD23	18:N:117:ILE:HD13	1.95	0.47
41:p:7:LEU:HD12	51:a:383:U:H5''	1.96	0.47
46:A:248:G:O2'	46:A:431:A:N1	2.40	0.47
46:A:2315:A:H4'	46:A:2316:A:O4'	2.14	0.47
51:a:19:U:H2'	51:a:20:C:C6	2.48	0.47
51:a:412:G:N7	53:d:2:ALA:N	2.62	0.47
51:a:649:A:C6	51:a:650:A:C6	3.03	0.47
9:C:157:SER:O	9:C:158:ALA:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:18:VAL:HG23	14:J:138:PRO:HB2	1.96	0.47
46:A:685:U:H2'	46:A:686:C:C6	2.49	0.47
46:A:2291:U:H4'	46:A:2357:A:C2	2.50	0.47
46:A:2343:A:H2'	46:A:2344:U:C6	2.49	0.47
51:a:1187:G:N2	51:a:1189:A:H3'	2.29	0.47
46:A:1308:A:C2	46:A:2042:A:C4	3.03	0.47
46:A:2715:G:C6	46:A:2716:U:C4	3.03	0.47
14:J:44:THR:O	14:J:45:TYR:C	2.56	0.47
25:U:10:MET:HB2	25:U:71:LEU:HD21	1.97	0.47
46:A:1759:U:HO2'	46:A:1760:A:H8	1.63	0.47
9:C:225:MET:HE2	46:A:829:A:C6	2.49	0.47
18:N:62:ALA:HB3	18:N:80:LEU:HD11	1.97	0.47
22:R:14:VAL:HB	22:R:97:ILE:HG13	1.96	0.47
46:A:2752:C:N4	46:A:2753:U:C4	2.83	0.47
51:a:1234:A:N3	51:a:1235:C:C5	2.82	0.47
51:a:1365:G:H2'	51:a:1366:A:C8	2.50	0.47
10:D:107:ILE:CG2	10:D:173:ASN:HA	2.45	0.47
14:J:36:ILE:HD11	14:J:141:TYR:CZ	2.50	0.47
46:A:469:A:C6	46:A:470:A:C6	3.03	0.47
51:a:1475:C:H2'	51:a:1476:C:O4'	2.15	0.47
46:A:340:U:H2'	46:A:341:G:O4'	2.15	0.47
46:A:1844:A:OP1	46:A:1851:G:H4'	2.14	0.47
46:A:2321:U:H2'	46:A:2322:C:O4'	2.15	0.47
46:A:614:G:H2'	46:A:2059:A:N7	2.30	0.47
46:A:2767:A:N1	46:A:2768:U:C2	2.82	0.47
47:b:39:TYR:HB2	47:b:189:THR:HG21	1.96	0.47
37:l:79:TYR:CG	37:l:100:VAL:HG21	2.50	0.46
46:A:1203:G:H5'	46:A:1203:G:C8	2.49	0.46
46:A:1311:G:OP2	46:A:1693:C:OP1	2.33	0.46
14:J:46:THR:HB	14:J:49:VAL:HG12	1.98	0.46
46:A:2752:C:C4	46:A:2753:U:C5	3.03	0.46
46:A:1303:U:C4	46:A:1304:G:C6	3.03	0.46
16:L:58:PHE:CD2	16:L:58:PHE:C	2.93	0.46
46:A:2048:U:H2'	46:A:2049:A:O5'	2.15	0.46
46:A:2767:A:C2	46:A:2768:U:H1'	2.50	0.46
48:s:19:ILE:HG21	48:s:44:PHE:CD1	2.51	0.46
46:A:2726:G:C2	46:A:2740:A:C2	3.04	0.46
10:D:153:ARG:HA	46:A:2081:G:N3	2.30	0.46
23:S:7:ALA:HB2	23:S:50:VAL:HG22	1.98	0.46
46:A:1096:A:C2	46:A:2780:G:C4	3.04	0.46
46:A:1366:C:H2'	46:A:1367:G:O4'	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:A:2319:G:C5	46:A:2320:U:C5	3.04	0.46
46:A:2291:U:H4'	46:A:2357:A:H2	1.81	0.46
46:A:2785:U:C5	46:A:2787:A:N7	2.84	0.46
10:D:13:THR:OG1	10:D:14:GLN:N	2.49	0.46
14:J:29:LEU:HD21	14:J:57:ILE:HD13	1.98	0.46
46:A:2309:G:C6	46:A:2310:C:C5	3.04	0.46
41:p:22:VAL:HG11	41:p:59:TRP:CD2	2.51	0.45
46:A:632:U:H2'	46:A:633:U:C6	2.51	0.45
46:A:2362:A:C5'	46:A:2364:A:H1'	2.46	0.45
51:a:271:A:H2'	51:a:272:C:C6	2.51	0.45
51:a:1531:G:C2	51:a:1532:U:C2	3.04	0.45
7:6:27:VAL:HG21	12:F:59:PHE:HA	1.97	0.45
15:K:22:ILE:HG23	46:A:1981:A:C2	2.51	0.45
32:g:26:LEU:HD22	32:g:62:PHE:CZ	2.51	0.45
34:i:130:ARG:NH2	45:v:33:U:OP2	2.46	0.45
4:3:4:MET:HE1	4:3:60:GLN:HE21	1.81	0.45
10:D:59:LYS:NZ	46:A:2857:U:OP1	2.34	0.45
46:A:1411:U:O2'	46:A:2241:A:H8	1.96	0.45
46:A:831:U:O2	46:A:831:U:O4'	2.35	0.45
46:A:1304:G:C6	46:A:1305:A:N6	2.85	0.45
47:b:110:ARG:HB3	47:b:148:LEU:HD11	1.99	0.45
52:W:42:GLY:O	52:W:43:SER:C	2.60	0.45
10:D:29:GLU:HA	10:D:185:LEU:HD23	1.99	0.45
46:A:2733:C:C4	46:A:2734:A:C5	3.04	0.45
46:A:2769:A:C6	46:A:2770:A:C6	3.05	0.45
51:a:959:A:C4	51:a:1242:G:N2	2.85	0.45
51:a:1067:G:C4	51:a:1213:A:C2	3.05	0.45
30:e:21:VAL:HG11	51:a:1090:A:C5'	2.47	0.45
15:K:43:VAL:HG21	15:K:52:VAL:HG12	1.98	0.45
16:L:79:LEU:HG	16:L:113:GLY:HA2	1.99	0.45
46:A:227:G:C6	46:A:228:C:C5	3.05	0.45
46:A:1074:A:N6	46:A:1171:G:H2'	2.32	0.45
50:9:8:U:O2	50:9:8:U:O4'	2.35	0.45
11:E:131:LEU:HD21	11:E:142:ILE:HD12	1.99	0.45
46:A:2769:A:C2	46:A:2770:A:C4	3.04	0.45
41:p:20:ILE:N	41:p:38:GLY:O	2.49	0.45
9:C:158:ALA:O	46:A:1849:U:O2'	2.32	0.44
10:D:160:LEU:HB3	10:D:161:PRO:CD	2.47	0.44
11:E:113:VAL:HG12	11:E:186:VAL:HG11	1.98	0.44
18:N:108:ARG:NH2	46:A:1366:C:O3'	2.50	0.44
35:j:56:HIS:ND1	35:j:56:HIS:C	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:A:227:G:C6	46:A:228:C:C4	3.05	0.44
11:E:139:MET:HG2	11:E:167:ALA:HB2	2.00	0.44
21:Q:94:MET:O	21:Q:95:LEU:C	2.60	0.44
41:p:22:VAL:HG11	41:p:59:TRP:CE3	2.53	0.44
51:a:69:C:H2'	51:a:70:G:C8	2.52	0.44
46:A:840:A:OP2	46:A:2101:G:H5'	2.17	0.44
46:A:1396:C:H2'	46:A:1397:G:O4'	2.17	0.44
46:A:2055:U:H2'	46:A:2056:G:O4'	2.17	0.44
35:j:50:THR:HG23	35:j:64:GLN:HG2	2.00	0.44
46:A:661:A:O5'	46:A:661:A:H8	2.01	0.44
46:A:1419:G:C2	46:A:1420:G:C8	3.06	0.44
46:A:1424:A:C4	46:A:1425:C:C5	3.05	0.44
51:a:447:U:C5	51:a:448:U:C6	3.06	0.44
14:J:32:GLU:OE1	14:J:144:ARG:N	2.51	0.44
19:O:35:ARG:HH11	19:O:35:ARG:HG2	1.82	0.44
46:A:1527:C:H3'	46:A:1528:U:H5''	1.99	0.44
46:A:578:A:H2'	46:A:578:A:N3	2.33	0.44
46:A:1756:U:C4	46:A:1757:G:C5	3.05	0.44
46:A:1895:A:C2	46:A:1905:A:C4	3.06	0.44
46:A:790:A:H2'	46:A:791:C:O4'	2.18	0.43
46:A:1515:C:H2'	46:A:1569:A:H61	1.83	0.43
46:A:2300:G:OP1	52:W:26:ALA:HB1	2.16	0.43
46:A:2723:G:C5	46:A:2724:U:C5	3.06	0.43
46:A:2895:C:C4	46:A:2896:U:C4	3.05	0.43
51:a:1514:G:H4'	51:a:1515:G:C4	2.53	0.43
1:0:18:THR:HG22	46:A:15:G:H4'	2.00	0.43
15:K:66:LYS:HA	15:K:79:PHE:O	2.18	0.43
34:i:65:VAL:HG11	34:i:79:ILE:HG12	2.00	0.43
46:A:2871:G:H2'	46:A:2872:U:C6	2.54	0.43
14:J:45:TYR:CD2	21:Q:63:THR:HG21	2.54	0.43
14:J:54:HIS:HA	14:J:122:LYS:HB3	2.01	0.43
46:A:150:A:H61	46:A:179:A:H2	1.63	0.43
46:A:2231:C:O2'	46:A:2233:C:OP1	2.31	0.43
2:1:6:THR:HG23	2:1:48:THR:HB	2.00	0.43
34:i:18:ARG:NH1	51:a:1156:C:O2	2.51	0.43
46:A:742:G:OP1	46:A:1419:G:O2'	2.35	0.43
46:A:831:U:H5'	46:A:832:G:OP1	2.18	0.43
50:9:19:C:H3'	50:9:20:U:C5'	2.48	0.43
21:Q:74:LEU:HD23	21:Q:79:LEU:HD13	2.01	0.43
23:S:21:MET:CE	23:S:103:ILE:HG23	2.49	0.43
46:A:259:A:H2'	46:A:260:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:a:1318:G:C5	51:a:1338:G:C2	3.06	0.43
46:A:2438:G:C6	46:A:2439:G:C5	3.07	0.43
51:a:613:G:H2'	51:a:614:U:O4'	2.19	0.43
36:k:38:ASP:OD1	36:k:42:ASN:N	2.52	0.43
51:a:150:A:H2'	51:a:151:A:O4'	2.19	0.43
2:1:12:CYS:SG	2:1:36:CYS:SG	3.17	0.43
9:C:221:ARG:HH22	9:C:224:VAL:HG11	1.82	0.43
15:K:12:ASP:HA	15:K:97:ARG:O	2.18	0.43
46:A:796:A:N1	46:A:800:G:O2'	2.41	0.43
10:D:3:LYS:HB3	10:D:101:ILE:HD12	2.01	0.42
51:a:1093:U:H3'	51:a:1094:G:C8	2.54	0.42
53:d:94:LEU:HD23	53:d:114:VAL:CG1	2.49	0.42
15:K:23:LYS:NZ	46:A:2590:A:N3	2.61	0.42
46:A:2370:G:H2'	46:A:2371:C:O4'	2.19	0.42
46:A:1021:A:H1'	46:A:1036:A:C2	2.54	0.42
46:A:1349:G:H1'	46:A:1656:C:H5'	2.01	0.42
8:B:7:G:OP1	19:O:19:ARG:NH1	2.52	0.42
46:A:2875:A:C2	46:A:2876:A:C4	3.06	0.42
38:m:110:LYS:NZ	51:a:1235:C:O2'	2.51	0.42
46:A:2060:A:C6	46:A:2527:C:H1'	2.54	0.42
46:A:2621:G:H2'	46:A:2622:U:O4'	2.20	0.42
28:Z:13:ILE:HD11	46:A:1035:G:C8	2.54	0.42
39:n:3:LYS:HG3	51:a:1059:U:H2'	2.02	0.42
46:A:1055:A:N3	46:A:1199:C:O2'	2.48	0.42
51:a:536:G:C6	51:a:537:C:C5	3.07	0.42
51:a:673:G:H22	51:a:750:G:H1	1.67	0.42
51:a:1314:G:O2'	51:a:1315:A:H8	2.02	0.42
21:Q:76:TYR:CZ	21:Q:80:MET:HG3	2.55	0.42
30:e:21:VAL:HG11	51:a:1090:A:H5''	2.01	0.42
17:M:54:MET:HE1	17:M:104:PHE:CG	2.55	0.42
