



Full wwPDB EM Validation Report ⓘ

Oct 5, 2024 – 03:51 pm BST

PDB ID : 5NWY
EMDB ID : EMD-3713
Title : 2.9 Å cryo-EM structure of VemP-stalled ribosome-nascent chain complex
Authors : Su, T.; Cheng, J.; Sohmen, D.; Hedman, R.; Berninghausen, O.; von Heijne, G.; Wilson, D.N.; Beckmann, R.
Deposited on : 2017-05-08
Resolution : 2.90 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

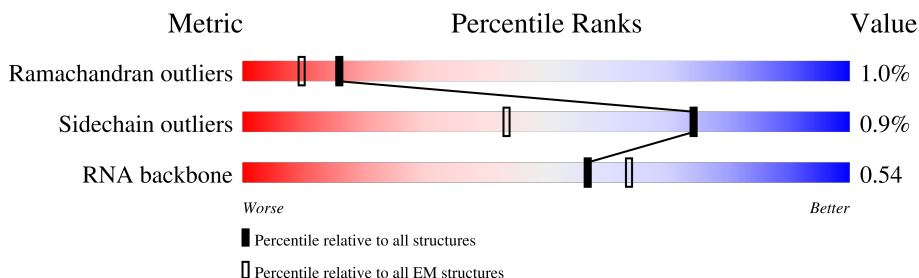
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	s	179	
2	M	75	
3	O	120	
4	P	273	
5	Q	209	
6	R	201	
7	S	179	
8	T	177	

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Mol	Chain	Length	Quality of chain
9	U	149	
10	V	142	
11	W	142	
12	X	123	
13	Y	144	
14	Z	136	
15	a	127	
16	b	117	
17	c	115	
18	d	118	
19	e	103	
20	f	110	
21	g	100	
22	h	104	
23	i	94	
24	j	85	
25	k	78	
26	l	63	
27	m	59	
28	n	57	
29	o	55	
30	p	46	
31	q	65	
32	r	38	
33	N	2903	

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Mol	Chain	Length	Quality of chain
34	L	70	
35	0	1539	
36	1	233	
37	2	233	
38	3	206	
39	4	166	
40	5	131	
41	6	156	
42	7	130	
43	8	130	
44	9	103	
45	A	129	
46	B	124	
47	C	118	
48	D	101	
49	E	89	
50	F	82	
51	G	84	
52	H	75	
53	I	92	
54	J	87	
55	K	71	
56	t	4	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 144142 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 VemP nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	s	37	Total	C	N	O	S	0	0
			316	198	58	58	2		

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
s	-2	MET	-	initiating methionine	UNP A0A0P7EF65
s	-1	HIS	-	expression tag	UNP A0A0P7EF65
s	0	HIS	-	expression tag	UNP A0A0P7EF65
s	1	HIS	-	expression tag	UNP A0A0P7EF65
s	2	HIS	-	expression tag	UNP A0A0P7EF65
s	3	HIS	-	expression tag	UNP A0A0P7EF65
s	4	HIS	-	expression tag	UNP A0A0P7EF65
s	5	HIS	-	expression tag	UNP A0A0P7EF65
s	6	HIS	-	expression tag	UNP A0A0P7EF65
s	7	HIS	-	expression tag	UNP A0A0P7EF65
s	8	HIS	-	expression tag	UNP A0A0P7EF65
s	9	GLY	-	expression tag	UNP A0A0P7EF65
s	10	ASP	-	expression tag	UNP A0A0P7EF65
s	11	TYR	-	expression tag	UNP A0A0P7EF65
s	12	LYS	-	expression tag	UNP A0A0P7EF65
s	13	ASP	-	expression tag	UNP A0A0P7EF65
s	14	ASP	-	expression tag	UNP A0A0P7EF65
s	15	ASP	-	expression tag	UNP A0A0P7EF65
s	16	ASP	-	expression tag	UNP A0A0P7EF65
s	17	LYS	-	expression tag	UNP A0A0P7EF65
s	18	GLU	-	expression tag	UNP A0A0P7EF65
s	19	ASN	-	expression tag	UNP A0A0P7EF65
s	20	LEU	-	expression tag	UNP A0A0P7EF65
s	21	TYR	-	expression tag	UNP A0A0P7EF65
s	22	PHE	-	expression tag	UNP A0A0P7EF65
s	23	GLN	-	expression tag	UNP A0A0P7EF65
s	24	GLY	-	expression tag	UNP A0A0P7EF65
s	25	SER	-	expression tag	UNP A0A0P7EF65

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Chain	Residue	Modelled	Actual	Comment	Reference
s	30	GLN	HIS	conflict	UNP A0A0P7EF65
s	59	ALA	VAL	conflict	UNP A0A0P7EF65
s	160	LEU	-	expression tag	UNP A0A0P7EF65
s	161	GLU	-	expression tag	UNP A0A0P7EF65
s	162	VAL	-	expression tag	UNP A0A0P7EF65
s	163	LEU	-	expression tag	UNP A0A0P7EF65
s	164	PHE	-	expression tag	UNP A0A0P7EF65
s	165	GLN	-	expression tag	UNP A0A0P7EF65
s	166	GLY	-	expression tag	UNP A0A0P7EF65
s	167	PRO	-	expression tag	UNP A0A0P7EF65
s	168	TYR	-	expression tag	UNP A0A0P7EF65
s	169	PRO	-	expression tag	UNP A0A0P7EF65
s	170	TYR	-	expression tag	UNP A0A0P7EF65
s	171	ASP	-	expression tag	UNP A0A0P7EF65
s	172	VAL	-	expression tag	UNP A0A0P7EF65
s	173	PRO	-	expression tag	UNP A0A0P7EF65
s	174	ASP	-	expression tag	UNP A0A0P7EF65
s	175	TYR	-	expression tag	UNP A0A0P7EF65
s	176	ALA	-	expression tag	UNP A0A0P7EF65

- Molecule 2 is a RNA chain called Gln-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	75	Total	C	N	O	P	0	0
			1594	711	281	527	75		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	209	Total	C	N	O	S	0	0
			1564	979	288	293	4		

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	176	Total	C	N	O	S	0	0
			1322	832	243	245	2		

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U	47	Total	C	N	O	S	0	0
			359	233	62	63	1		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	141	Total	C	N	O	S	0	0
			1031	651	179	195	6		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	142	Total	C	N	O	S	0	0
			1128	714	212	198	4		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	143	Total	C	N	O	S	0	0
			1044	649	206	188	1		

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	136	Total	C	N	O	S	0	0
			1073	686	205	176	6		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	b	116	Total	C	N	O	0	0
			891	552	178	161		

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	114	Total	C	N	O	S	0	0
			915	573	179	162	1		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	d	117	Total	C	N	O	0	0
			946	604	192	150		

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	103	Total	C	N	O	S	0	0
			815	516	153	144	2		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	i	94	Total	C	N	O	S	0	0
			752	479	137	133	3		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	j	75	Total	C	N	O	S	0	0
			568	353	113	101	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	k	77	Total	C	N	O	S	0	0
			624	388	129	105	2		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	l	63	Total	C	N	O	S	0	0
			508	313	99	94	2		

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	m	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	n	56	Total	C	N	O	S	0	0
			443	269	94	79	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	o	50	Total	C	N	O	0	0
			409	263	75	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	p	46	Total	C	N	O	S	0	0
			376	228	90	56	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	q	64	Total	C	N	O	S	0	0
			503	323	105	73	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	r	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 33 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	N	2897	Total	C	N	O	P	1	0
			62215	27754	11448	20115	2898		

- Molecule 34 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 35 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	0	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	2	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	3	205	Total	C	N	O	S	0	0
			1642	1026	315	297	4		

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	4	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	5	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	6	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	7	129	Total	C	N	O	S	0	0
			978	616	173	183	6		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	8	127	Total	C	N	O	S	0	0
			1021	634	206	178	3		

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	9	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	A	117	Total	C	N	O	S	0	0
			876	540	174	159	3		

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	B	123	Total	C	N	O	S	0	0
			954	590	196	164	4		

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	C	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 48 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	D	96	Total	C	N	O	S	0	0
			773	483	160	127	3		

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	E	88	Total	C	N	O	S	0	0
			709	437	143	128	1		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	F	82	Total	C	N	O	S	0	0
			648	406	128	113	1		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	G	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	H	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	I	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	J	85	Total	C	N	O	S	0	0
			664	411	137	113	3		

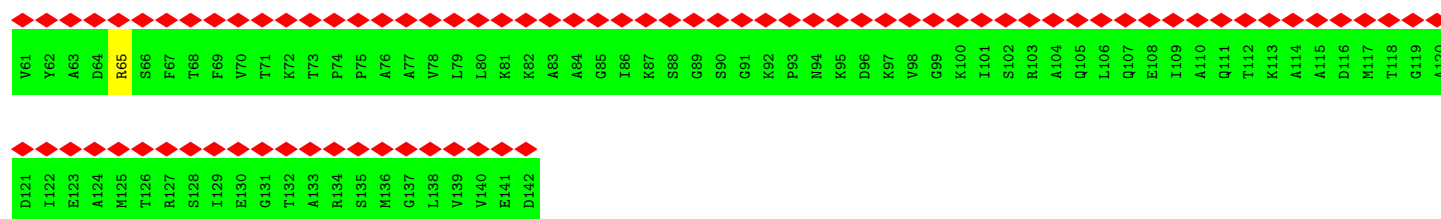
- Molecule 55 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	K	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

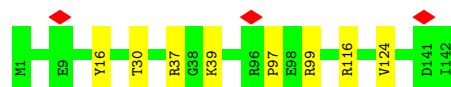
- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	t	4	Total	C	N	O	P	0	0
			85	38	15	28	4		

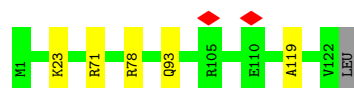
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| NET | A2 | K3 | K4 | V5 | Q6 | A7 | Y8 | V9 | K10 | L11 | Q12 | V13 | A14 | A15 | G16 | M17 | A18 | N19 | P20 | S21 | P22 | P23 | V24 | G25 | P26 | A27 | L28 | G29 | Q30 | Q31 | G32 | V33 | N34 | I35 | M36 | E37 | F38 | C39 | K40 | A41 | F42 | N43 | A44 | K45 | T46 | D47 | S48 | I49 | E50 | K51 | G52 | L53 | P54 | I55 | P56 | V57 | V58 | I59 | S60 |
|-----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



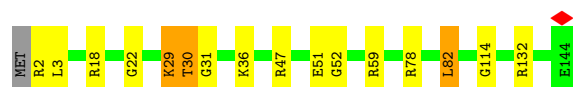
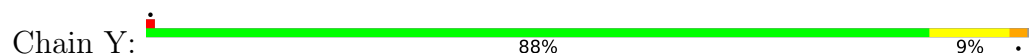
• Molecule 11: 50S ribosomal protein L13