46:A:1028:C:O2	46:A:1028:C:O5'	2.37	0.42
46:A:2316:A:C5	46:A:2318:G:C8	3.07	0.42
51:a:579:G:C6	51:a:883:A:C2	3.08	0.42
51:a:774:G:C6	51:a:821:G:C4	3.08	0.42
9:C:180:GLU:OE1	46:A:1828:G:O2'	2.33	0.42
22:R:5:ILE:HD11	22:R:12:ILE:HD11	2.00	0.42
30:e:110:PRO:HG2	30:e:136:MET:HE3	2.02	0.42
46:A:1314:A:H4'	46:A:1315:G:OP1	2.20	0.42
49:7:406:U:H2'	49:7:407:U:O4'	2.20	0.42
17:M:68:ILE:HD13	17:M:103:LEU:HD22	2.01	0.42
46:A:2050:G:N3	46:A:2050:G:H2'	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:A:2319:G:C6	46:A:2320:U:C4	3.08	0.42
46:A:2768:U:C5	46:A:2792:G:C5	3.08	0.42
51:a:1166:A:C4	51:a:1190:G:C6	3.08	0.42
11:E:46:GLN:HG2	11:E:48:THR:HG23	2.02	0.41
11:E:126:LEU:HD11	11:E:129:LEU:HB2	2.02	0.41
28:Z:14:GLY:HA2	46:A:1015:G:O3'	2.20	0.41
46:A:247:A:C2	46:A:258:A:C5	3.08	0.41
46:A:1618:A:H2'	46:A:1619:A:C8	2.55	0.41
46:A:2235:G:C5	46:A:2236:C:C5	3.08	0.41
51:a:839:G:C6	51:a:840:U:C4	3.08	0.41
18:N:99:THR:O	46:A:2906:U:O2'	2.38	0.41
46:A:2302:A:H2'	46:A:2303:A:C8	2.55	0.41
9:C:13:ARG:HG2	9:C:13:ARG:HH11	1.84	0.41
10:D:17:ALA:HB2	10:D:23:ILE:CD1	2.51	0.41
21:Q:75:SER:O	21:Q:76:TYR:C	2.62	0.41
51:a:589:C:H2'	51:a:590:G:O4'	2.20	0.41
51:a:937:G:O2'	51:a:1513:A:N7	2.49	0.41
1:O:3:VAL:HG12	46:A:2044:A:C2	2.55	0.41
39:n:44:PHE:CZ	39:n:56:VAL:HG11	2.56	0.41
6:5:101:VAL:HG11	46:A:793:U:H1'	2.02	0.41
9:C:63:ARG:HH21	46:A:1616:G:P	2.44	0.41
46:A:652:A:N1	46:A:653:A:C2	2.89	0.41
46:A:784:C:H2'	46:A:785:C:O4'	2.21	0.41
46:A:2381:A:C4	46:A:2395:A:C2	3.09	0.41
46:A:2550:C:C4	46:A:2551:U:C4	3.08	0.41
46:A:2555:G:C6	46:A:2556:C:C4	3.08	0.41
46:A:2716:U:H6	46:A:2716:U:O5'	2.02	0.41
46:A:2766:G:C6	46:A:2767:A:C5	3.08	0.41
47:b:96:TRP:CZ2	47:b:100:THR:HB	2.55	0.41
2:1:17:TYR:OH	46:A:2376:C:O2'	2.29	0.41
4:3:27:ALA:O	4:3:29:THR:HG23	2.19	0.41
12:F:79:LEU:HD21	12:F:85:ILE:HG21	2.03	0.41
46:A:2839:C:C5	46:A:2840:C:C4	3.08	0.41
51:a:974:A:N3	51:a:979:A:O2'	2.52	0.41
46:A:1759:U:O2'	46:A:1760:A:H8	2.03	0.41
46:A:2555:G:C5	46:A:2556:C:C5	3.09	0.41
46:A:2879:G:C2	46:A:2889:A:C2	3.07	0.41
5:4:6:SER:OG	46:A:2496:C:OP1	2.33	0.41
14:J:100:LYS:O	14:J:101:MET:C	2.61	0.41
46:A:1830:G:H3'	46:A:1831:A:H5''	2.03	0.41
51:a:1234:A:N3	51:a:1234:A:H2'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:11:ARG:NH1	19:O:98:GLY:O	2.53	0.41
32:g:119:ARG:NH2	51:a:1249:U:OP1	2.54	0.41
46:A:613:U:O2'	46:A:1029:A:N1	2.48	0.41
46:A:1823:U:H2'	46:A:1824:C:C6	2.56	0.41
46:A:2558:G:H5'	46:A:2558:G:C8	2.55	0.41
51:a:724:A:H2'	51:a:725:A:C8	2.55	0.41
51:a:932:G:C6	51:a:933:A:C6	3.09	0.41
51:a:945:A:C2	51:a:946:C:C2	3.09	0.41
51:a:1004:A:C8	51:a:1225:A:H4'	2.55	0.41
51:a:1377:G:C6	51:a:1378:C:C5	3.09	0.41
23:S:74:ALA:CB	23:S:105:ILE:HD13	2.51	0.41
46:A:1874:G:H2'	46:A:1875:G:O4'	2.21	0.41
46:A:1883:A:H2'	46:A:1884:G:O4'	2.20	0.41
51:a:61:A:N3	51:a:61:A:H2'	2.36	0.41
51:a:363:C:C4	51:a:364:A:N7	2.89	0.41
51:a:1358:A:H1'	51:a:1383:A:N6	2.36	0.41
34:i:22:VAL:HG21	34:i:64:LEU:HD12	2.02	0.40
46:A:844:U:H2'	46:A:845:G:O4'	2.21	0.40
46:A:1634:U:C2	46:A:1635:G:C8	3.09	0.40
46:A:1983:G:O2'	46:A:1985:U:O4	2.33	0.40
46:A:2767:A:N6	46:A:2768:U:C4	2.89	0.40
51:a:536:G:O2'	51:a:544:A:N1	2.42	0.40
51:a:725:A:C6	51:a:726:C:C4	3.09	0.40
53:d:15:LEU:HD13	53:d:56:LYS:HA	2.02	0.40
9:C:145:GLU:HB2	9:C:188:CYS:HB3	2.02	0.40
10:D:191:ASN:HD22	46:A:2709:C:H1'	1.86	0.40
21:Q:15:LYS:O	21:Q:16:LYS:C	2.64	0.40
26:X:54:LEU:HD22	26:X:61:ARG:HD3	2.03	0.40
51:a:1197:A:H2'	51:a:1198:U:O4'	2.21	0.40
51:a:1227:C:H2'	51:a:1228:U:C6	2.56	0.40
51:a:1321:G:C2	51:a:1335:U:C2	3.09	0.40
10:D:52:GLY:HA3	10:D:77:LYS:HG3	2.03	0.40
46:A:1819:C:H2'	46:A:1820:A:C4	2.57	0.40
51:a:1359:A:C5	51:a:1360:U:C5	3.09	0.40
10:D:35:VAL:HG13	10:D:49:ILE:HG23	2.04	0.40
15:K:19:VAL:HG11	15:K:86:ILE:HD11	2.03	0.40
19:O:39:HIS:HA	19:O:68:THR:O	2.21	0.40
46:A:1245:G:N3	46:A:1245:G:O4'	2.55	0.40
46:A:1752:G:C2	46:A:1753:C:C2	3.09	0.40
46:A:1822:G:H2'	46:A:1823:U:O4'	2.22	0.40
46:A:2362:A:O4'	46:A:2364:A:C4	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:a:900:G:O2'	51:a:916:G:O6	2.37	0.40
51:a:1380:G:C5	51:a:1381:U:C4	3.09	0.40
11:E:34:PHE:CE2	16:L:8:PRO:HB3	2.57	0.40
21:Q:3:ARG:NH1	46:A:493:G:OP1	2.50	0.40
46:A:905:G:N3	46:A:2297:A:H2'	2.36	0.40
46:A:2665:U:H2'	46:A:2666:U:C6	2.57	0.40
51:a:40:G:N2	51:a:405:A:C4	2.90	0.40
51:a:549:G:H2'	51:a:550:G:O4'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	52/59 (88%)	47 (90%)	3 (6%)	2 (4%)	2	9
2	1	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
3	2	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
4	3	62/66 (94%)	56 (90%)	6 (10%)	0	100	100
5	4	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
6	5	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	6	44/66 (67%)	38 (86%)	6 (14%)	0	100	100
9	C	271/277 (98%)	253 (93%)	16 (6%)	2 (1%)	18	47
10	D	205/209 (98%)	188 (92%)	15 (7%)	2 (1%)	12	38
11	E	204/207 (99%)	187 (92%)	17 (8%)	0	100	100
12	F	176/179 (98%)	160 (91%)	14 (8%)	2 (1%)	11	36
13	G	173/179 (97%)	150 (87%)	21 (12%)	2 (1%)	10	34
14	J	142/145 (98%)	133 (94%)	8 (6%)	1 (1%)	18	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	K	120/122 (98%)	103 (86%)	17 (14%)	0	100	100
16	L	144/146 (99%)	134 (93%)	9 (6%)	1 (1%)	18	47
17	M	133/144 (92%)	129 (97%)	4 (3%)	0	100	100
18	N	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	7	25
19	O	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
20	P	112/115 (97%)	103 (92%)	7 (6%)	2 (2%)	6	23
21	Q	116/119 (98%)	110 (95%)	5 (4%)	1 (1%)	14	41
22	R	99/102 (97%)	94 (95%)	5 (5%)	0	100	100
23	S	108/113 (96%)	103 (95%)	3 (3%)	2 (2%)	6	22
24	T	89/95 (94%)	79 (89%)	10 (11%)	0	100	100
25	U	100/103 (97%)	91 (91%)	8 (8%)	1 (1%)	12	38
26	X	59/62 (95%)	55 (93%)	4 (7%)	0	100	100
27	Y	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
28	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
29	c	202/218 (93%)	180 (89%)	19 (9%)	3 (2%)	8	28
30	e	162/166 (98%)	153 (94%)	9 (6%)	0	100	100
31	f	91/95 (96%)	77 (85%)	14 (15%)	0	100	100
32	g	149/156 (96%)	135 (91%)	13 (9%)	1 (1%)	18	47
33	h	128/132 (97%)	116 (91%)	10 (8%)	2 (2%)	7	27
34	i	126/130 (97%)	112 (89%)	13 (10%)	1 (1%)	16	44
35	j	95/102 (93%)	86 (90%)	9 (10%)	0	100	100
36	k	113/131 (86%)	105 (93%)	8 (7%)	0	100	100
37	l	132/138 (96%)	123 (93%)	8 (6%)	1 (1%)	16	44
38	m	116/121 (96%)	105 (90%)	11 (10%)	0	100	100
39	n	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	25
40	o	85/89 (96%)	78 (92%)	7 (8%)	0	100	100
41	p	85/90 (94%)	73 (86%)	12 (14%)	0	100	100
42	q	82/87 (94%)	74 (90%)	7 (8%)	1 (1%)	10	34
43	r	63/79 (80%)	61 (97%)	1 (2%)	1 (2%)	7	27
44	t	84/88 (96%)	83 (99%)	1 (1%)	0	100	100
47	b	191/246 (78%)	172 (90%)	13 (7%)	6 (3%)	3	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	s	81/92 (88%)	74 (91%)	5 (6%)	2 (2%)	4	16
52	W	81/94 (86%)	77 (95%)	3 (4%)	1 (1%)	10	34
53	d	197/200 (98%)	176 (89%)	21 (11%)	0	100	100
All	All	5244/5556 (94%)	4806 (92%)	398 (8%)	40 (1%)	18	44