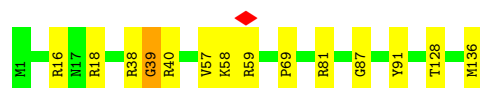
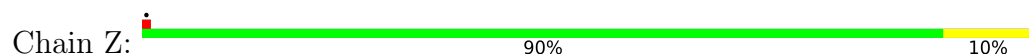
• Molecule 12: 50S ribosomal protein L14



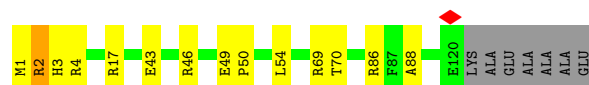
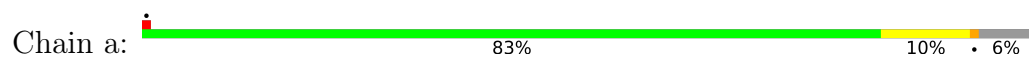
• Molecule 13: 50S ribosomal protein L15



• Molecule 14: 50S ribosomal protein L16

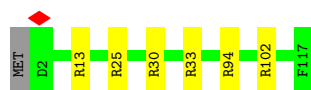


• Molecule 15: 50S ribosomal protein L17

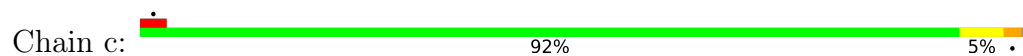


• Molecule 16: 50S ribosomal protein L18

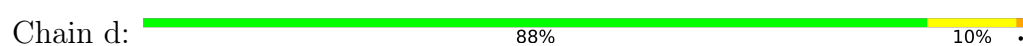




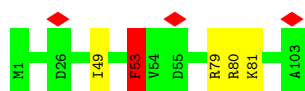
- Molecule 17: 50S ribosomal protein L19



- Molecule 18: 50S ribosomal protein L20



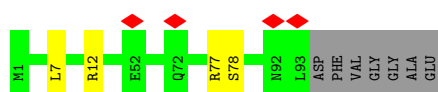
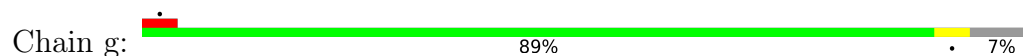
- Molecule 19: 50S ribosomal protein L21



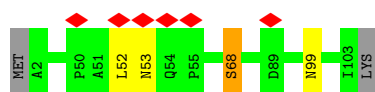
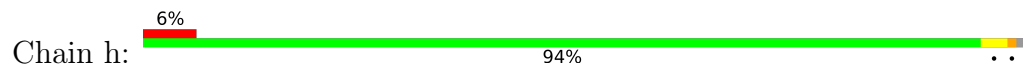
- Molecule 20: 50S ribosomal protein L22



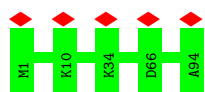
- Molecule 21: 50S ribosomal protein L23



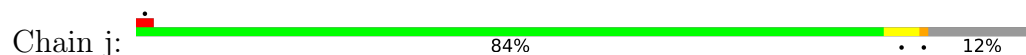
- Molecule 22: 50S ribosomal protein L24



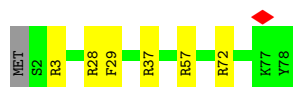
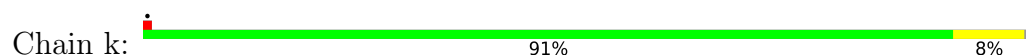
- Molecule 23: 50S ribosomal protein L25



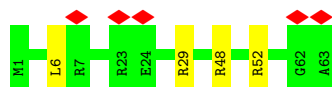
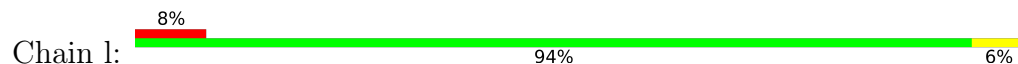
- Molecule 24: 50S ribosomal protein L27



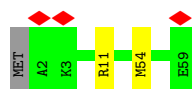
- Molecule 25: 50S ribosomal protein L28



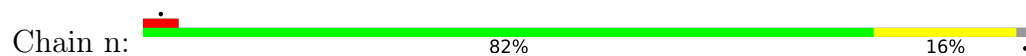
- Molecule 26: 50S ribosomal protein L29



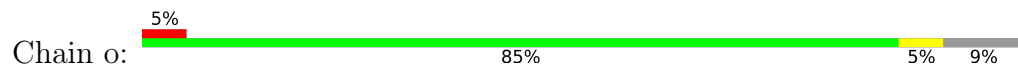
- Molecule 27: 50S ribosomal protein L30



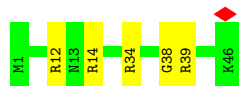
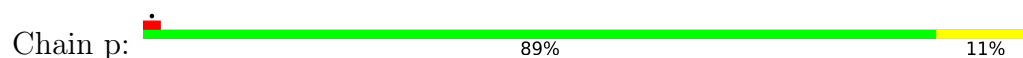
- Molecule 28: 50S ribosomal protein L32



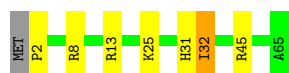
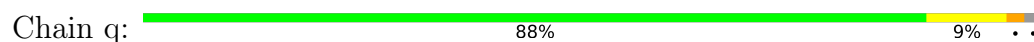
- Molecule 29: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L34



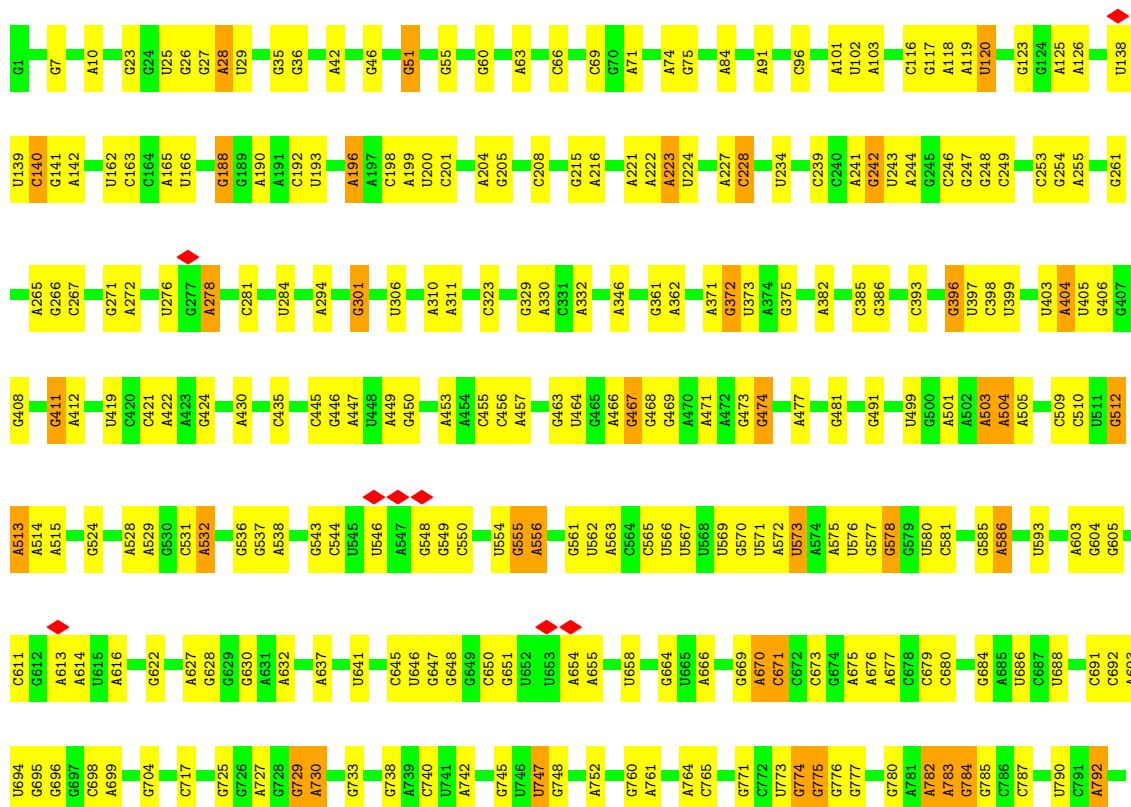
- Molecule 31: 50S ribosomal protein L35



- Molecule 32: 50S ribosomal protein L36

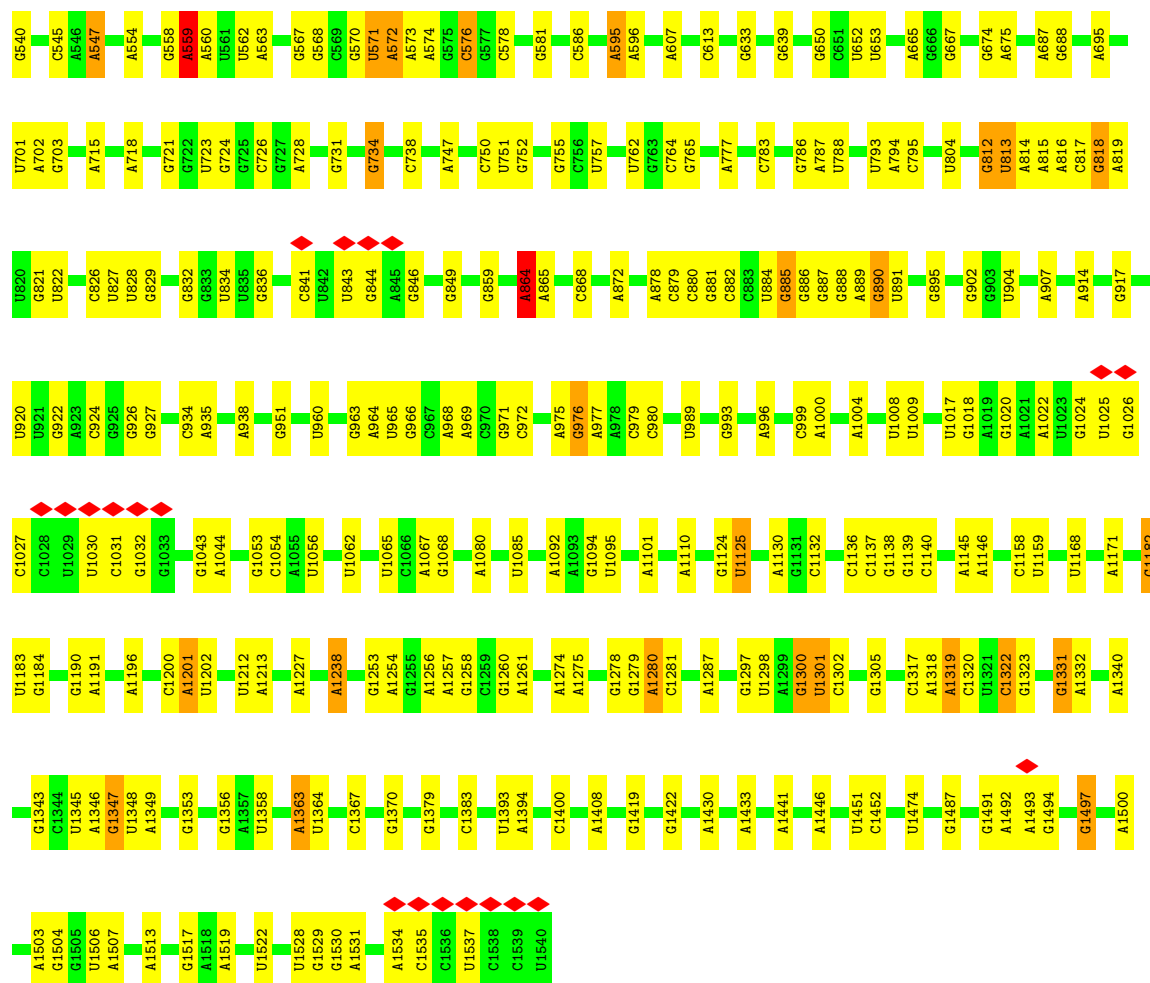


- Molecule 33: 23S rRNA

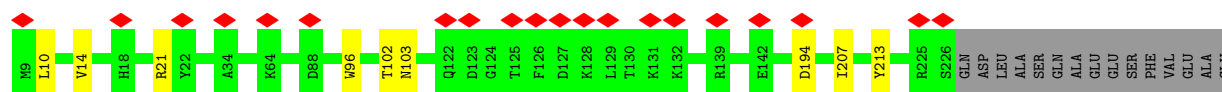
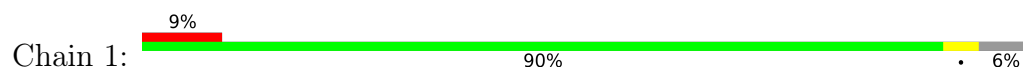




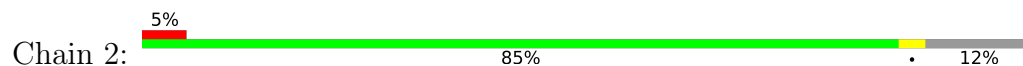




• Molecule 36: 30S ribosomal protein S2



• Molecule 37: 30S ribosomal protein S3

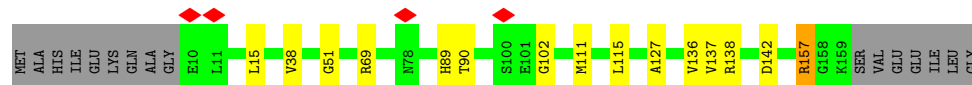
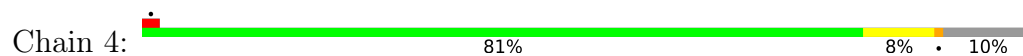


• Molecule 38: 30S ribosomal protein S4

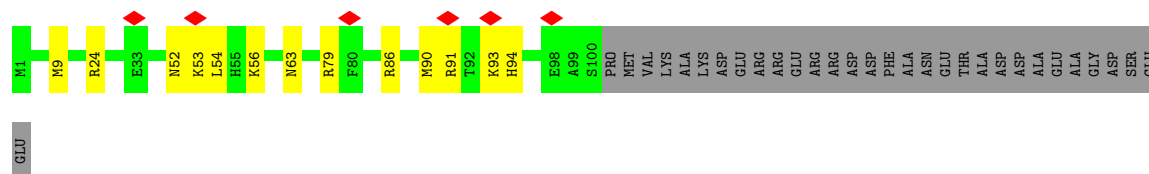




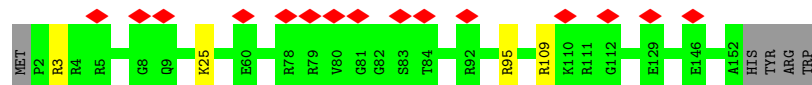
- Molecule 39: 30S ribosomal protein S5



- Molecule 40: 30S ribosomal protein S6



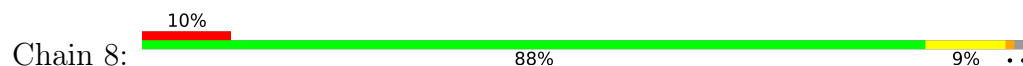
- Molecule 41: 30S ribosomal protein S7



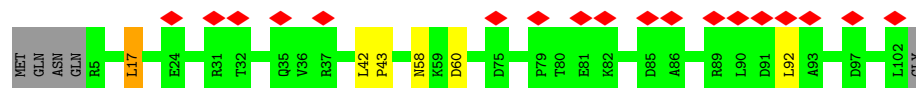
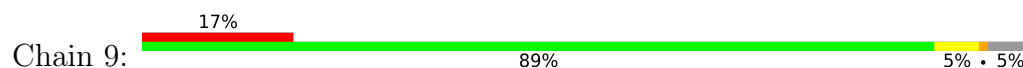
- Molecule 42: 30S ribosomal protein S8




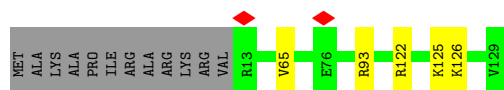
- Molecule 43: 30S ribosomal protein S9



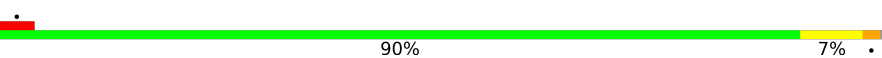
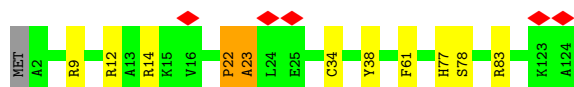
- Molecule 44: 30S ribosomal protein S10



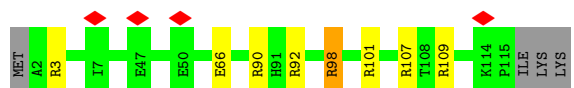
• Molecule 45: 30S ribosomal protein S11

Chain A:  87% 9%


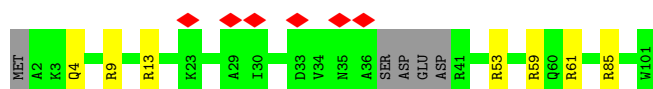
• Molecule 46: 30S ribosomal protein S12

Chain B:  90% 7% ..

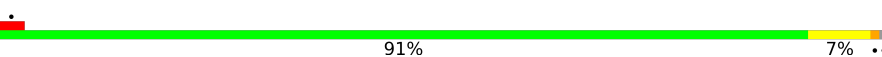
• Molecule 47: 30S ribosomal protein S13

Chain C:  90% 6% ..

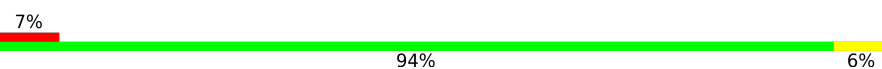
• Molecule 48: 30S ribosomal protein S14

Chain D:  88% 7% 5%


• Molecule 49: 30S ribosomal protein S15

Chain E:  91% 7% ..

• Molecule 50: 30S ribosomal protein S16

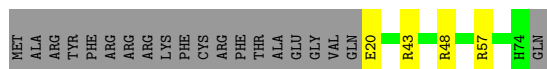
Chain F:  94% 6% 7%

• Molecule 51: 30S ribosomal protein S17

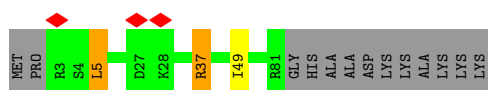
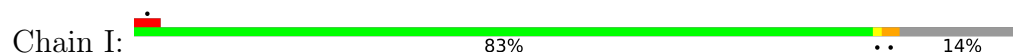
Chain G:  88% 7% 5%



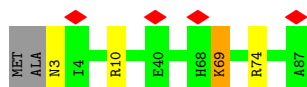
- Molecule 52: 30S ribosomal protein S18



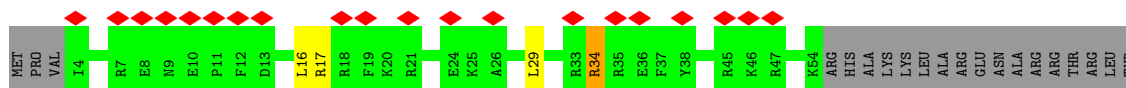
- Molecule 53: 30S ribosomal protein S19



- Molecule 54: 30S ribosomal protein S20



- Molecule 55: 30S ribosomal protein S21



- Molecule 56: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	400024	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.318	Depositor
Minimum map value	-0.174	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	398.912, 398.912, 398.912	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	s	0.89	1/326 (0.3%)	0.80	1/441 (0.2%)
2	M	0.63	3/1779 (0.2%)	0.83	2/2768 (0.1%)
3	O	0.79	2/2828 (0.1%)	0.87	6/4410 (0.1%)
4	P	1.41	22/2121 (1.0%)	1.32	27/2852 (0.9%)
5	Q	1.18	3/1585 (0.2%)	1.13	8/2134 (0.4%)
6	R	0.97	3/1571 (0.2%)	1.02	9/2113 (0.4%)
7	S	0.67	0/1434	0.85	0/1926
8	T	0.67	0/1342	0.83	4/1816 (0.2%)
9	U	0.76	0/364	1.05	1/490 (0.2%)
10	V	0.52	0/1045	0.65	0/1410
11	W	1.10	4/1151 (0.3%)	1.10	7/1551 (0.5%)
12	X	1.15	0/947	1.19	5/1268 (0.4%)
13	Y	1.30	3/1053 (0.3%)	1.38	13/1403 (0.9%)
14	Z	1.13	2/1092 (0.2%)	1.19	7/1460 (0.5%)
15	a	1.28	3/973 (0.3%)	1.30	10/1301 (0.8%)
16	b	0.84	2/901 (0.2%)	1.08	8/1209 (0.7%)
17	c	1.09	3/927 (0.3%)	1.19	7/1240 (0.6%)
18	d	1.32	5/959 (0.5%)	1.37	15/1278 (1.2%)
19	e	1.08	2/828 (0.2%)	1.08	3/1107 (0.3%)
20	f	1.02	1/864 (0.1%)	1.09	1/1156 (0.1%)
21	g	0.91	0/744	1.01	2/994 (0.2%)
22	h	0.82	1/787 (0.1%)	0.89	0/1051
23	i	0.78	0/765	0.86	0/1025
24	j	1.21	2/575 (0.3%)	1.29	6/762 (0.8%)
25	k	1.09	1/634 (0.2%)	1.15	6/848 (0.7%)
26	l	0.71	0/509	1.05	4/677 (0.6%)
27	m	0.86	0/452	1.08	2/605 (0.3%)
28	n	1.16	2/449 (0.4%)	1.42	7/599 (1.2%)
29	o	1.31	7/416 (1.7%)	0.96	1/554 (0.2%)
30	p	1.38	3/379 (0.8%)	1.75	6/498 (1.2%)
31	q	1.14	0/512	1.26	6/676 (0.9%)
32	r	1.15	1/302 (0.3%)	1.35	5/397 (1.3%)
33	N	1.24	512/69681 (0.7%)	1.04	347/108706 (0.3%)
34	L	0.61	0/531	0.85	0/709