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	P	37	ARG
33	h	79	ARG
47	b	100	THR
47	b	154	MET
10	D	184	ASN
12	F	126	GLY
18	N	42	SER
34	i	109	ARG
42	q	57	ILE
9	C	158	ALA
13	G	21	ASP
16	L	29	LYS
23	S	12	ILE
47	b	98	GLY
52	W	65	ASP
1	0	45	ALA
1	0	49	TYR
13	G	56	PRO
18	N	10	SER
23	S	9	THR
25	U	74	LYS
29	c	25	GLY
32	g	130	ASN
39	n	38	LYS
43	r	24	THR
47	b	64	GLY
47	b	107	ILE
48	s	4	SER
20	P	28	VAL
33	h	84	GLY
10	D	54	ASP
37	l	122	ASN
48	s	9	PRO

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Mol	Chain	Res	Type
12	F	174	GLY
14	J	132	PRO
47	b	25	PRO
9	C	155	VAL
21	Q	9	VAL
29	c	14	VAL
29	c	144	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	48/53 (91%)	45 (94%)	3 (6%)	16	45
2	1	46/47 (98%)	43 (94%)	3 (6%)	15	43
3	2	39/39 (100%)	38 (97%)	1 (3%)	40	75
4	3	54/56 (96%)	52 (96%)	2 (4%)	30	65
5	4	35/35 (100%)	34 (97%)	1 (3%)	37	73
6	5	38/38 (100%)	38 (100%)	0	100	100
7	6	39/55 (71%)	36 (92%)	3 (8%)	12	36
9	C	221/225 (98%)	213 (96%)	8 (4%)	31	66
10	D	168/170 (99%)	164 (98%)	4 (2%)	43	77
11	E	169/170 (99%)	164 (97%)	5 (3%)	36	72
12	F	153/154 (99%)	152 (99%)	1 (1%)	76	91
13	G	148/151 (98%)	146 (99%)	2 (1%)	59	85
14	J	122/123 (99%)	117 (96%)	5 (4%)	27	62
15	K	101/101 (100%)	95 (94%)	6 (6%)	18	48
16	L	110/110 (100%)	109 (99%)	1 (1%)	70	89
17	M	109/116 (94%)	108 (99%)	1 (1%)	70	89
18	N	99/100 (99%)	97 (98%)	2 (2%)	48	80
19	O	93/93 (100%)	86 (92%)	7 (8%)	12	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	P	98/100 (98%)	95 (97%)	3 (3%)	35	70
21	Q	97/98 (99%)	95 (98%)	2 (2%)	47	79
22	R	84/84 (100%)	81 (96%)	3 (4%)	31	66
23	S	91/93 (98%)	89 (98%)	2 (2%)	45	78
24	T	82/85 (96%)	82 (100%)	0	100	100
25	U	86/87 (99%)	83 (96%)	3 (4%)	32	67
26	X	49/50 (98%)	47 (96%)	2 (4%)	27	62
27	Y	57/57 (100%)	56 (98%)	1 (2%)	51	82
28	Z	52/53 (98%)	51 (98%)	1 (2%)	50	81
29	c	167/178 (94%)	162 (97%)	5 (3%)	36	72
30	e	128/130 (98%)	127 (99%)	1 (1%)	73	90
31	f	82/84 (98%)	80 (98%)	2 (2%)	43	77
32	g	127/132 (96%)	125 (98%)	2 (2%)	55	83
33	h	110/112 (98%)	108 (98%)	2 (2%)	51	82
34	i	101/102 (99%)	100 (99%)	1 (1%)	68	88
35	j	88/92 (96%)	86 (98%)	2 (2%)	44	78
36	k	87/100 (87%)	85 (98%)	2 (2%)	44	78
37	l	112/115 (97%)	107 (96%)	5 (4%)	24	58
38	m	101/104 (97%)	100 (99%)	1 (1%)	68	88
39	n	53/54 (98%)	52 (98%)	1 (2%)	50	81
40	o	82/83 (99%)	81 (99%)	1 (1%)	63	87
41	p	74/76 (97%)	71 (96%)	3 (4%)	27	62
42	q	77/80 (96%)	77 (100%)	0	100	100
43	r	56/64 (88%)	55 (98%)	1 (2%)	51	82
44	t	69/70 (99%)	68 (99%)	1 (1%)	59	85
47	b	167/212 (79%)	161 (96%)	6 (4%)	31	66
48	s	72/81 (89%)	71 (99%)	1 (1%)	59	85
52	W	64/74 (86%)	61 (95%)	3 (5%)	23	57
53	d	172/173 (99%)	168 (98%)	4 (2%)	44	78
All	All	4477/4659 (96%)	4361 (97%)	116 (3%)	41	75

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	3	VAL
1	0	8	THR
1	0	39	SER
2	1	6	THR
2	1	19	SER
2	1	42	SER
3	2	25	LYS
4	3	43	LYS
4	3	64	ASN
5	4	28	GLU
7	6	11	LYS
7	6	30	GLU
7	6	38	GLU
9	C	49	LEU
9	C	153	GLN
9	C	182	ARG
9	C	246	PRO
9	C	247	MET
9	C	255	LEU
9	C	271	VAL
9	C	274	ARG
10	D	40	THR
10	D	92	GLU
10	D	174	LEU
10	D	177	VAL
11	E	32	VAL
11	E	38	LEU
11	E	80	SER
11	E	181	ILE
11	E	194	ILE
12	F	17	MET
13	G	70	ARG
13	G	172	ARG
14	J	3	THR
14	J	40	LYS
14	J	49	VAL
14	J	127	ARG
14	J	130	GLU
15	K	19	VAL
15	K	20	LEU
15	K	80	ASP
15	K	112	MET
15	K	115	VAL

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Mol	Chain	Res	Type
15	K	116	SER
16	L	9	SER
17	M	5	LYS
18	N	66	ILE
18	N	108	ARG
19	O	6	SER
19	O	22	LEU
19	O	55	SER
19	O	63	LEU
19	O	66	GLU
19	O	79	GLU
19	O	109	LEU
20	P	48	ILE
20	P	61	VAL
20	P	88	ARG
21	Q	11	ARG
21	Q	30	THR
22	R	13	LYS
22	R	22	ILE
22	R	52	THR
23	S	29	VAL
23	S	82	LEU
25	U	33	VAL
25	U	45	SER
25	U	73	PRO
26	X	27	ARG
26	X	61	ARG
27	Y	2	LYS
28	Z	30	LYS
29	c	4	LYS
29	c	17	ASP
29	c	36	LEU
29	c	53	LYS
29	c	62	ARG
30	e	58	GLU
31	f	10	ILE
31	f	54	ASP
32	g	75	VAL
32	g	76	LYS
33	h	22	HIS
33	h	57	GLN
34	i	34	GLU

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Mol	Chain	Res	Type
35	j	56	HIS
35	j	74	ILE
36	k	17	ASN
36	k	108	GLU
37	l	10	LYS
37	l	18	ASN
37	l	39	SER
37	l	58	PRO
37	l	117	THR
38	m	104	ASN
39	n	5	SER
40	o	24	SER
41	p	3	VAL
41	p	21	VAL
41	p	60	LEU
43	r	69	GLN
44	t	82	LYS
47	b	10	LEU
47	b	25	PRO
47	b	75	GLN
47	b	92	VAL
47	b	106	THR
47	b	155	LYS
48	s	37	ARG
52	W	13	LYS
52	W	19	LYS
52	W	84	ARG
53	d	12	SER
53	d	41	ARG
53	d	63	VAL
53	d	132	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	50	ASN
2	1	4	ASN
4	3	31	HIS
4	3	35	ASN
4	3	38	GLN
4	3	60	GLN
6	5	103	GLN

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Mol	Chain	Res	Type
7	6	6	HIS
7	6	8	ASN
7	6	20	ASN
9	C	143	ASN
10	D	140	HIS
11	E	46	GLN
11	E	169	ASN
12	F	172	GLN
13	G	22	ASN
15	K	4	GLN
15	K	34	ASN
15	K	82	ASN
15	K	110	ASN
16	L	114	ASN
18	N	57	HIS
18	N	77	GLN
19	O	32	ASN
19	O	49	ASN
19	O	64	ASN
22	R	86	GLN
23	S	67	ASN
23	S	73	GLN
23	S	95	GLN
24	T	55	ASN
24	T	58	ASN
25	U	51	ASN
25	U	53	GLN
25	U	58	ASN
25	U	99	GLN
26	X	23	ASN
27	Y	31	GLN
28	Z	59	GLN
29	c	91	ASN
29	c	135	GLN
32	g	129	ASN
32	g	148	ASN
36	k	121	ASN
37	l	5	ASN
38	m	100	GLN
38	m	118	ASN
40	o	72	ASN
41	p	72	ASN

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Mol	Chain	Res	Type
43	r	21	ASN
43	r	69	GLN
47	b	55	ASN
48	s	57	HIS
48	s	69	HIS
53	d	115	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	v	75/76 (98%)	19 (25%)	0
46	A	2710/2928 (92%)	526 (19%)	103 (3%)
49	7	8/9 (88%)	2 (25%)	0
50	9	72/85 (84%)	33 (45%)	8 (11%)
51	a	1532/1554 (98%)	312 (20%)	0
8	B	111/112 (99%)	27 (24%)	9 (8%)
All	All	4508/4764 (94%)	919 (20%)	120 (2%)

All (919) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	B	4	G
8	B	7	G
8	B	10	G
8	B	11	A
8	B	12	U
8	B	13	A
8	B	23	U
8	B	32	U
8	B	33	U
8	B	38	U
8	B	40	C
8	B	43	A
8	B	49	G
8	B	50	A
8	B	51	A
8	B	53	U
8	B	54	U
8	B	55	A
8	B	63	C
8	B	64	A

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Mol	Chain	Res	Type
8	B	86	U
8	B	87	U
8	B	88	C
8	B	94	G
8	B	97	A
8	B	107	G
8	B	108	C
45	v	8	U
45	v	9	A
45	v	10	G
45	v	14	A
45	v	17	U
45	v	18	G
45	v	19	G
45	v	20	U
45	v	21	A
45	v	22	G
45	v	46	G
45	v	47	U
45	v	48	C
45	v	52	G
45	v	57	G
45	v	58	A
45	v	65	C
45	v	69	A
45	v	76	A
46	A	12	A
46	A	13	A
46	A	15	G
46	A	34	U
46	A	45	G
46	A	46	C
46	A	60	G
46	A	63	G
46	A	71	A
46	A	75	G
46	A	80	G
46	A	91	A
46	A	93	C
46	A	117	A
46	A	118	A
46	A	119	U

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Mol	Chain	Res	Type
46	A	129	C
46	A	164	U
46	A	166	A
46	A	175	G
46	A	176	A
46	A	177	G
46	A	183	A
46	A	184	G
46	A	199	A
46	A	202	A
46	A	203	U
46	A	207	A
46	A	216	A
46	A	219	A
46	A	225	A
46	A	226	A
46	A	229	A
46	A	236	A
46	A	248	G
46	A	251	G
46	A	252	C
46	A	258	A
46	A	262	G
46	A	270	C
46	A	271	C
46	A	272	C
46	A	275	A
46	A	293	U
46	A	299	U
46	A	300	G
46	A	301	U
46	A	302	A
46	A	309	U
46	A	310	C
46	A	334	G
46	A	342	A
46	A	346	G
46	A	350	U
46	A	355	A
46	A	368	G
46	A	373	A
46	A	374	A

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Mol	Chain	Res	Type
46	A	398	U
46	A	407	A
46	A	411	G
46	A	412	A
46	A	418	A
46	A	419	G
46	A	422	C
46	A	430	C
46	A	432	C
46	A	433	G
46	A	458	G
46	A	459	A
46	A	471	G
46	A	481	U
46	A	482	C
46	A	487	G
46	A	490	A
46	A	491	C
46	A	493	G
46	A	503	C
46	A	504	A
46	A	528	G
46	A	537	A
46	A	547	A
46	A	550	G
46	A	551	A
46	A	554	U
46	A	568	G
46	A	575	A
46	A	576	G
46	A	577	U
46	A	578	A
46	A	579	G
46	A	591	U
46	A	595	G
46	A	599	G
46	A	600	A
46	A	602	G
46	A	605	G
46	A	606	U
46	A	607	G
46	A	608	C

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Mol	Chain	Res	Type
46	A	615	U
46	A	616	A
46	A	617	G
46	A	619	A
46	A	622	A
46	A	630	A
46	A	631	G
46	A	647	A
46	A	657	G
46	A	658	A
46	A	659	A
46	A	666	G
46	A	673	A
46	A	680	G
46	A	683	A
46	A	691	U
46	A	692	A
46	A	701	G
46	A	702	A
46	A	732	A
46	A	733	U
46	A	742	G
46	A	777	C
46	A	783	C
46	A	793	U
46	A	794	U
46	A	795	G
46	A	811	A
46	A	812	G
46	A	822	G
46	A	829	A
46	A	831	U
46	A	832	G
46	A	837	U
46	A	839	G
46	A	841	A
46	A	852	G
46	A	859	C
46	A	864	C
46	A	866	A
46	A	874	U
46	A	875	U

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Mol	Chain	Res	Type
46	A	876	A
46	A	877	G
46	A	881	U
46	A	882	A
46	A	892	U
46	A	905	G
46	A	906	G
46	A	913	A
46	A	915	U
46	A	916	G
46	A	920	G
46	A	930	C
46	A	931	C
46	A	948	A
46	A	952	A
46	A	954	U
46	A	957	A
46	A	959	C
46	A	964	A
46	A	973	G
46	A	976	U
46	A	987	A
46	A	991	A
46	A	992	G
46	A	1007	G
46	A	1017	C
46	A	1020	A
46	A	1029	A
46	A	1031	C
46	A	1032	C
46	A	1042	A
46	A	1051	C
46	A	1055	A
46	A	1058	U
46	A	1059	A
46	A	1068	G
46	A	1071	G
46	A	1072	A
46	A	1073	A
46	A	1079	U
46	A	1084	A
46	A	1092	A