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	0	0.96	132/36966 (0.4%)	0.93	107/57666 (0.2%)
36	1	0.82	2/1735 (0.1%)	0.94	3/2338 (0.1%)
37	2	0.85	1/1651 (0.1%)	0.95	4/2225 (0.2%)
38	3	0.75	0/1664	0.98	6/2227 (0.3%)
39	4	1.11	1/1118 (0.1%)	1.21	6/1504 (0.4%)
40	5	0.90	1/835 (0.1%)	1.04	4/1128 (0.4%)
41	6	0.66	0/1195	0.95	5/1602 (0.3%)
42	7	0.88	0/988	0.99	2/1326 (0.2%)
43	8	0.85	0/1033	1.13	7/1375 (0.5%)
44	9	0.74	0/796	1.01	3/1077 (0.3%)
45	A	0.85	1/892 (0.1%)	1.03	3/1205 (0.2%)
46	B	1.09	3/968 (0.3%)	1.22	7/1300 (0.5%)
47	C	0.85	1/892 (0.1%)	1.12	9/1193 (0.8%)
48	D	0.86	0/784	1.14	7/1043 (0.7%)
49	E	0.94	0/717	1.14	8/959 (0.8%)
50	F	0.94	0/658	1.16	5/884 (0.6%)
51	G	0.82	0/657	1.02	0/881
52	H	0.98	1/462 (0.2%)	1.11	2/621 (0.3%)
53	I	0.81	0/652	1.05	3/877 (0.3%)
54	J	0.89	0/670	1.06	3/888 (0.3%)
55	K	1.07	1/430 (0.2%)	1.24	4/570 (0.7%)
56	t	0.87	0/94	0.96	1/144 (0.7%)
All	All	1.10	732/156683 (0.5%)	1.03	725/234467 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	P	0	3
5	Q	0	1
7	S	0	2
9	U	0	1
10	V	0	1
13	Y	0	2
14	Z	0	2
22	h	0	1
31	q	0	1
33	N	0	7
35	0	0	5
36	1	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
37	2	0	2
39	4	0	5
40	5	0	2
43	8	0	4
45	A	0	1
46	B	0	2
51	G	0	2
53	I	0	1
54	J	0	1
55	K	0	1
All	All	0	50