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Mol	Chain	Res	Type
46	A	1093	G
46	A	1098	C
46	A	1153	G
46	A	1158	G
46	A	1160	G
46	A	1172	A
46	A	1174	A
46	A	1175	A
46	A	1178	U
46	A	1179	A
46	A	1180	C
46	A	1181	C
46	A	1182	G
46	A	1188	A
46	A	1189	A
46	A	1203	G
46	A	1204	C
46	A	1246	G
46	A	1247	G
46	A	1250	G
46	A	1251	U
46	A	1258	A
46	A	1260	A
46	A	1278	G
46	A	1284	A
46	A	1288	G
46	A	1290	G
46	A	1293	A
46	A	1296	G
46	A	1309	G
46	A	1311	G
46	A	1312	A
46	A	1314	A
46	A	1315	G
46	A	1339	A
46	A	1340	A
46	A	1341	U
46	A	1344	C
46	A	1346	A
46	A	1352	U
46	A	1364	C
46	A	1372	C

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Mol	Chain	Res	Type
46	A	1377	G
46	A	1380	U
46	A	1388	A
46	A	1389	C
46	A	1391	U
46	A	1404	A
46	A	1418	U
46	A	1426	A
46	A	1435	U
46	A	1449	C
46	A	1450	C
46	A	1461	A
46	A	1462	G
46	A	1465	A
46	A	1466	U
46	A	1470	G
46	A	1473	A
46	A	1474	C
46	A	1480	A
46	A	1481	G
46	A	1489	U
46	A	1490	A
46	A	1499	A
46	A	1500	U
46	A	1501	U
46	A	1502	G
46	A	1505	U
46	A	1506	A
46	A	1507	U
46	A	1508	C
46	A	1514	C
46	A	1516	A
46	A	1521	G
46	A	1525	G
46	A	1526	G
46	A	1527	C
46	A	1528	U
46	A	1529	G
46	A	1531	G
46	A	1536	A
46	A	1540	A
46	A	1542	A

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Mol	Chain	Res	Type
46	A	1543	U
46	A	1544	C
46	A	1553	A
46	A	1557	G
46	A	1558	G
46	A	1559	C
46	A	1560	U
46	A	1563	G
46	A	1568	G
46	A	1570	U
46	A	1573	C
46	A	1576	G
46	A	1590	C
46	A	1602	U
46	A	1603	U
46	A	1607	C
46	A	1608	A
46	A	1614	A
46	A	1617	A
46	A	1626	U
46	A	1630	G
46	A	1631	A
46	A	1632	G
46	A	1633	G
46	A	1640	G
46	A	1653	A
46	A	1654	A
46	A	1655	A
46	A	1691	A
46	A	1693	C
46	A	1705	C
46	A	1719	G
46	A	1720	C
46	A	1743	A
46	A	1748	G
46	A	1752	G
46	A	1757	G
46	A	1758	U
46	A	1759	U
46	A	1760	A
46	A	1767	A
46	A	1770	C

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Mol	Chain	Res	Type
46	A	1771	C
46	A	1776	A
46	A	1777	G
46	A	1779	G
46	A	1791	A
46	A	1792	G
46	A	1793	G
46	A	1801	G
46	A	1802	A
46	A	1805	G
46	A	1811	C
46	A	1829	C
46	A	1830	G
46	A	1831	A
46	A	1832	A
46	A	1838	A
46	A	1845	A
46	A	1858	A
46	A	1859	C
46	A	1867	C
46	A	1876	A
46	A	1877	A
46	A	1886	G
46	A	1887	G
46	A	1888	A
46	A	1898	G
46	A	1899	U
46	A	1900	A
46	A	1901	A
46	A	1902	G
46	A	1911	C
46	A	1914	A
46	A	1935	G
46	A	1936	G
46	A	1941	A
46	A	1942	A
46	A	1944	U
46	A	1945	A
46	A	1946	U
46	A	1958	G
46	A	1959	G
46	A	1966	A

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Mol	Chain	Res	Type
46	A	1967	A
46	A	1984	U
46	A	1992	C
46	A	1996	C
46	A	1999	A
46	A	2000	A
46	A	2001	G
46	A	2020	U
46	A	2022	U
46	A	2025	C
46	A	2026	A
46	A	2035	C
46	A	2036	U
46	A	2049	A
46	A	2052	A
46	A	2054	C
46	A	2056	G
46	A	2060	A
46	A	2061	G
46	A	2062	A
46	A	2070	U
46	A	2072	C
46	A	2080	A
46	A	2081	G
46	A	2084	C
46	A	2085	G
46	A	2086	G
46	A	2089	A
46	A	2090	G
46	A	2091	A
46	A	2098	G
46	A	2099	G
46	A	2121	U
46	A	2122	G
46	A	2128	U
46	A	2129	G
46	A	2131	U
46	A	2219	G
46	A	2227	A
46	A	2232	G
46	A	2233	C
46	A	2240	U

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Mol	Chain	Res	Type
46	A	2241	A
46	A	2254	A
46	A	2255	C
46	A	2267	G
46	A	2268	G
46	A	2296	A
46	A	2304	C
46	A	2305	G
46	A	2312	C
46	A	2313	C
46	A	2315	A
46	A	2316	A
46	A	2319	G
46	A	2324	C
46	A	2334	U
46	A	2338	A
46	A	2341	U
46	A	2342	C
46	A	2348	C
46	A	2349	A
46	A	2351	A
46	A	2354	G
46	A	2356	A
46	A	2362	A
46	A	2363	C
46	A	2364	A
46	A	2366	G
46	A	2375	A
46	A	2376	C
46	A	2379	C
46	A	2383	A
46	A	2404	G
46	A	2406	A
46	A	2408	G
46	A	2412	G
46	A	2414	C
46	A	2416	U
46	A	2417	A
46	A	2420	G
46	A	2431	U
46	A	2432	C
46	A	2435	C

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Mol	Chain	Res	Type
46	A	2440	A
46	A	2443	G
46	A	2451	C
46	A	2452	U
46	A	2453	C
46	A	2454	A
46	A	2455	A
46	A	2457	G
46	A	2458	G
46	A	2459	A
46	A	2463	A
46	A	2464	A
46	A	2468	A
46	A	2469	C
46	A	2470	C
46	A	2477	A
46	A	2497	A
46	A	2498	A
46	A	2503	C
46	A	2513	G
46	A	2525	C
46	A	2531	G
46	A	2533	U
46	A	2534	G
46	A	2547	A
46	A	2558	G
46	A	2559	U
46	A	2563	C
46	A	2568	C
46	A	2569	C
46	A	2570	A
46	A	2571	A
46	A	2572	G
46	A	2581	U
46	A	2583	U
46	A	2595	A
46	A	2596	G
46	A	2602	C
46	A	2614	U
46	A	2631	A
46	A	2632	G
46	A	2638	U

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Mol	Chain	Res	Type
46	A	2642	U
46	A	2685	U
46	A	2692	G
46	A	2695	C
46	A	2698	G
46	A	2702	G
46	A	2706	G
46	A	2712	C
46	A	2718	PSU
46	A	2720	C
46	A	2742	C
46	A	2743	G
46	A	2747	G
46	A	2750	A
46	A	2764	G
46	A	2773	G
46	A	2777	A
46	A	2780	G
46	A	2786	A
46	A	2793	A
46	A	2794	A
46	A	2806	G
46	A	2807	A
46	A	2818	C
46	A	2820	U
46	A	2823	C
46	A	2828	G
46	A	2833	U
46	A	2838	U
46	A	2845	A
46	A	2858	U
46	A	2859	G
46	A	2860	A
46	A	2861	U
46	A	2862	A
46	A	2872	U
46	A	2875	A
46	A	2886	C
46	A	2891	G
46	A	2892	G
46	A	2893	A
46	A	2897	G

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Mol	Chain	Res	Type
46	A	2898	A
46	A	2899	C
46	A	2904	A
46	A	2905	C
46	A	2911	G
46	A	2918	G
49	7	406	U
49	7	412	A
50	9	4	G
50	9	6	G
50	9	7	G
50	9	8	U
50	9	9	A
50	9	13	A
50	9	16	U
50	9	17	G
50	9	18	G
50	9	19	C
50	9	20	U
50	9	21	A
50	9	22	A
50	9	23	A
50	9	24	C
50	9	26	C
50	9	27	G
50	9	35	G
50	9	37	A
50	9	42	C
50	9	43	G
50	9	45	U
50	9	66	G
50	9	69	U
50	9	70	C
50	9	72	G
50	9	75	C
50	9	76	C
50	9	78	C
50	9	79	U
50	9	82	A
50	9	83	C
50	9	84	C
51	a	9	G

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Mol	Chain	Res	Type
51	a	10	A
51	a	11	G
51	a	24	G
51	a	34	A
51	a	41	G
51	a	49	C
51	a	50	C
51	a	51	U
51	a	52	A
51	a	53	A
51	a	61	A
51	a	67	A
51	a	68	G
51	a	72	A
51	a	73	C
51	a	76	A
51	a	77	U
51	a	83	C
51	a	84	U
51	a	85	U
51	a	86	G
51	a	87	C
51	a	88	U
51	a	89	C
51	a	90	C
51	a	92	U
51	a	93	G
51	a	119	C
51	a	128	A
51	a	143	C
51	a	153	U
51	a	158	G
51	a	162	C
51	a	172	U
51	a	176	G
51	a	181	G
51	a	182	U
51	a	188	G
51	a	189	A
51	a	194	C
51	a	195	A
51	a	207	U

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Mol	Chain	Res	Type
51	a	209	A
51	a	210	A
51	a	219	U
51	a	220	C
51	a	222	G
51	a	234	A
51	a	248	C
51	a	253	U
51	a	255	G
51	a	259	G
51	a	260	U
51	a	267	G
51	a	274	G
51	a	275	C
51	a	280	C
51	a	297	G
51	a	313	G
51	a	314	A
51	a	325	U
51	a	329	A
51	a	336	C
51	a	337	A
51	a	338	C
51	a	340	G
51	a	353	C
51	a	354	G
51	a	355	G
51	a	360	C
51	a	362	G
51	a	373	U
51	a	374	C
51	a	375	U
51	a	380	C
51	a	381	A
51	a	385	G
51	a	392	G
51	a	414	G
51	a	420	U
51	a	421	G
51	a	429	U
51	a	430	C
51	a	431	G

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Mol	Chain	Res	Type
51	a	432	G
51	a	434	U
51	a	435	C
51	a	436	G
51	a	437	U
51	a	438	A
51	a	461	C
51	a	465	U
51	a	467	C
51	a	475	A
51	a	479	G
51	a	485	A
51	a	493	G
51	a	494	G
51	a	496	A
51	a	506	A
51	a	508	A
51	a	510	C
51	a	520	C
51	a	524	G
51	a	527	C
51	a	533	G
51	a	536	G
51	a	539	G
51	a	540	U
51	a	541	A
51	a	542	A
51	a	550	G
51	a	554	C
51	a	556	A
51	a	568	A
51	a	569	A
51	a	570	U
51	a	571	U
51	a	576	G
51	a	581	A
51	a	582	A
51	a	585	G
51	a	586	G
51	a	604	A
51	a	605	A
51	a	629	C

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Mol	Chain	Res	Type
51	a	642	U
51	a	651	A
51	a	662	U
51	a	663	G
51	a	674	A
51	a	680	G
51	a	691	C
51	a	728	C
51	a	732	U
51	a	733	G
51	a	740	G
51	a	743	A
51	a	757	A
51	a	758	A
51	a	762	A
51	a	764	G
51	a	772	G
51	a	786	A
51	a	790	A
51	a	803	A
51	a	813	U
51	a	824	A
51	a	826	C
51	a	841	G
51	a	845	G
51	a	849	G
51	a	850	U
51	a	852	U
51	a	853	C
51	a	855	G
51	a	856	C
51	a	861	U
51	a	862	A
51	a	863	G
51	a	868	G
51	a	869	C
51	a	886	A
51	a	897	G
51	a	899	A
51	a	912	G
51	a	924	A
51	a	944	C

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Mol	Chain	Res	Type
51	a	945	A
51	a	952	G
51	a	965	U
51	a	966	U
51	a	970	U
51	a	975	A
51	a	978	A
51	a	979	A
51	a	981	G
51	a	985	A
51	a	986	G
51	a	987	A
51	a	988	A
51	a	993	A
51	a	994	C
51	a	1002	U
51	a	1003	G
51	a	1004	A
51	a	1008	C
51	a	1009	C
51	a	1010	U
51	a	1012	U
51	a	1013	G
51	a	1019	C
51	a	1020	C
51	a	1028	A
51	a	1030	G
51	a	1034	U
51	a	1035	C
51	a	1036	C
51	a	1039	U
51	a	1040	U
51	a	1041	C
51	a	1042	G
51	a	1043	G
51	a	1044	G
51	a	1045	G
51	a	1046	G
51	a	1049	G
51	a	1050	A
51	a	1051	G
51	a	1054	A

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Mol	Chain	Res	Type
51	a	1060	G
51	a	1063	G
51	a	1066	U
51	a	1075	U
51	a	1076	C
51	a	1084	G
51	a	1095	U
51	a	1099	G
51	a	1104	G
51	a	1105	U
51	a	1111	A
51	a	1114	G
51	a	1119	C
51	a	1135	U
51	a	1140	A
51	a	1142	C
51	a	1144	U
51	a	1145	U
51	a	1149	U
51	a	1157	U
51	a	1166	A
51	a	1168	U
51	a	1169	G
51	a	1176	A
51	a	1178	A
51	a	1180	A
51	a	1193	G
51	a	1205	A
51	a	1206	A
51	a	1220	U
51	a	1221	U
51	a	1222	A
51	a	1235	C
51	a	1236	A
51	a	1237	C
51	a	1238	A
51	a	1247	A
51	a	1263	G
51	a	1265	C
51	a	1266	A
51	a	1267	G
51	a	1269	G

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Mol	Chain	Res	Type
51	a	1270	A
51	a	1287	C
51	a	1289	A
51	a	1290	U
51	a	1291	C
51	a	1295	C
51	a	1296	A
51	a	1302	G
51	a	1309	G
51	a	1310	U
51	a	1311	U
51	a	1312	C
51	a	1314	G
51	a	1317	C
51	a	1321	G
51	a	1329	C
51	a	1331	C
51	a	1344	C
51	a	1345	U
51	a	1347	G
51	a	1349	A
51	a	1355	A
51	a	1362	G
51	a	1366	A
51	a	1367	U
51	a	1373	U
51	a	1379	G
51	a	1388	G
51	a	1398	C
51	a	1405	A
51	a	1406	C
51	a	1407	A
51	a	1432	G
51	a	1435	A
51	a	1449	U
51	a	1451	A
51	a	1455	A
51	a	1459	U
51	a	1462	U
51	a	1463	A
51	a	1464	G
51	a	1494	U

Continued on next page...

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Mol	Chain	Res	Type
51	a	1497	G
51	a	1502	A
51	a	1503	A
51	a	1504	G
51	a	1507	G
51	a	1509	A
51	a	1513	A
51	a	1516	U
51	a	1517	A
51	a	1518	G
51	a	1527	G
51	a	1529	A
51	a	1530	G
51	a	1534	C
51	a	1538	U
51	a	1539	G
51	a	1540	G

All (120) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	B	10	G
8	B	11	A
8	B	32	U
8	B	37	A
8	B	48	G
8	B	49	G
8	B	63	C
8	B	86	U
8	B	87	U
46	A	12	A
46	A	45	G
46	A	67	A
46	A	92	G
46	A	122	G
46	A	175	G
46	A	181	G
46	A	202	A
46	A	225	A
46	A	299	U
46	A	300	G
46	A	344	G

Continued on next page...

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Mol	Chain	Res	Type
46	A	411	G
46	A	458	G
46	A	466	C
46	A	481	U
46	A	493	G
46	A	539	G
46	A	549	A
46	A	575	A
46	A	599	G
46	A	615	U
46	A	666	G
46	A	691	U
46	A	701	G
46	A	732	A
46	A	793	U
46	A	811	A
46	A	831	U
46	A	848	G
46	A	855	G
46	A	876	A
46	A	905	G
46	A	978	A
46	A	986	G
46	A	990	C
46	A	1025	A
46	A	1030	G
46	A	1041	C
46	A	1092	A
46	A	1179	A
46	A	1188	A
46	A	1203	G
46	A	1244	A
46	A	1245	G
46	A	1246	G
46	A	1250	G
46	A	1266	A
46	A	1296	G
46	A	1325	A
46	A	1339	A
46	A	1344	C
46	A	1350	U
46	A	1474	C

Continued on next page...

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Mol	Chain	Res	Type
46	A	1480	A
46	A	1505	U
46	A	1525	G
46	A	1530	G
46	A	1535	U
46	A	1542	A
46	A	1543	U
46	A	1558	G
46	A	1602	U
46	A	1606	A
46	A	1631	A
46	A	1653	A
46	A	1705	C
46	A	1751	U
46	A	1757	G
46	A	1791	A
46	A	1813	A
46	A	1830	G
46	A	1887	G
46	A	1941	A
46	A	1944	U
46	A	2064	G
46	A	2080	A
46	A	2098	G
46	A	2121	U
46	A	2127	U
46	A	2254	A
46	A	2304	C
46	A	2315	A
46	A	2349	A
46	A	2374	G
46	A	2375	A
46	A	2420	G
46	A	2435	C
46	A	2451	C
46	A	2452	U
46	A	2459	A
46	A	2468	A
46	A	2487	U
46	A	2497	A
46	A	2558	G
46	A	2569	C

Continued on next page...

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Mol	Chain	Res	Type
46	A	2571	A
46	A	2631	A
46	A	2785	U
46	A	2805	A
46	A	2892	G
46	A	2898	A
46	A	2904	A
50	9	3	A
50	9	18	G
50	9	20	U
50	9	21	A
50	9	69	U
50	9	75	C
50	9	78	C
50	9	83	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
46	OMG	A	2280	45,46	23,26,27	0.41	0	33,38,41	0.60	0
46	PSU	A	2718	46	18,21,22	0.92	2 (11%)	22,30,33	0.93	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	OMG	A	2280	45,46	-	0/9/27/28	0/3/3/3
46	PSU	A	2718	46	-	1/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A	2718	PSU	C4-C5	-2.44	1.37	1.44
46	A	2718	PSU	C6-C5	2.33	1.38	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	2718	PSU	O2'-C2'-C3'	2.27	119.16	111.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	2718	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

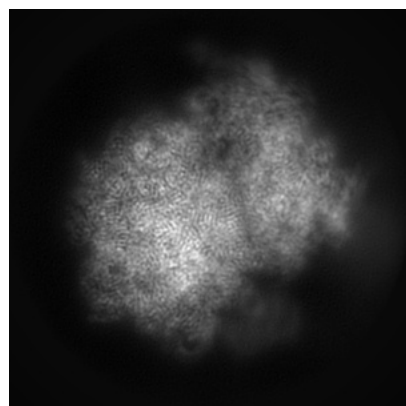
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50858. These allow visual inspection of the internal detail of the map and identification of artifacts.

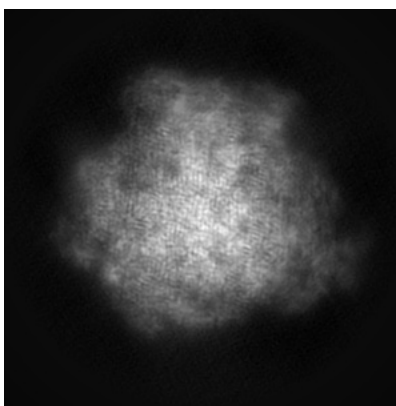
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

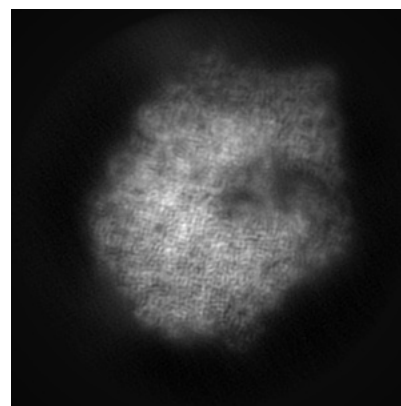
6.1.1 Primary map



X

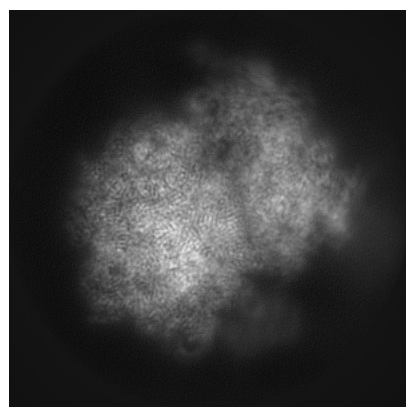


Y

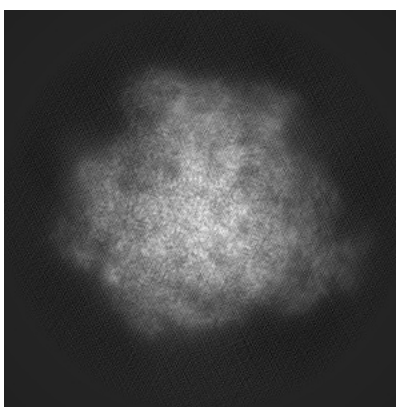


Z

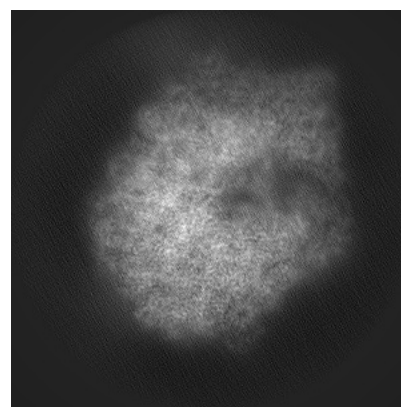
6.1.2 Raw map



X



Y

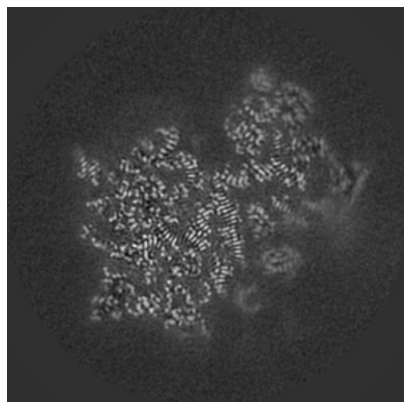


Z

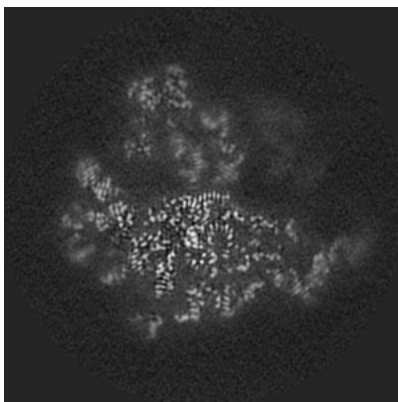
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

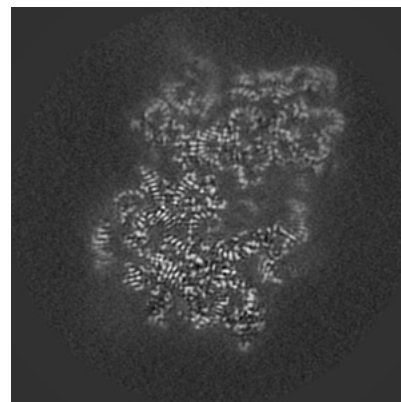
6.2.1 Primary map



X Index: 192

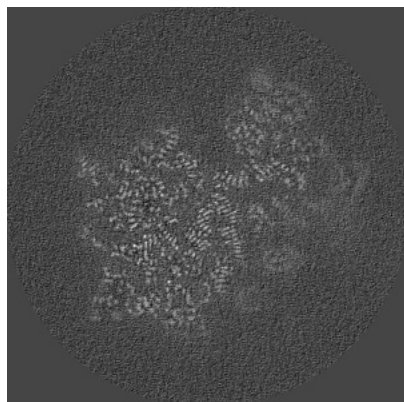


Y Index: 192

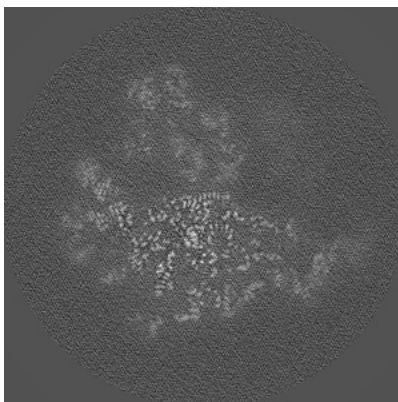


Z Index: 192

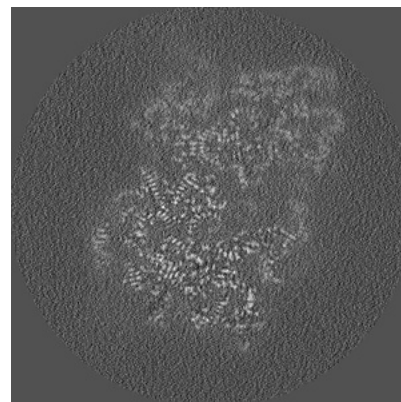
6.2.2 Raw map



X Index: 192



Y Index: 192

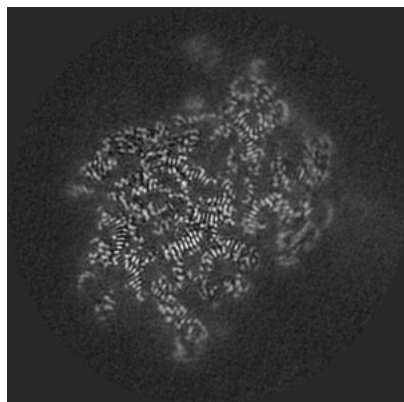


Z Index: 192

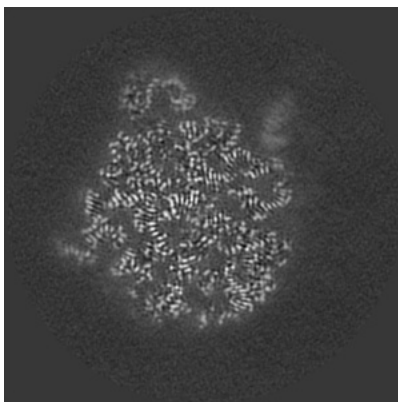
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