All (732) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	2873	A	C6-N1	-20.61	1.21	1.35
33	N	2765	A	C6-N1	-18.53	1.22	1.35
33	N	2502	G	P-OP2	16.69	1.77	1.49
33	N	503	A	C6-N1	-15.32	1.24	1.35
33	N	1156	A	P-OP2	15.22	1.74	1.49
35	0	1238	A	C6-N1	-13.84	1.25	1.35
4	P	213	TRP	CD2-CE2	13.73	1.57	1.41
35	0	24	U	N3-C4	-13.70	1.26	1.38
33	N	1333	G	P-OP2	12.86	1.70	1.49
33	N	783	A	P-OP2	12.70	1.70	1.49
33	N	945	A	P-OP2	12.30	1.69	1.49
33	N	1639	C	P-OP1	12.14	1.69	1.49
33	N	945	A	P-OP1	11.86	1.69	1.49
33	N	1664	A	P-OP2	11.84	1.69	1.49
33	N	310	A	C6-N1	-11.57	1.27	1.35
33	N	1670	C	P-OP1	11.52	1.68	1.49
4	P	213	TRP	CZ3-CH2	11.46	1.58	1.40
33	N	1141	U	N3-C4	-11.46	1.28	1.38
33	N	2074	U	P-OP1	11.41	1.68	1.49
35	0	559	A	N1-C2	11.40	1.44	1.34
33	N	234	U	N3-C4	-11.32	1.28	1.38
35	0	368	U	N3-C4	-11.28	1.28	1.38
35	0	37	U	N3-C4	-11.18	1.28	1.38
4	P	213	TRP	CB-CG	-11.07	1.30	1.50
33	N	2588	G	P-OP1	11.05	1.67	1.49
33	N	828	U	O3'-P	-10.91	1.48	1.61
33	N	2005	A	P-OP1	10.76	1.67	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	2349	G	O3'-P	-10.76	1.48	1.61
33	N	2445	G	O3'-P	-10.72	1.48	1.61
33	N	2272	U	N3-C4	-10.66	1.28	1.38
33	N	827	U	P-OP1	10.63	1.67	1.49
33	N	450	G	P-OP2	10.62	1.67	1.49
33	N	963	U	O3'-P	-10.48	1.48	1.61
33	N	932	U	N3-C4	-10.39	1.29	1.38
33	N	1777	U	O3'-P	-10.32	1.48	1.61
33	N	943	A	P-OP2	10.25	1.66	1.49
33	N	2589	A	O3'-P	-10.25	1.48	1.61
22	h	68	SER	CB-OG	10.19	1.55	1.42
33	N	2025	C	P-OP2	10.15	1.66	1.49
2	M	1	U	OP3-P	-10.13	1.49	1.61
35	0	757	U	O3'-P	-10.06	1.49	1.61
33	N	567	U	P-OP1	10.04	1.66	1.49
33	N	2060	A	O3'-P	-10.03	1.49	1.61
35	0	1301	U	N3-C4	10.03	1.47	1.38
35	0	1358	U	N3-C4	-10.02	1.29	1.38
35	0	578	C	P-OP1	9.99	1.66	1.49
33	N	800	A	P-OP1	9.97	1.66	1.49
33	N	787	C	O3'-P	-9.88	1.49	1.61
29	o	21	TYR	CE2-CZ	-9.84	1.25	1.38
33	N	782	A	O3'-P	-9.82	1.49	1.61
35	0	24	U	C2-N3	9.82	1.44	1.37
33	N	1968	G	O3'-P	-9.82	1.49	1.61
33	N	692	C	O3'-P	-9.79	1.49	1.61
35	0	20	U	O3'-P	-9.78	1.49	1.61
33	N	1604	C	P-OP1	9.72	1.65	1.49
33	N	2522	U	C2-N3	9.71	1.44	1.37
33	N	2687	U	O3'-P	-9.69	1.49	1.61
33	N	585	G	O3'-P	-9.68	1.49	1.61
33	N	825	A	O3'-P	-9.68	1.49	1.61
33	N	1009	A	O3'-P	-9.68	1.49	1.61
33	N	2615	U	P-OP1	9.66	1.65	1.49
35	0	21	G	P-OP1	9.66	1.65	1.49
33	N	1774	C	P-OP1	9.64	1.65	1.49
33	N	2720	U	C2-N3	9.60	1.44	1.37
33	N	1257	C	O3'-P	-9.52	1.49	1.61
33	N	2344	U	N3-C4	-9.36	1.30	1.38
33	N	963	U	P-OP1	9.34	1.64	1.49
33	N	554	U	O3'-P	-9.32	1.50	1.61
33	N	809	G	O3'-P	-9.30	1.50	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	1828	G	P-OP2	9.29	1.64	1.49
33	N	2550	G	O3'-P	-9.26	1.50	1.61
33	N	2019	A	O3'-P	-9.24	1.50	1.61
33	N	116	C	O3'-P	-9.24	1.50	1.61
33	N	2025	C	O3'-P	-9.23	1.50	1.61
33	N	2593	U	O3'-P	-9.19	1.50	1.61
33	N	576	U	P-OP1	9.15	1.64	1.49
33	N	2050	C	O3'-P	-9.15	1.50	1.61
33	N	445	C	O3'-P	-9.14	1.50	1.61
33	N	306	U	N3-C4	9.08	1.46	1.38
35	0	667	G	O3'-P	-9.07	1.50	1.61
33	N	948	C	P-OP1	9.06	1.64	1.49
33	N	1152	C	O3'-P	-9.01	1.50	1.61
33	N	984	A	O3'-P	-9.01	1.50	1.61
33	N	1269	A	P-OP2	9.01	1.64	1.49
35	0	882	C	O3'-P	-8.99	1.50	1.61
33	N	1375	U	O3'-P	-8.99	1.50	1.61
33	N	2588	G	O3'-P	-8.92	1.50	1.61
33	N	397	U	O3'-P	-8.84	1.50	1.61
33	N	673	C	O3'-P	-8.81	1.50	1.61
35	0	827	U	N3-C4	-8.80	1.30	1.38
33	N	2588	G	P-OP2	8.78	1.63	1.49
33	N	2543	G	P-OP1	8.77	1.63	1.49
33	N	1019	U	O3'-P	-8.70	1.50	1.61
33	N	859	G	O3'-P	8.69	1.71	1.61
33	N	2052	A	O3'-P	-8.67	1.50	1.61
33	N	2576	G	P-OP1	8.64	1.63	1.49
33	N	120	U	P-OP1	8.64	1.63	1.49
33	N	1612	C	O3'-P	-8.57	1.50	1.61
33	N	2635	A	O3'-P	-8.55	1.50	1.61
33	N	1664	A	P-OP1	8.53	1.63	1.49
33	N	200	U	O3'-P	-8.53	1.50	1.61
33	N	2698	U	O3'-P	-8.52	1.50	1.61
33	N	1774	C	O3'-P	-8.52	1.50	1.61
33	N	2714	G	P-OP2	8.51	1.63	1.49
33	N	1994	C	O3'-P	-8.45	1.51	1.61
32	r	38	GLY	N-CA	8.44	1.58	1.46
4	P	195	VAL	CB-CG1	-8.38	1.35	1.52
33	N	503	A	N1-C2	8.35	1.41	1.34
33	N	2466	C	O3'-P	-8.32	1.51	1.61
35	0	812	G	O3'-P	8.29	1.71	1.61
35	0	1500	A	O3'-P	-8.28	1.51	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	1751	U	O3'-P	-8.27	1.51	1.61
33	N	2503	A	P-OP2	8.27	1.63	1.49
33	N	1658	C	O3'-P	-8.26	1.51	1.61
33	N	499	U	N3-C4	8.25	1.45	1.38
33	N	641	U	O3'-P	-8.23	1.51	1.61
33	N	1900	A	O3'-P	8.23	1.71	1.61
33	N	2498	C	P-OP2	8.21	1.62	1.49
33	N	1831	G	O3'-P	-8.20	1.51	1.61
33	N	826	U	P-OP1	8.19	1.62	1.49
33	N	2740	A	O3'-P	-8.17	1.51	1.61
33	N	2613	U	N3-C4	-8.17	1.31	1.38
13	Y	18	ARG	CZ-NH1	8.16	1.43	1.33
33	N	955	U	O3'-P	-8.16	1.51	1.61
33	N	453	A	P-OP1	8.15	1.62	1.49
33	N	1353	A	O3'-P	-8.15	1.51	1.61
33	N	1780	A	P-OP1	8.14	1.62	1.49
33	N	2022	U	P-OP1	8.14	1.62	1.49
33	N	1254	A	O3'-P	-8.01	1.51	1.61
33	N	2489	U	O3'-P	-7.98	1.51	1.61
33	N	2605	U	O3'-P	-7.96	1.51	1.61
33	N	1658	C	P-OP1	7.96	1.62	1.49
33	N	2437	G	O3'-P	-7.91	1.51	1.61
33	N	2502	G	O5'-C5'	-7.91	1.30	1.42
33	N	2264	C	O3'-P	-7.90	1.51	1.61
33	N	1813	G	O3'-P	-7.87	1.51	1.61
33	N	2006	C	P-OP1	7.83	1.62	1.49
33	N	372	G	O3'-P	7.79	1.70	1.61
33	N	2590	A	O3'-P	-7.79	1.51	1.61
33	N	1782	U	P-OP1	7.79	1.62	1.49
33	N	839	U	O3'-P	-7.79	1.51	1.61
33	N	2062	A	P-OP2	7.75	1.62	1.49
35	O	726	C	O3'-P	-7.75	1.51	1.61
33	N	192	C	P-OP1	7.74	1.62	1.49
33	N	733	G	O3'-P	-7.72	1.51	1.61
33	N	2265	U	O3'-P	-7.71	1.51	1.61
33	N	1189	A	O3'-P	-7.71	1.51	1.61
4	P	204	VAL	CB-CG2	-7.70	1.36	1.52
33	N	1268	A	P-OP1	7.70	1.62	1.49
33	N	1794	A	O3'-P	-7.69	1.51	1.61
33	N	192	C	O3'-P	-7.69	1.51	1.61
33	N	2572	A	O3'-P	-7.67	1.51	1.61
33	N	2447	G	O3'-P	-7.65	1.51	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	832	U	O3'-P	-7.65	1.51	1.61
33	N	1778	U	O3'-P	-7.63	1.51	1.61
33	N	2518	A	P-OP2	7.62	1.61	1.49
33	N	810	U	P-OP1	7.60	1.61	1.49
33	N	997	G	O3'-P	-7.59	1.52	1.61
33	N	515	A	O3'-P	-7.59	1.52	1.61
33	N	1790	C	O3'-P	-7.59	1.52	1.61
35	0	884	U	C4-O4	-7.59	1.17	1.23
33	N	464	U	O3'-P	-7.55	1.52	1.61
33	N	569	U	O3'-P	-7.53	1.52	1.61
33	N	1771	C	O3'-P	-7.50	1.52	1.61
33	N	254	G	O3'-P	-7.50	1.52	1.61
33	N	676	A	O3'-P	-7.50	1.52	1.61
33	N	821	A	O3'-P	-7.49	1.52	1.61
13	Y	51	GLU	C-O	7.48	1.37	1.23
33	N	1970	A	P-OP2	7.48	1.61	1.49
33	N	2620	C	O3'-P	-7.47	1.52	1.61
33	N	2822	G	O3'-P	-7.47	1.52	1.61
13	Y	22	GLY	C-O	-7.47	1.11	1.23
33	N	1828	G	P-OP1	7.46	1.61	1.49
33	N	2081	U	O3'-P	-7.46	1.52	1.61
35	0	1238	A	N1-C2	7.46	1.41	1.34
33	N	2031	A	P-OP1	-7.46	1.36	1.49
35	0	1367	C	O3'-P	-7.46	1.52	1.61
33	N	2272	U	C4-O4	-7.45	1.17	1.23
33	N	2061	G	C2'-O2'	7.45	1.51	1.41
33	N	2867	G	O3'-P	7.44	1.70	1.61
40	5	63	ASN	C-O	-7.44	1.09	1.23
16	b	30	ARG	CZ-NH1	7.43	1.42	1.33
35	0	1393	U	O3'-P	-7.43	1.52	1.61
33	N	2625	G	O3'-P	-7.42	1.52	1.61
33	N	1678	A	P-OP2	7.40	1.61	1.49
33	N	2637	U	O3'-P	-7.39	1.52	1.61
33	N	975	A	P-OP2	7.37	1.61	1.49
33	N	2072	C	O3'-P	-7.33	1.52	1.61
33	N	538	A	O3'-P	-7.33	1.52	1.61
33	N	2232	C	O3'-P	-7.33	1.52	1.61
33	N	2837	A	O3'-P	-7.33	1.52	1.61
33	N	2444	G	O3'-P	-7.32	1.52	1.61
33	N	566	U	O3'-P	-7.29	1.52	1.61
33	N	2344	U	C2-N3	-7.29	1.32	1.37
33	N	2359	C	O3'-P	-7.28	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	2457	U	O3'-P	-7.27	1.52	1.61
33	N	1822	C	O3'-P	-7.26	1.52	1.61
33	N	2247	A	O3'-P	-7.24	1.52	1.61
4	P	221	ARG	CB-CG	-7.24	1.33	1.52
33	N	198	C	O3'-P	-7.24	1.52	1.61
33	N	572	A	P-OP1	7.21	1.61	1.49
35	O	387	U	O3'-P	-7.20	1.52	1.61
33	N	2684	U	O3'-P	-7.18	1.52	1.61
35	O	22	G	O3'-P	-7.18	1.52	1.61
33	N	2602	A	O3'-P	7.17	1.69	1.61
33	N	2598	A	O3'-P	-7.17	1.52	1.61
33	N	1261	C	O3'-P	-7.17	1.52	1.61
33	N	2542	A	O3'-P	-7.15	1.52	1.61
33	N	1298	C	O3'-P	-7.14	1.52	1.61
33	N	966	G	O3'-P	-7.13	1.52	1.61
33	N	1805	A	O3'-P	-7.13	1.52	1.61
33	N	2013	A	O3'-P	-7.12	1.52	1.61
33	N	126	A	O3'-P	-7.11	1.52	1.61
29	o	21	TYR	CG-CD1	-7.11	1.29	1.39
33	N	2013	A	C6-N6	-7.11	1.28	1.33
33	N	940	G	O3'-P	-7.10	1.52	1.61
33	N	1681	G	O3'-P	-7.08	1.52	1.61
33	N	671	C	P-OP2	7.08	1.60	1.49
33	N	29	U	O3'-P	-7.07	1.52	1.61
33	N	818	G	P-OP2	7.07	1.60	1.49
33	N	571	U	O3'-P	-7.07	1.52	1.61
33	N	2016	U	O3'-P	-7.06	1.52	1.61
35	O	563	A	C6-N6	-7.06	1.28	1.33
46	B	34	CYS	CB-SG	-7.05	1.70	1.82
33	N	2406	A	P-OP1	7.03	1.60	1.49
33	N	25	U	O3'-P	-7.03	1.52	1.61
35	O	505	G	O3'-P	-7.03	1.52	1.61
33	N	1795	C	O3'-P	-7.01	1.52	1.61
3	O	83	G	O3'-P	-7.01	1.52	1.61
35	O	1358	U	C4-O4	-7.01	1.18	1.23
33	N	2419	U	C4-O4	7.01	1.29	1.23
33	N	2385	C	P-OP1	7.00	1.60	1.49
33	N	773	U	O3'-P	-7.00	1.52	1.61
33	N	796	C	O3'-P	-6.99	1.52	1.61
33	N	1141	U	C2-N3	-6.97	1.32	1.37
33	N	1949	G	O3'-P	-6.97	1.52	1.61
33	N	2049	G	O3'-P	-6.97	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	680	C	O3'-P	-6.96	1.52	1.61
33	N	2499	C	P-OP2	6.95	1.60	1.49
29	o	21	TYR	CG-CD2	-6.94	1.30	1.39
33	N	2829	A	O3'-P	-6.89	1.52	1.61
35	0	764	C	O3'-P	-6.88	1.52	1.61