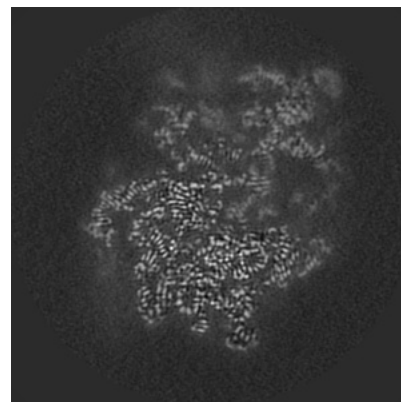
6.3.1 Primary map



X Index: 163

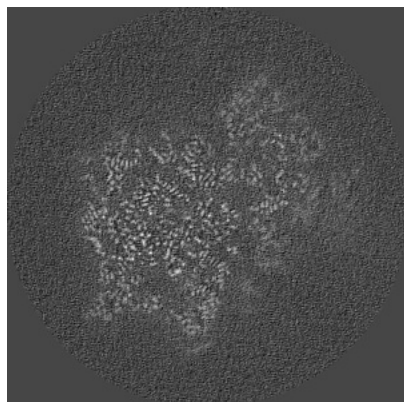


Y Index: 157

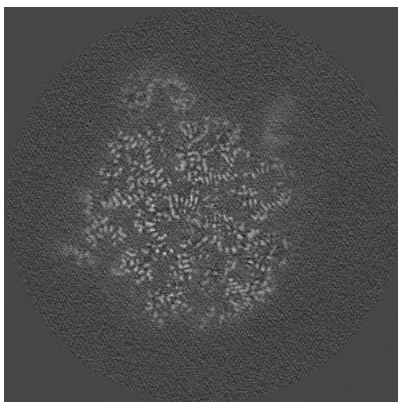


Z Index: 179

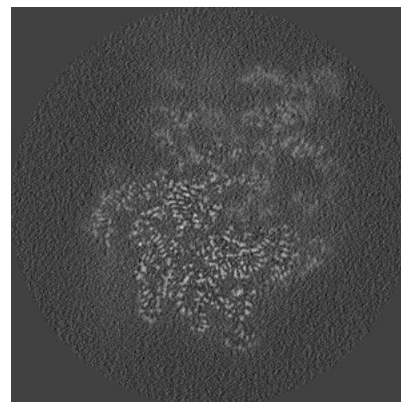
6.3.2 Raw map



X Index: 183



Y Index: 156

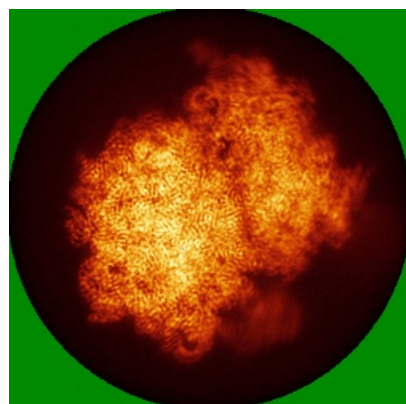


Z Index: 178

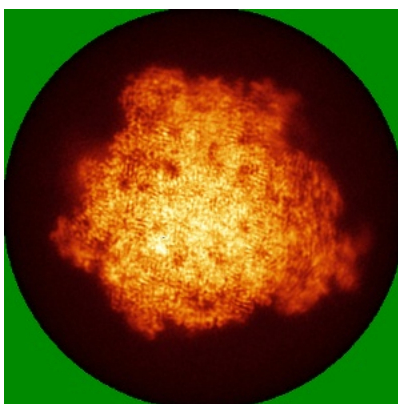
The images above show the largest variance slices of the map in three orthogonal directions.

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

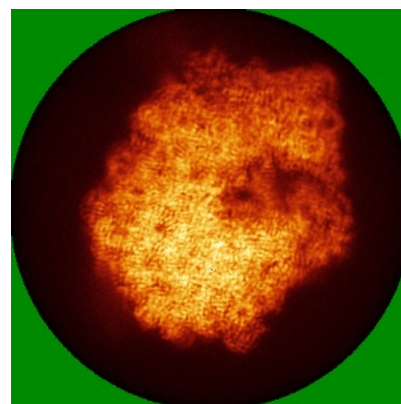
6.4.1 Primary map



X

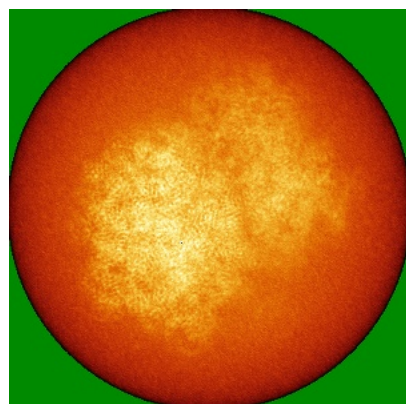


Y

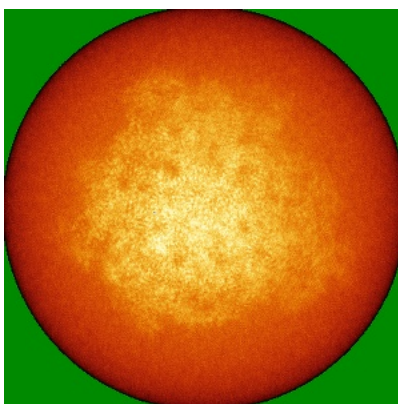


Z

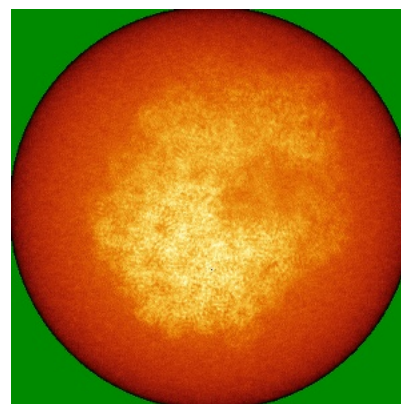
6.4.2 Raw map



X



Y

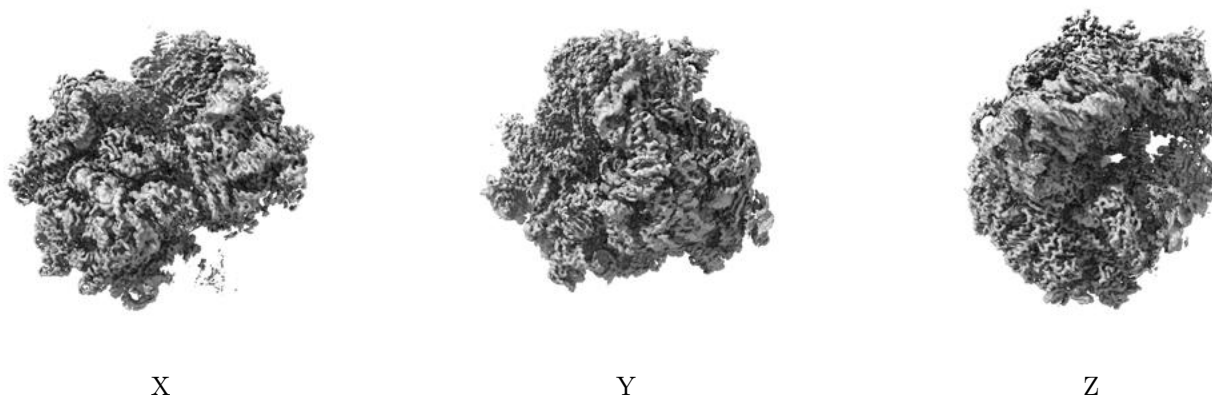


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

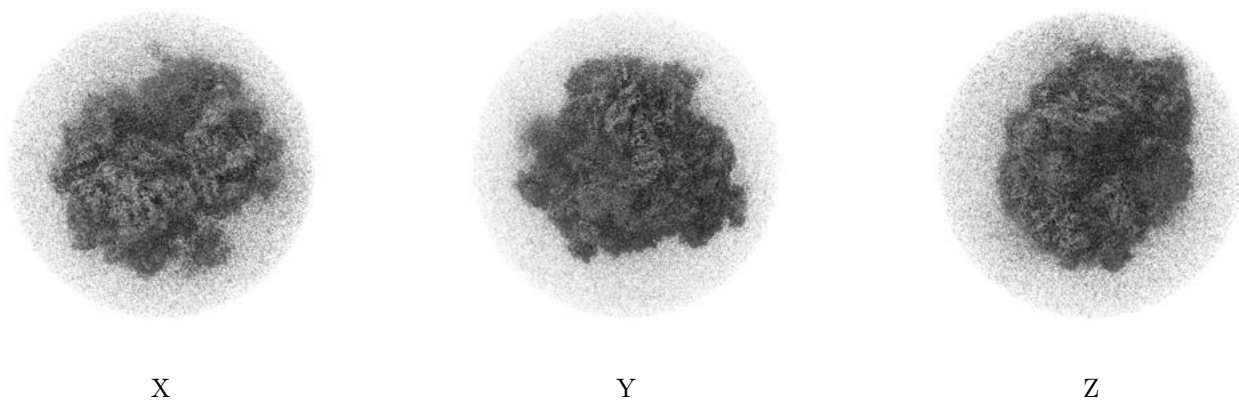
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

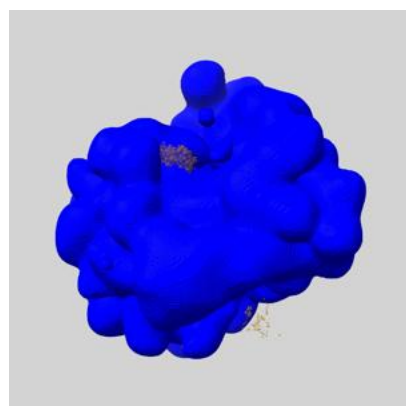
6.6 Mask visualisation [i](#)

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

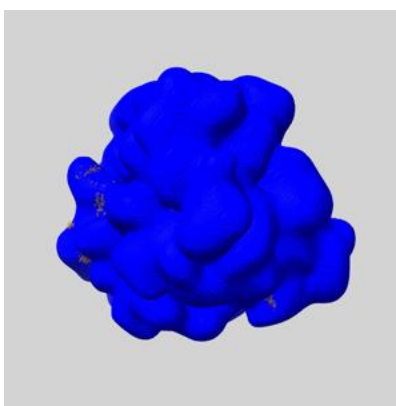
A mask typically either:

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

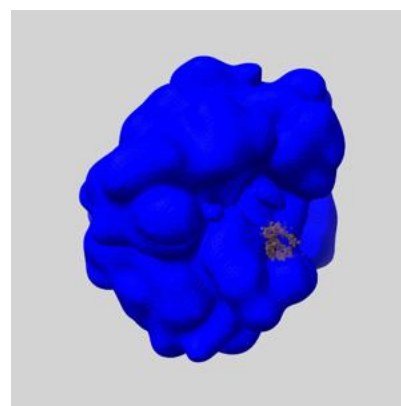
6.6.1 emd_50858_msk_1.map [i](#)



X



Y

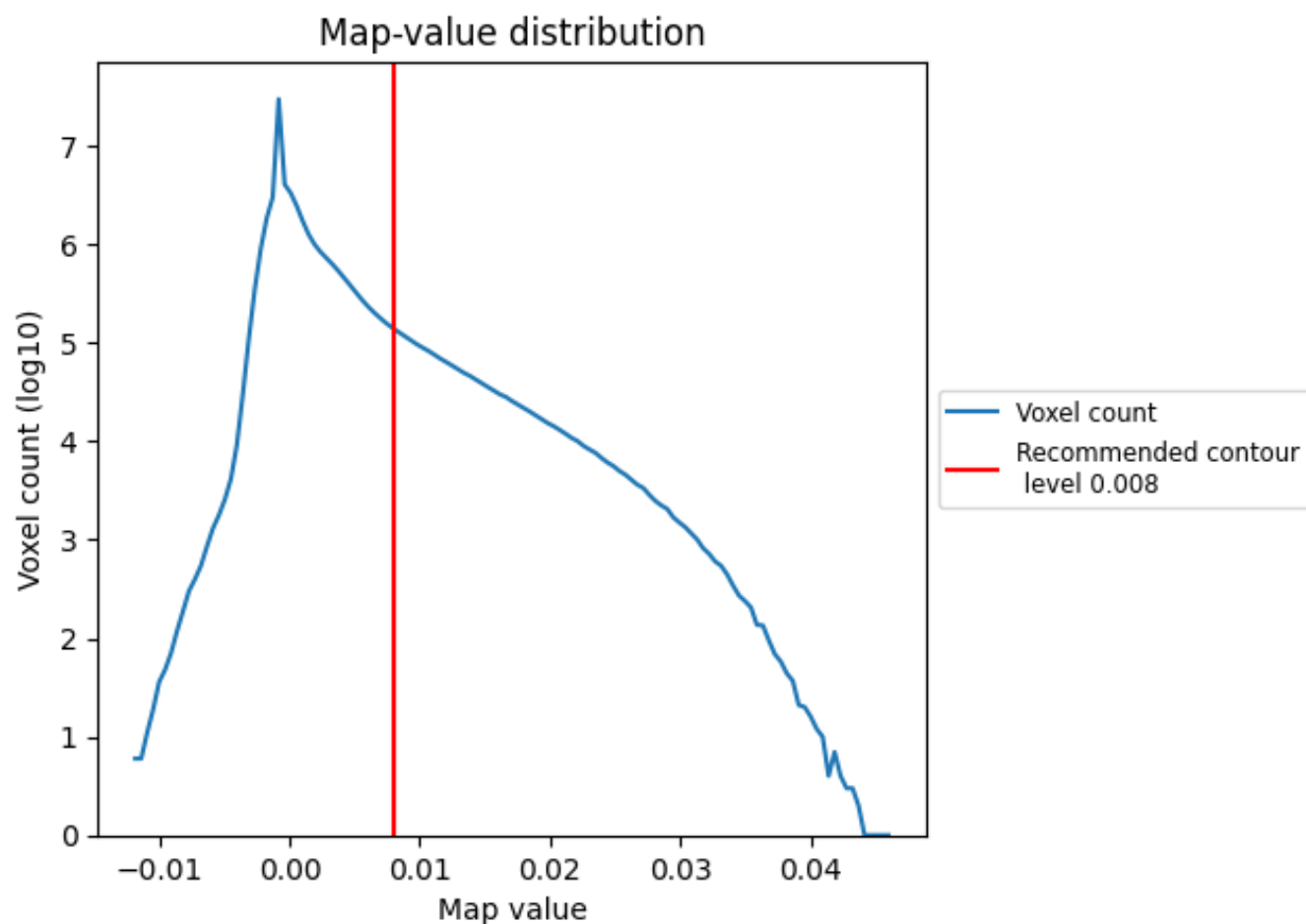


Z

7 Map analysis [i](#)

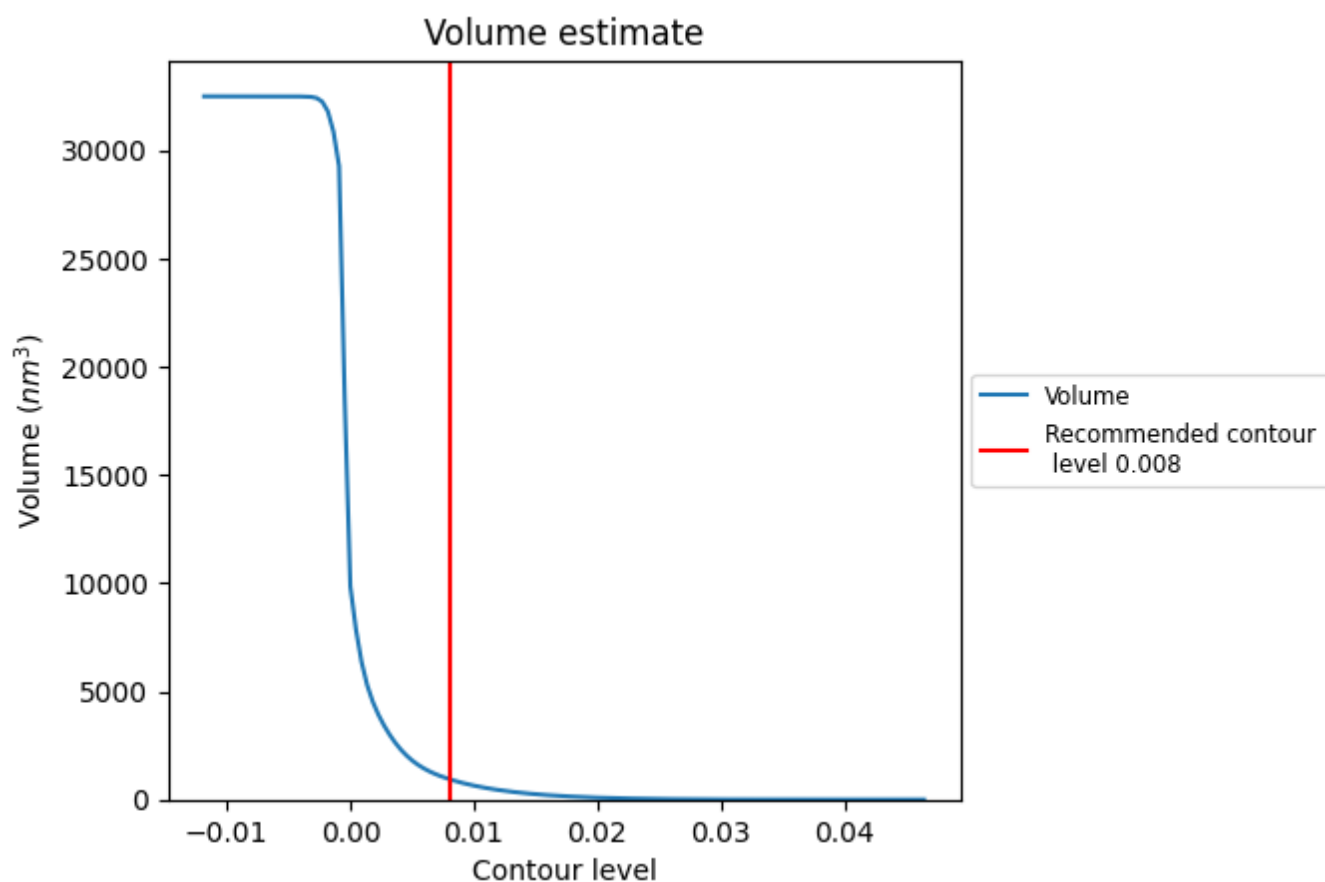
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

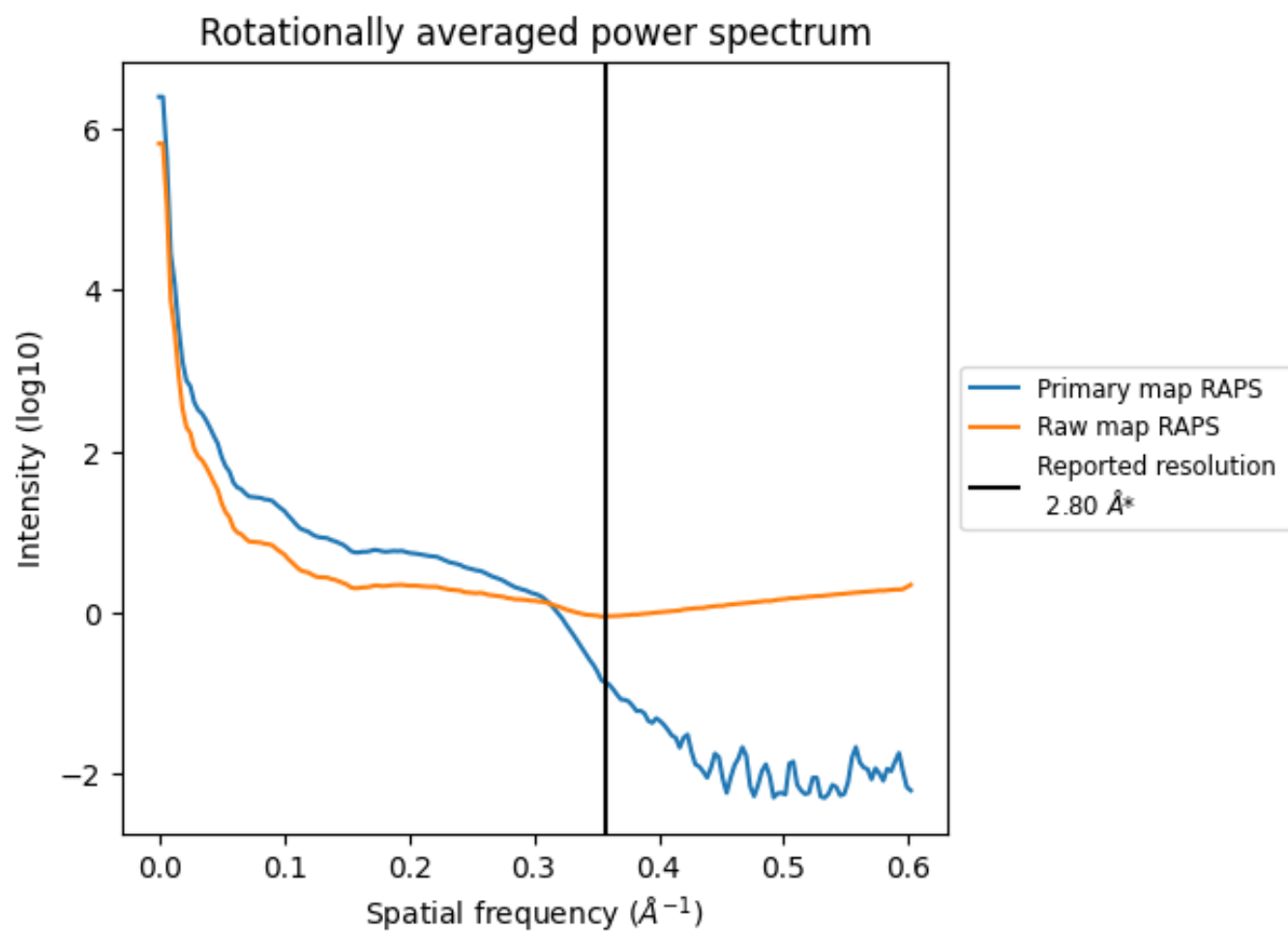
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 946 nm³; this corresponds to an approximate mass of 855 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