35	0	765	G	O3'-P	-6.87	1.52	1.61
33	N	2051	A	O3'-P	6.86	1.69	1.61
33	N	2332	C	O3'-P	-6.86	1.52	1.61
15	a	1	MET	C-O	6.86	1.36	1.23
33	N	730	A	P-OP2	6.86	1.60	1.49
33	N	2436	G	O3'-P	-6.85	1.52	1.61
33	N	2443	C	C4'-C3'	-6.84	1.45	1.53
35	0	980	C	P-OP1	6.83	1.60	1.49
33	N	1394	U	O3'-P	-6.79	1.53	1.61
33	N	239	C	O3'-P	-6.79	1.53	1.61
33	N	1824	G	P-OP2	6.78	1.60	1.49
33	N	688	U	O3'-P	-6.77	1.53	1.61
33	N	927	A	N1-C2	6.76	1.40	1.34
33	N	923	G	O3'-P	-6.76	1.53	1.61
33	N	2572	A	P-OP1	-6.75	1.37	1.49
33	N	784	G	O3'-P	6.74	1.69	1.61
33	N	2048	G	O3'-P	-6.71	1.53	1.61
33	N	2268	A	P-OP1	6.71	1.60	1.49
33	N	2516	A	O3'-P	-6.70	1.53	1.61
33	N	2285	C	O3'-P	-6.70	1.53	1.61
33	N	578	G	P-OP2	6.69	1.60	1.49
35	0	814	A	P-OP2	6.68	1.60	1.49
33	N	1782	U	O3'-P	-6.68	1.53	1.61
33	N	419	U	O3'-P	-6.68	1.53	1.61
33	N	2499	C	P-OP1	6.68	1.60	1.49
4	P	10	SER	CA-CB	6.66	1.62	1.52
33	N	1662	U	P-OP2	6.65	1.60	1.49
4	P	271	ARG	CZ-NH1	6.65	1.41	1.33
35	0	37	U	C2-N3	-6.64	1.33	1.37
33	N	2074	U	O3'-P	-6.64	1.53	1.61
33	N	2045	C	O3'-P	-6.64	1.53	1.61
33	N	2260	C	O3'-P	-6.62	1.53	1.61
35	0	1182	G	O3'-P	6.62	1.69	1.61
33	N	2694	G	O3'-P	-6.60	1.53	1.61
33	N	1234	U	O3'-P	-6.60	1.53	1.61
33	N	1649	G	O3'-P	-6.59	1.53	1.61
33	N	1977	A	O3'-P	-6.59	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	139	SER	CB-OG	-6.59	1.33	1.42
24	j	42	GLY	N-CA	6.58	1.55	1.46
33	N	1960	A	O3'-P	-6.58	1.53	1.61
30	p	34	ARG	CG-CD	-6.57	1.35	1.51
33	N	783	A	C4'-O4'	6.56	1.54	1.45
33	N	2072	C	P-OP1	6.56	1.60	1.49
35	0	864	A	N1-C2	6.56	1.40	1.34
33	N	932	U	C4-O4	-6.56	1.18	1.23
18	d	24	TYR	CG-CD1	6.55	1.47	1.39
33	N	698	C	O3'-P	-6.54	1.53	1.61
33	N	2289	G	O3'-P	-6.54	1.53	1.61
33	N	117	G	O3'-P	-6.54	1.53	1.61
33	N	1009	A	P-OP2	6.54	1.60	1.49
33	N	761	A	P-OP1	6.54	1.60	1.49
17	c	98	TYR	CE1-CZ	6.53	1.47	1.38
33	N	193	U	O3'-P	-6.53	1.53	1.61
33	N	2452	C	O3'-P	-6.53	1.53	1.61
33	N	1334	G	O3'-P	-6.53	1.53	1.61
33	N	499	U	C4-O4	-6.52	1.18	1.23
39	4	127	ALA	C-O	-6.51	1.10	1.23
33	N	1432	G	O3'-P	-6.50	1.53	1.61
33	N	2028	U	O3'-P	-6.49	1.53	1.61
33	N	2723	C	O3'-P	-6.48	1.53	1.61
33	N	1191	G	O3'-P	-6.48	1.53	1.61
33	N	1010	A	P-OP2	6.48	1.59	1.49
33	N	2727	A	O3'-P	-6.48	1.53	1.61
33	N	960	A	O3'-P	-6.47	1.53	1.61
33	N	393	C	P-OP1	6.46	1.59	1.49
33	N	2426	A	O3'-P	-6.45	1.53	1.61
33	N	1142	A	O3'-P	6.45	1.68	1.61
33	N	2699	C	O3'-P	-6.45	1.53	1.61
33	N	1993	U	O5'-C5'	-6.44	1.32	1.42
33	N	694	U	O3'-P	-6.43	1.53	1.61
33	N	2248	C	P-OP2	6.43	1.59	1.49
33	N	2262	U	O3'-P	-6.43	1.53	1.61
30	p	38	GLY	CA-C	-6.41	1.41	1.51
33	N	1677	A	O3'-P	-6.41	1.53	1.61
33	N	1296	G	O3'-P	-6.41	1.53	1.61
5	Q	125	TRP	CE3-CZ3	-6.41	1.27	1.38
35	0	368	U	C4-O4	-6.40	1.18	1.23
33	N	2502	G	O3'-P	-6.40	1.53	1.61
18	d	49	ASP	CB-CG	6.39	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	1186	G	P-OP2	6.39	1.59	1.49
35	O	715	A	O3'-P	-6.39	1.53	1.61
33	N	28	A	P-O5'	-6.38	1.53	1.59
33	N	1652	A	O3'-P	-6.38	1.53	1.61
35	O	368	U	C2-N3	-6.38	1.33	1.37
33	N	1186	G	O3'-P	-6.38	1.53	1.61
33	N	1680	U	O3'-P	-6.38	1.53	1.61
33	N	2243	U	P-OP1	6.37	1.59	1.49
33	N	1367	A	O3'-P	-6.35	1.53	1.61
35	O	1062	U	O3'-P	-6.35	1.53	1.61
4	P	219	THR	C-O	6.34	1.35	1.23
33	N	2444	G	C2'-C1'	-6.33	1.46	1.53
33	N	745	G	O3'-P	-6.33	1.53	1.61
33	N	1671	U	P-OP2	6.33	1.59	1.49
33	N	632	A	O3'-P	-6.33	1.53	1.61
33	N	1141	U	C4-O4	-6.33	1.18	1.23
33	N	208	C	O3'-P	-6.32	1.53	1.61
4	P	213	TRP	CD1-NE1	6.31	1.48	1.38
33	N	408	G	O3'-P	-6.31	1.53	1.61
55	K	34	ARG	CZ-NH1	6.31	1.41	1.33
33	N	2554	U	P-OP2	-6.30	1.38	1.49
29	O	49	TYR	CE1-CZ	-6.30	1.30	1.38
35	O	812	G	C3'-C2'	-6.29	1.45	1.52
35	O	37	U	C4-O4	-6.29	1.18	1.23
33	N	1327	A	P-OP2	6.29	1.59	1.49
35	O	19	A	O3'-P	-6.28	1.53	1.61
33	N	247	G	O3'-P	-6.28	1.53	1.61
33	N	1650	A	O3'-P	-6.28	1.53	1.61
35	O	787	A	O3'-P	-6.28	1.53	1.61
33	N	946	C	P-OP2	6.28	1.59	1.49
33	N	2000	C	O3'-P	-6.27	1.53	1.61
33	N	783	A	C5-C6	-6.26	1.35	1.41
33	N	1004	U	O3'-P	-6.26	1.53	1.61
33	N	1026	G	P-OP2	-6.26	1.38	1.49
35	O	439	U	C2-N3	6.26	1.42	1.37
11	W	16	TYR	CG-CD1	-6.25	1.31	1.39
33	N	576	U	O3'-P	-6.25	1.53	1.61
35	O	1301	U	N1-C2	6.24	1.44	1.38
33	N	1342	A	P-OP2	6.24	1.59	1.49
35	O	884	U	N3-C4	-6.24	1.32	1.38
33	N	7	G	O3'-P	-6.23	1.53	1.61
4	P	214	ARG	CZ-NH1	6.23	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	567	U	O3'-P	-6.22	1.53	1.61
35	0	572	A	P-OP1	6.22	1.59	1.49
33	N	1827	U	O3'-P	-6.21	1.53	1.61
35	0	613	C	O3'-P	-6.21	1.53	1.61
33	N	1816	C	O3'-P	-6.21	1.53	1.61
33	N	253	C	O3'-P	-6.21	1.53	1.61
35	0	920	U	O3'-P	-6.20	1.53	1.61
33	N	2543	G	O5'-C5'	-6.19	1.32	1.42
33	N	26	G	O3'-P	-6.19	1.53	1.61
35	0	568	G	O3'-P	-6.19	1.53	1.61
33	N	411	G	P-OP1	6.18	1.59	1.49
33	N	430	A	C6-N6	-6.18	1.29	1.33
46	B	23	ALA	N-CA	6.18	1.58	1.46
33	N	1196	C	O3'-P	-6.18	1.53	1.61
33	N	120	U	P-OP2	6.17	1.59	1.49
35	0	498	A	N1-C2	6.17	1.40	1.34
33	N	398	C	O3'-P	-6.17	1.53	1.61
35	0	1358	U	C2-N3	-6.17	1.33	1.37
33	N	1142	A	C5-C6	-6.16	1.35	1.41
33	N	593	U	O3'-P	-6.16	1.53	1.61
33	N	2263	C	O3'-P	-6.16	1.53	1.61
33	N	932	U	C2-N3	-6.16	1.33	1.37
17	c	93	ARG	CD-NE	-6.15	1.35	1.46
33	N	2682	A	P-OP2	6.15	1.59	1.49
33	N	777	G	O3'-P	-6.15	1.53	1.61
35	0	1474	U	O3'-P	-6.14	1.53	1.61
33	N	1006	C	O3'-P	-6.14	1.53	1.61
35	0	581	G	O3'-P	-6.14	1.53	1.61
33	N	123	G	O3'-P	-6.13	1.53	1.61
33	N	234	U	C2-N3	-6.12	1.33	1.37
33	N	2035	G	O5'-C5'	-6.12	1.33	1.42
33	N	725	G	O3'-P	-6.11	1.53	1.61
33	N	1968	G	P-OP1	6.11	1.59	1.49
33	N	1370	C	O3'-P	-6.11	1.53	1.61
15	a	2	ARG	C-O	-6.11	1.11	1.23
33	N	1957	C	O3'-P	-6.10	1.53	1.61
33	N	244	A	O3'-P	-6.09	1.53	1.61
33	N	1153	C	P-OP2	6.09	1.59	1.49
35	0	1080	A	O3'-P	-6.08	1.53	1.61
33	N	1636	U	O3'-P	-6.07	1.53	1.61
35	0	356	A	O3'-P	-6.07	1.53	1.61
35	0	1110	A	P-OP2	6.06	1.59	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	0	46	G	O3'-P	-6.05	1.53	1.61
33	N	1368	G	O3'-P	-6.05	1.53	1.61
33	N	1905	C	O3'-P	-6.04	1.53	1.61
35	0	816	A	O3'-P	-6.04	1.53	1.61
33	N	1793	C	O3'-P	-6.04	1.53	1.61
33	N	2571	U	O3'-P	-6.04	1.53	1.61
33	N	190	A	O3'-P	-6.03	1.53	1.61
33	N	1756	G	O3'-P	-6.03	1.53	1.61
33	N	2642	G	O3'-P	-6.03	1.53	1.61
35	0	1522	U	O3'-P	-6.03	1.53	1.61
33	N	2503	A	P-OP1	6.01	1.59	1.49
33	N	1134	A	O3'-P	6.01	1.68	1.61
33	N	2003	A	O3'-P	-6.01	1.53	1.61
33	N	727	A	P-OP1	6.00	1.59	1.49
35	0	834	U	O3'-P	-6.00	1.53	1.61
33	N	2277	G	O3'-P	-6.00	1.53	1.61
33	N	963	U	P-OP2	6.00	1.59	1.49
33	N	1205	A	O3'-P	5.99	1.68	1.61
33	N	1648	U	P-OP2	5.99	1.59	1.49
33	N	699	A	O3'-P	-5.97	1.53	1.61
35	0	917	G	O3'-P	-5.97	1.53	1.61
33	N	2847	U	O3'-P	-5.97	1.53	1.61
33	N	2776	A	C5-C6	-5.97	1.35	1.41
35	0	1513	A	O3'-P	-5.95	1.54	1.61
33	N	1676	A	O3'-P	-5.95	1.54	1.61
35	0	813	U	P-O5'	-5.94	1.53	1.59
35	0	500	G	O3'-P	-5.94	1.54	1.61
33	N	2442	C	O3'-P	-5.94	1.54	1.61
35	0	118	U	O3'-P	-5.93	1.54	1.61
2	M	72	G	O3'-P	-5.92	1.54	1.61
33	N	1187	G	P-OP2	5.92	1.59	1.49
6	R	80	SER	C-O	-5.92	1.12	1.23
35	0	879	C	O3'-P	-5.92	1.54	1.61
33	N	1323	C	O3'-P	-5.92	1.54	1.61
33	N	1007	C	O3'-P	-5.91	1.54	1.61
35	0	888	G	O3'-P	-5.91	1.54	1.61
33	N	2238	G	O3'-P	5.90	1.68	1.61
33	N	524	G	O3'-P	-5.90	1.54	1.61
33	N	2250	G	C5-C6	-5.90	1.36	1.42
33	N	2626	C	O3'-P	-5.89	1.54	1.61
33	N	1324	G	O3'-P	-5.88	1.54	1.61
35	0	498	A	C2-N3	5.88	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	1369	G	O3'-P	-5.88	1.54	1.61
35	0	559	A	C2-N3	5.88	1.38	1.33
33	N	2014	A	O3'-P	-5.87	1.54	1.61
33	N	310	A	C5-C6	-5.87	1.35	1.41
33	N	1264	A	O3'-P	-5.87	1.54	1.61
33	N	577	G	O3'-P	-5.87	1.54	1.61
35	0	1054	C	P-OP2	5.86	1.58	1.49
33	N	2639	A	O3'-P	-5.86	1.54	1.61
33	N	1610	A	O3'-P	-5.86	1.54	1.61
33	N	580	U	O3'-P	-5.84	1.54	1.61
33	N	1647	U	P-OP2	5.84	1.58	1.49
35	0	804	U	O3'-P	-5.83	1.54	1.61
37	2	2	GLY	N-CA	5.82	1.54	1.46
33	N	1676	A	P-OP2	5.82	1.58	1.49
33	N	774	G	C2'-O2'	5.81	1.49	1.41
33	N	2541	A	O3'-P	-5.80	1.54	1.61
33	N	2779	U	O3'-P	-5.80	1.54	1.61
33	N	2025	C	O5'-C5'	-5.80	1.33	1.42
35	0	116	A	P-OP2	5.80	1.58	1.49
33	N	628	G	O3'-P	-5.79	1.54	1.61
33	N	2688	G	O3'-P	-5.79	1.54	1.61
33	N	2072	C	O5'-C5'	-5.79	1.33	1.42
35	0	788	U	O3'-P	-5.78	1.54	1.61
33	N	2272	U	O3'-P	-5.78	1.54	1.61
33	N	1796	U	O3'-P	-5.77	1.54	1.61
33	N	2054	A	O3'-P	-5.76	1.54	1.61
35	0	545	C	O3'-P	-5.76	1.54	1.61
33	N	562	U	O3'-P	-5.76	1.54	1.61
33	N	565	C	O3'-P	-5.76	1.54	1.61
33	N	1665	A	P-OP2	5.76	1.58	1.49
33	N	1602	U	C4-O4	5.75	1.28	1.23
33	N	234	U	C4-O4	-5.75	1.19	1.23
35	0	786	G	O3'-P	-5.75	1.54	1.61
35	0	1068	G	O3'-P	-5.75	1.54	1.61
33	N	605	G	O3'-P	-5.74	1.54	1.61
33	N	2612	C	O3'-P	-5.74	1.54	1.61
33	N	499	U	O3'-P	-5.74	1.54	1.61
33	N	2011	U	O3'-P	-5.74	1.54	1.61
33	N	2429	G	P-OP2	5.74	1.58	1.49
35	0	868	C	O3'-P	-5.74	1.54	1.61
33	N	2545	G	O3'-P	-5.74	1.54	1.61