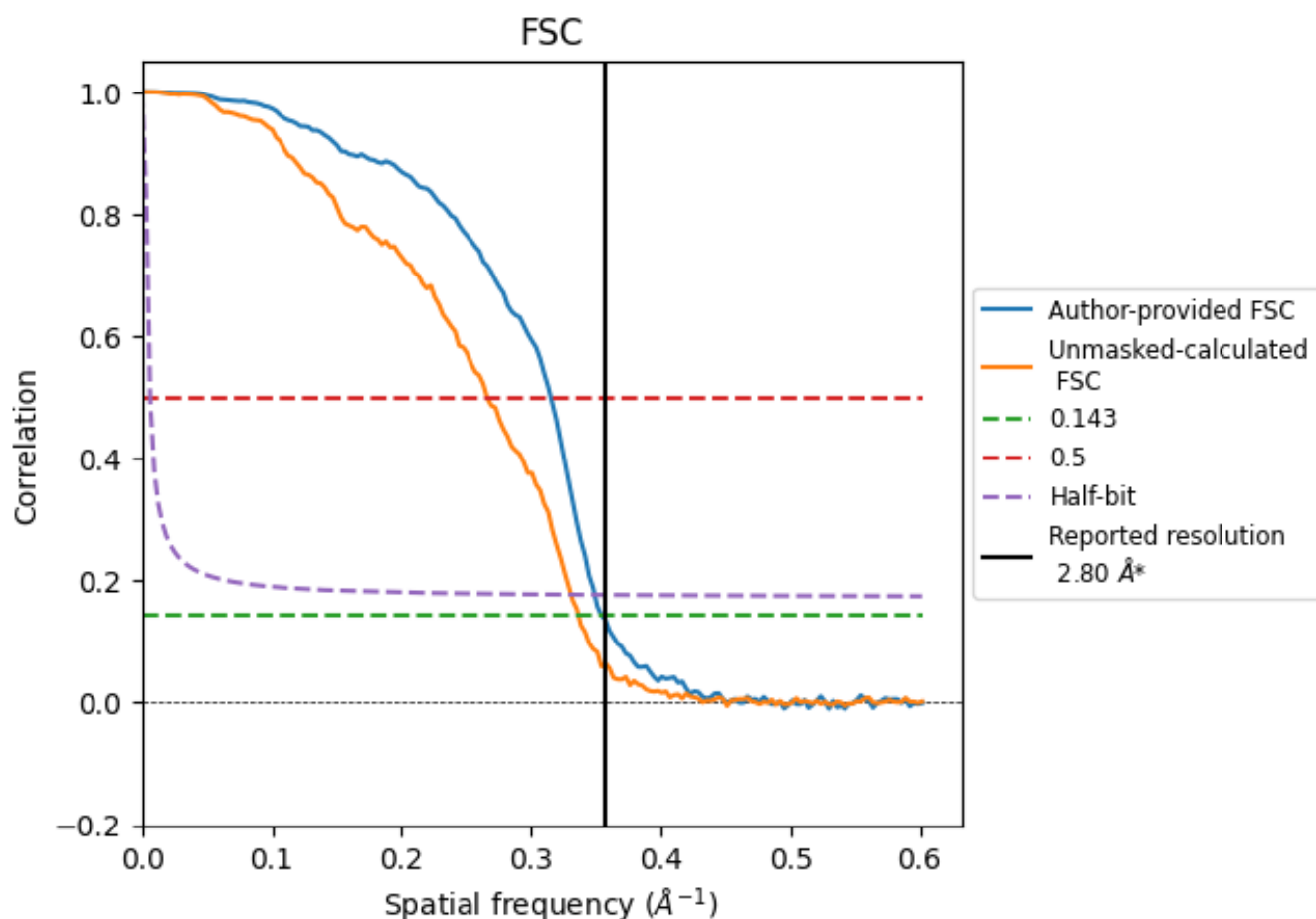


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

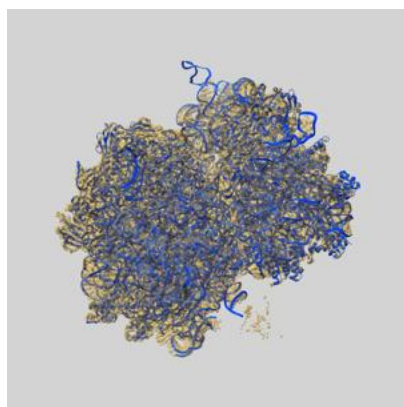
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.17	2.87
Unmasked-calculated*	2.97	3.76	3.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

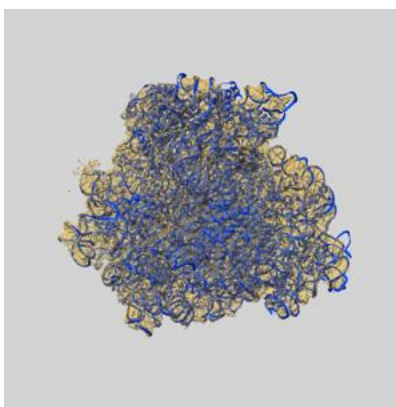
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50858 and PDB model 9FY3. Per-residue inclusion information can be found in section [3](#) on page [14](#).

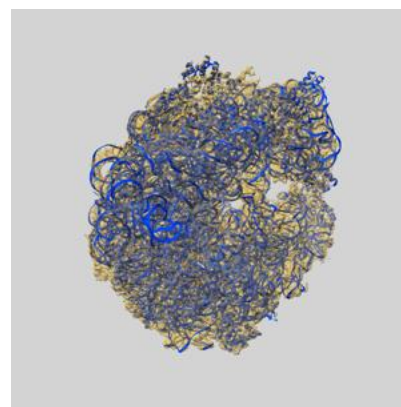
9.1 Map-model overlay [i](#)



X



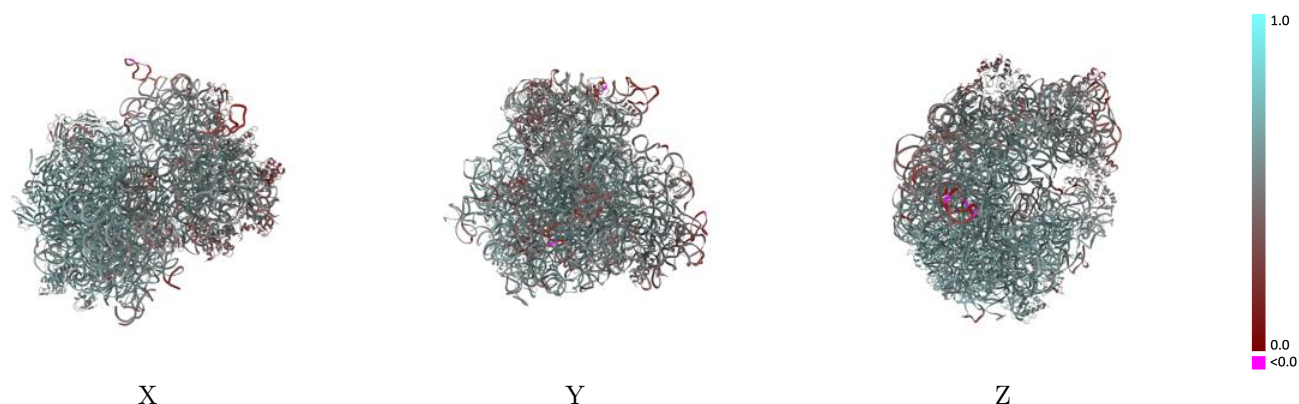
Y



Z

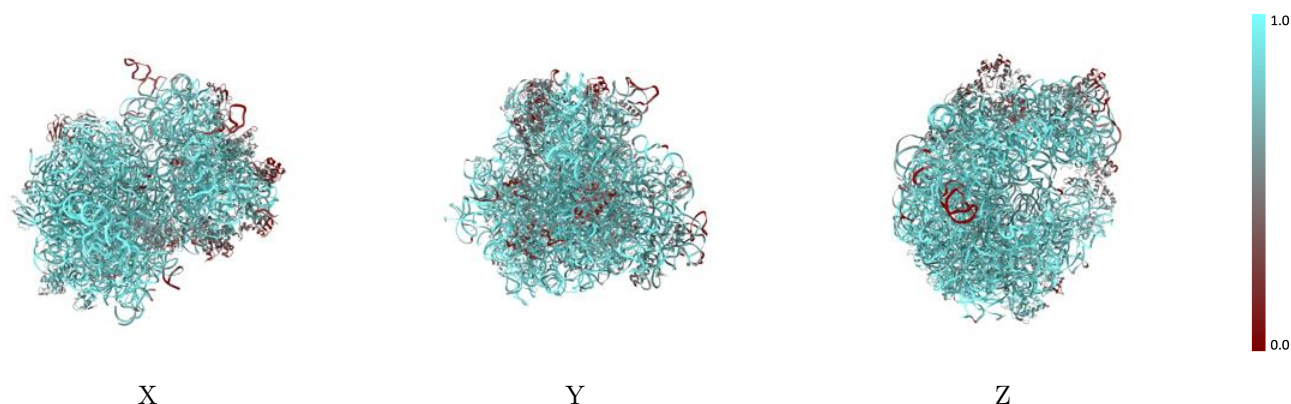
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



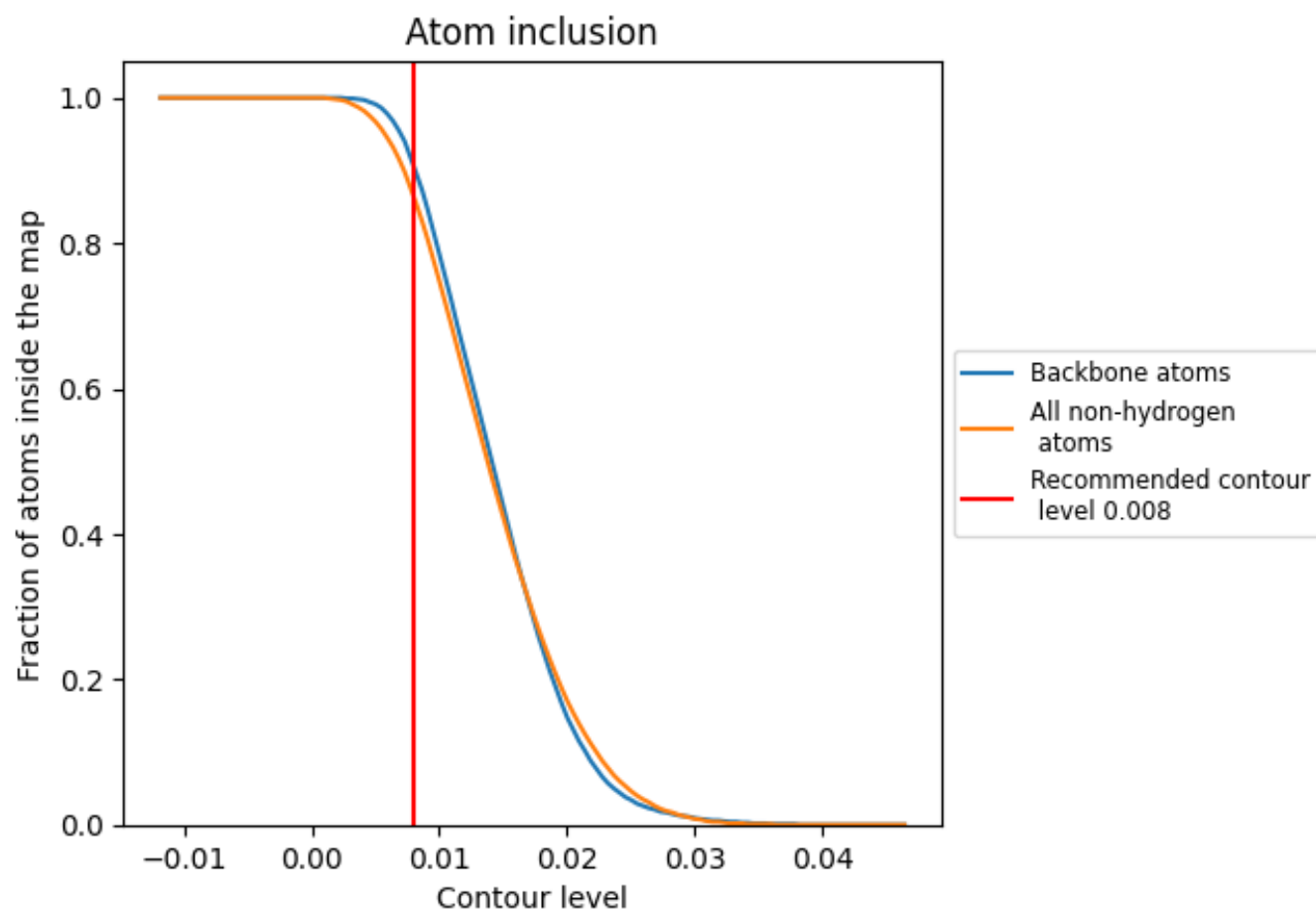
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8640	 0.5500
0	 0.8740	 0.5870
1	 0.7840	 0.5600
2	 0.9710	 0.6360
3	 0.9300	 0.6150
4	 0.8970	 0.5890
5	 0.8490	 0.5700
6	 0.3010	 0.3820
7	 0.9470	 0.5760
9	 0.7770	 0.4730
A	 0.9660	 0.6000
B	 0.9080	 0.5320
C	 0.8960	 0.6000
D	 0.8540	 0.6000
E	 0.7930	 0.5730
F	 0.5190	 0.4360
G	 0.5880	 0.4850
J	 0.8550	 0.5920
K	 0.8790	 0.5970
L	 0.8080	 0.5790
M	 0.8950	 0.6000
N	 0.8730	 0.5860
O	 0.6520	 0.5010
P	 0.7930	 0.5660
Q	 0.8860	 0.6080
R	 0.7930	 0.5920
S	 0.8740	 0.6000
T	 0.8230	 0.5710
U	 0.7270	 0.5560
W	 0.8770	 0.5930
X	 0.7150	 0.5510
Y	 0.7200	 0.5220
Z	 0.8270	 0.5760
a	 0.8800	 0.5060
b	 0.4130	 0.4040



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Chain	Atom inclusion	Q-score
c	 0.6540	 0.4870
d	 0.5420	 0.4510
e	 0.6930	 0.5190
f	 0.3660	 0.3530
g	 0.5050	 0.4150
h	 0.6730	 0.4840
i	 0.5100	 0.4270
j	 0.4850	 0.4110
k	 0.4960	 0.3980
l	 0.8400	 0.5840
m	 0.6020	 0.4540
n	 0.7990	 0.5370
o	 0.6910	 0.4840
p	 0.6250	 0.4590
q	 0.6460	 0.4840
r	 0.4880	 0.3870
s	 0.6470	 0.4710
t	 0.5890	 0.4590
v	 0.8910	 0.5130