35	0	233	C	O3'-P	-5.74	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	n	29	SER	CB-OG	-5.73	1.34	1.42
33	N	2503	A	O3'-P	-5.73	1.54	1.61
35	O	323	U	O3'-P	-5.72	1.54	1.61
33	N	1605	C	O3'-P	-5.72	1.54	1.61
25	k	29	PHE	CG-CD1	-5.71	1.30	1.38
4	P	213	TRP	CE3-CZ3	5.71	1.48	1.38
11	W	30	THR	CB-CG2	-5.70	1.33	1.52
35	O	1430	A	O3'-P	-5.70	1.54	1.61
35	O	319	G	O3'-P	-5.69	1.54	1.61
4	P	221	ARG	CA-C	-5.68	1.38	1.52
33	N	2560	A	O3'-P	-5.68	1.54	1.61
4	P	238	ARG	C-O	5.68	1.34	1.23
33	N	824	U	O3'-P	-5.68	1.54	1.61
33	N	28	A	O3'-P	-5.68	1.54	1.61
33	N	382	A	O3'-P	-5.68	1.54	1.61
35	O	439	U	C4-O4	-5.67	1.19	1.23
35	O	404	G	O3'-P	-5.67	1.54	1.61
35	O	24	U	C4-O4	-5.67	1.19	1.23
33	N	1351	C	O3'-P	-5.66	1.54	1.61
33	N	2509	G	O3'-P	-5.66	1.54	1.61
35	O	1363	A	C6-N6	-5.65	1.29	1.33
33	N	310	A	N1-C2	5.65	1.39	1.34
33	N	536	G	O3'-P	-5.65	1.54	1.61
33	N	1568	G	O3'-P	-5.64	1.54	1.61
33	N	2732	G	C3'-O3'	5.63	1.50	1.42
33	N	2591	C	O3'-P	-5.62	1.54	1.61
33	N	570	G	O3'-P	-5.62	1.54	1.61
33	N	1338	G	O3'-P	-5.62	1.54	1.61
33	N	1790	C	N1-C2	-5.62	1.34	1.40
35	O	878	A	O3'-P	-5.62	1.54	1.61
35	O	750	C	O3'-P	-5.62	1.54	1.61
33	N	691	C	O3'-P	-5.62	1.54	1.61
33	N	810	U	O3'-P	-5.62	1.54	1.61
11	W	16	TYR	CE1-CZ	-5.61	1.31	1.38
33	N	1446	C	O3'-P	-5.60	1.54	1.61
35	O	570	G	O3'-P	-5.60	1.54	1.61
35	O	826	C	O3'-P	-5.58	1.54	1.61
33	N	464	U	C4'-O4'	-5.58	1.38	1.45
35	O	1238	A	C5-C6	-5.57	1.36	1.41
35	O	547	A	P-OP1	5.57	1.58	1.49
33	N	1189	A	P-OP2	5.56	1.58	1.49
6	R	81	GLY	N-CA	-5.55	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	222	GLY	C-O	-5.55	1.14	1.23
33	N	2732	G	C2'-O2'	5.55	1.48	1.41
33	N	2272	U	C2-N3	-5.54	1.33	1.37
33	N	1802	A	C5-C6	-5.54	1.36	1.41
33	N	2685	G	O3'-P	-5.54	1.54	1.61
33	N	1742	U	O3'-P	-5.52	1.54	1.61
20	f	101	SER	CB-OG	-5.52	1.35	1.42
33	N	2645	G	O3'-P	-5.52	1.54	1.61
35	0	907	A	O3'-P	-5.52	1.54	1.61
18	d	45	TYR	CG-CD1	-5.52	1.31	1.39
35	0	895	G	O3'-P	-5.51	1.54	1.61
33	N	375	G	P-OP1	5.51	1.58	1.49
33	N	1783	A	O3'-P	-5.50	1.54	1.61
33	N	2448	A	P-OP1	5.50	1.58	1.49
35	0	963	G	O3'-P	-5.50	1.54	1.61
33	N	1648	U	O3'-P	-5.50	1.54	1.61
33	N	1708	C	O3'-P	-5.49	1.54	1.61
15	a	43	GLU	CG-CD	5.49	1.60	1.51
35	0	885	G	O3'-P	-5.48	1.54	1.61
33	N	246	C	O3'-P	-5.47	1.54	1.61
33	N	840	C	O3'-P	-5.47	1.54	1.61
33	N	2445	G	P-OP2	5.47	1.58	1.49
33	N	1973	G	O3'-P	-5.47	1.54	1.61
33	N	990	A	P-OP2	5.46	1.58	1.49
33	N	1670	C	O3'-P	-5.46	1.54	1.61
33	N	1328	A	O3'-P	-5.46	1.54	1.61
33	N	2266	A	P-OP1	5.45	1.58	1.49
33	N	2821	A	P-O5'	-5.45	1.54	1.59
33	N	1770	G	O3'-P	-5.45	1.54	1.61
35	0	927	G	O3'-P	-5.45	1.54	1.61
33	N	2062	A	O5'-C5'	-5.42	1.34	1.42
33	N	468	G	O3'-P	-5.42	1.54	1.61
33	N	2715	C	O3'-P	-5.41	1.54	1.61
33	N	188	G	O3'-P	-5.41	1.54	1.61
33	N	973	A	P-O5'	-5.41	1.54	1.59
33	N	787	C	P-OP1	5.41	1.58	1.49
33	N	693	A	O3'-P	-5.41	1.54	1.61
16	b	102	ARG	CZ-NH2	5.40	1.40	1.33
35	0	872	A	C6-N6	-5.40	1.29	1.33
33	N	1934	C	O3'-P	-5.39	1.54	1.61
33	N	2643	G	O3'-P	-5.39	1.54	1.61
35	0	391	G	O3'-P	-5.38	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	0	827	U	C4-O4	-5.38	1.19	1.23
2	M	73	C	O3'-P	-5.38	1.54	1.61
33	N	973	A	O3'-P	-5.38	1.54	1.61
33	N	1995	U	P-OP1	5.38	1.58	1.49
33	N	927	A	C2-N3	5.37	1.38	1.33
33	N	1255	U	O5'-C5'	-5.37	1.34	1.42
35	0	887	G	O3'-P	-5.36	1.54	1.61
33	N	1265	A	P-O5'	-5.36	1.54	1.59
33	N	771	G	O3'-P	-5.36	1.54	1.61
33	N	528	A	C5-C6	-5.36	1.36	1.41
33	N	1832	C	O3'-P	-5.35	1.54	1.61
33	N	2720	U	C4-O4	-5.35	1.19	1.23
33	N	1136	G	P-OP1	5.35	1.58	1.49
33	N	742	A	O3'-P	-5.34	1.54	1.61
33	N	1021	A	C6-N6	-5.34	1.29	1.33
35	0	528	C	O3'-P	-5.34	1.54	1.61
33	N	1833	C	O3'-P	-5.33	1.54	1.61
33	N	66	C	O3'-P	-5.33	1.54	1.61
33	N	2005	A	O3'-P	-5.33	1.54	1.61
35	0	24	U	O3'-P	-5.33	1.54	1.61
33	N	385	C	O3'-P	-5.32	1.54	1.61
33	N	561	G	O3'-P	-5.32	1.54	1.61
33	N	1272	A	O3'-P	-5.31	1.54	1.61
47	C	101	ARG	CZ-NH1	5.31	1.40	1.33
35	0	1497	G	O3'-P	-5.31	1.54	1.61
33	N	2549	G	O3'-P	-5.30	1.54	1.61
35	0	938	A	O3'-P	-5.30	1.54	1.61
33	N	2023	C	O3'-P	-5.29	1.54	1.61
33	N	978	G	O3'-P	-5.29	1.54	1.61
33	N	1786	A	O3'-P	-5.29	1.54	1.61
33	N	2724	U	O3'-P	-5.29	1.54	1.61
33	N	784	G	C4'-C3'	-5.29	1.47	1.52
24	j	41	ARG	CG-CD	5.29	1.65	1.51
4	P	11	PRO	N-CA	5.29	1.56	1.47
33	N	2243	U	N3-C4	-5.29	1.33	1.38
33	N	2274	A	O3'-P	-5.29	1.54	1.61
35	0	386	C	O3'-P	-5.29	1.54	1.61
28	n	20	ASP	CB-CG	5.28	1.62	1.51
33	N	783	A	N9-C4	-5.28	1.34	1.37
14	Z	39	GLY	C-O	-5.28	1.15	1.23
35	0	1507	A	O3'-P	-5.28	1.54	1.61
35	0	318	G	O3'-P	-5.28	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	0	586	C	O3'-P	-5.28	1.54	1.61
35	0	751	U	O3'-P	-5.28	1.54	1.61
33	N	1632	A	O3'-P	-5.27	1.54	1.61
33	N	1993	U	P-O5'	-5.27	1.54	1.59
33	N	1327	A	O3'-P	-5.27	1.54	1.61
33	N	2430	A	P-OP2	5.27	1.57	1.49
33	N	430	A	C6-N1	-5.26	1.31	1.35
33	N	2845	U	O3'-P	-5.26	1.54	1.61
35	0	1322	C	O3'-P	5.26	1.67	1.61
5	Q	127	PHE	CE1-CZ	-5.26	1.27	1.37
4	P	48	ARG	C-O	-5.25	1.13	1.23
33	N	1990	C	C2'-C1'	-5.25	1.47	1.53
33	N	2500	U	O3'-P	-5.25	1.54	1.61
35	0	964	A	P-OP1	5.25	1.57	1.49
33	N	2445	G	C2-N2	5.25	1.39	1.34
30	p	39	ARG	NE-CZ	5.25	1.39	1.33
33	N	1837	C	O3'-P	-5.25	1.54	1.61
33	N	2024	G	O3'-P	-5.25	1.54	1.61
52	H	20	GLU	CD-OE1	5.24	1.31	1.25
33	N	2766	A	O3'-P	-5.24	1.54	1.61
33	N	1141	U	C2-O2	-5.24	1.17	1.22
33	N	261	G	O3'-P	-5.23	1.54	1.61
33	N	976	G	O3'-P	-5.23	1.54	1.61
18	d	24	TYR	CE2-CZ	5.23	1.45	1.38
35	0	25	C	O3'-P	-5.23	1.54	1.61
17	c	53	ARG	CG-CD	-5.23	1.38	1.51
33	N	1637	A	O3'-P	-5.22	1.54	1.61
35	0	123	U	O3'-P	-5.22	1.54	1.61
46	B	38	TYR	CB-CG	-5.22	1.43	1.51
33	N	2267	A	P-OP1	5.22	1.57	1.49
33	N	469	G	O3'-P	-5.21	1.54	1.61
35	0	1301	U	C2-N3	5.21	1.41	1.37
33	N	2838	G	O3'-P	-5.21	1.54	1.61
33	N	2592	G	O3'-P	-5.21	1.54	1.61
35	0	291	U	O3'-P	-5.20	1.54	1.61
33	N	989	G	C3'-O3'	5.20	1.49	1.42
33	N	1991	U	O3'-P	-5.20	1.54	1.61
6	R	77	ILE	CB-CG1	-5.19	1.39	1.54
14	Z	91	TYR	CE2-CZ	-5.19	1.31	1.38
33	N	2387	U	O3'-P	-5.19	1.54	1.61
29	o	49	TYR	CE2-CZ	-5.18	1.31	1.38
33	N	2036	C	O3'-P	-5.18	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	0	554	A	O3'-P	-5.18	1.54	1.61
35	0	924	C	O3'-P	-5.18	1.54	1.61
4	P	234	GLY	C-O	-5.17	1.15	1.23
35	0	373	A	O3'-P	-5.17	1.54	1.61
33	N	69	C	O3'-P	-5.17	1.54	1.61
33	N	2875	C	O3'-P	-5.17	1.54	1.61
35	0	886	G	O3'-P	-5.17	1.54	1.61
33	N	800	A	N9-C4	-5.17	1.34	1.37
33	N	2448	A	P-OP2	5.16	1.57	1.49
35	0	397	A	C6-N6	-5.16	1.29	1.33
29	o	21	TYR	CE1-CZ	-5.16	1.31	1.38
33	N	981	A	P-OP1	5.16	1.57	1.49
35	0	783	C	O3'-P	-5.16	1.54	1.61
35	0	18	C	O3'-P	-5.15	1.54	1.61
33	N	1826	G	O3'-P	-5.15	1.54	1.61
45	A	65	VAL	CB-CG1	-5.15	1.42	1.52
4	P	213	TRP	CA-C	-5.15	1.39	1.52
5	Q	113	SER	CB-OG	-5.15	1.35	1.42
33	N	2839	G	O3'-P	-5.15	1.54	1.61
33	N	419	U	P-OP1	5.14	1.57	1.49
19	e	80	ARG	CB-CG	-5.14	1.38	1.52
33	N	1254	A	C2'-O2'	5.14	1.48	1.41
35	0	951	G	O3'-P	-5.14	1.54	1.61
35	0	1500	A	P-OP2	5.13	1.57	1.49
4	P	235	GLY	CA-C	-5.13	1.43	1.51
33	N	2078	C	O3'-P	-5.13	1.54	1.61
33	N	2490	G	O3'-P	-5.13	1.54	1.61
33	N	223	A	O3'-P	-5.12	1.55	1.61
33	N	1864	U	O3'-P	-5.11	1.55	1.61
33	N	2017	U	N1-C2	-5.11	1.33	1.38
33	N	467	G	O3'-P	-5.11	1.55	1.61
33	N	2361	G	O3'-P	-5.11	1.55	1.61
35	0	816	A	P-OP1	5.11	1.57	1.49
33	N	604	G	O3'-P	-5.10	1.55	1.61
33	N	513	A	P-O5'	-5.10	1.54	1.59
33	N	784	G	P-OP1	5.10	1.57	1.49
33	N	2241	A	O3'-P	-5.10	1.55	1.61
36	1	213	TYR	CB-CG	-5.10	1.44	1.51
33	N	2267	A	C6-N1	-5.10	1.31	1.35
1	s	132	TYR	CG-CD1	5.09	1.45	1.39
33	N	954	G	O3'-P	-5.09	1.55	1.61
35	0	979	C	O3'-P	-5.09	1.55	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	96	TRP	CG-CD1	5.09	1.43	1.36
33	N	1202	G	O3'-P	-5.08	1.55	1.61
33	N	449	A	O3'-P	-5.08	1.55	1.61
33	N	503	A	O3'-P	5.08	1.67	1.61
33	N	664	G	O3'-P	-5.08	1.55	1.61
35	0	1408	A	O3'-P	-5.08	1.55	1.61
35	0	827	U	O3'-P	-5.08	1.55	1.61
33	N	1679	A	O3'-P	-5.07	1.55	1.61
33	N	918	A	O3'-P	-5.07	1.55	1.61
33	N	787	C	P-O5'	-5.07	1.54	1.59
33	N	948	C	N1-C2	-5.06	1.35	1.40
33	N	2611	C	P-OP2	5.06	1.57	1.49
3	O	90	C	O3'-P	-5.06	1.55	1.61
33	N	1308	A	O3'-P	-5.04	1.55	1.61
29	o	49	TYR	CG-CD1	-5.04	1.32	1.39
33	N	1972	G	O3'-P	-5.04	1.55	1.61
33	N	1250	G	P-OP1	5.04	1.57	1.49
33	N	1985	C	O3'-P	-5.04	1.55	1.61
33	N	666	A	O3'-P	-5.04	1.55	1.61
33	N	2706	A	O3'-P	-5.04	1.55	1.61
35	0	881	G	O3'-P	-5.03	1.55	1.61
35	0	506	G	O3'-P	-5.03	1.55	1.61
33	N	1237	A	P-OP2	5.03	1.57	1.49
33	N	396	G	O3'-P	-5.03	1.55	1.61
33	N	1954	G	O3'-P	-5.03	1.55	1.61
35	0	827	U	C2-N3	-5.02	1.34	1.37
4	P	236	GLU	CD-OE2	5.02	1.31	1.25
35	0	1363	A	C6-N1	-5.02	1.32	1.35
33	N	2551	C	P-OP2	5.02	1.57	1.49
18	d	33	ARG	CB-CG	-5.01	1.39	1.52
33	N	2580	U	O3'-P	-5.01	1.55	1.61
11	W	97	PRO	C-O	5.01	1.33	1.23
19	e	53	PHE	CG-CD1	5.01	1.46	1.38

All (725) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	N	2506[A]	U	OP1-P-O3'	17.15	142.94	105.20
33	N	2506[B]	U	OP1-P-O3'	17.15	142.94	105.20
30	p	39	ARG	NE-CZ-NH1	16.10	128.35	120.30
30	p	39	ARG	NE-CZ-NH2	-14.77	112.91	120.30
2	M	73	C	O3'-P-O5'	14.38	131.32	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	N	2522	U	C2-N3-C4	-13.78	118.73	127.00
33	N	2720	U	C2-N3-C4	-13.62	118.83	127.00
33	N	2062	A	O5'-P-OP1	-13.24	93.78	105.70
33	N	467	G	O5'-P-OP1	-13.17	93.85	105.70
33	N	2836	U	O5'-P-OP1	-12.85	94.14	105.70
53	I	5	LEU	CB-CG-CD2	12.61	132.44	111.00
18	d	53	ARG	NE-CZ-NH1	12.47	126.53	120.30
33	N	1996	C	O5'-P-OP2	-12.27	94.66	105.70
33	N	2506[A]	U	O3'-P-O5'	-12.25	80.72	104.00
33	N	2506[B]	U	O3'-P-O5'	-12.25	80.72	104.00
24	j	41	ARG	NE-CZ-NH1	12.15	126.38	120.30
33	N	499	U	C2-N3-C4	-12.06	119.77	127.00
33	N	2873	A	N1-C6-N6	-12.01	111.39	118.60
33	N	2821	A	O5'-P-OP1	-11.87	95.02	105.70
25	k	28	ARG	NE-CZ-NH2	-11.63	114.48	120.30
13	Y	18	ARG	NE-CZ-NH2	-11.60	114.50	120.30
28	n	20	ASP	CB-CG-OD1	11.60	128.74	118.30
35	o	559	A	C6-N1-C2	-11.37	111.78	118.60
35	o	1301	U	C2-N3-C4	-11.35	120.19	127.00
33	N	1665	A	O5'-P-OP1	-11.28	95.55	105.70
33	N	2505	G	P-O3'-C3'	-11.09	106.39	119.70
33	N	228	C	O5'-P-OP1	-10.97	95.83	105.70
35	o	752	G	O5'-P-OP1	-10.96	95.84	105.70
11	W	116	ARG	NE-CZ-NH2	-10.89	114.85	120.30
33	N	2447	G	O5'-P-OP1	-10.88	95.91	105.70
14	Z	16	ARG	NE-CZ-NH2	-10.85	114.88	120.30
33	N	2765	A	N1-C6-N6	-10.83	112.10	118.60
30	p	34	ARG	NE-CZ-NH1	-10.72	114.94	120.30
45	A	122	ARG	NE-CZ-NH1	10.66	125.63	120.30
4	P	214	ARG	NE-CZ-NH2	-10.65	114.97	120.30
47	C	109	ARG	NE-CZ-NH1	10.62	125.61	120.30
33	N	1941	C	O5'-P-OP1	-10.62	96.14	105.70
33	N	27	G	O5'-P-OP1	-10.52	96.23	105.70
33	N	2067	G	O5'-P-OP1	-10.49	96.25	105.70
35	o	1497	G	O5'-P-OP2	-10.39	96.34	105.70
35	o	16	A	O5'-P-OP1	-10.37	96.37	105.70
18	d	53	ARG	NE-CZ-NH2	-10.31	115.15	120.30
55	K	34	ARG	NE-CZ-NH2	-10.28	115.16	120.30
33	N	1965	C	O5'-P-OP2	-10.14	96.58	105.70
5	Q	13	ARG	NE-CZ-NH2	10.12	125.36	120.30
18	d	6	ARG	NE-CZ-NH2	10.05	125.33	120.30
36	1	21	ARG	NE-CZ-NH1	10.00	125.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	N	953	G	O5'-P-OP1	-9.96	96.73	105.70
33	N	474	G	O5'-P-OP1	-9.92	96.77	105.70
35	O	21	G	O5'-P-OP1	9.87	122.54	110.70
33	N	2059	A	O5'-P-OP2	-9.84	96.84	105.70
33	N	2072	C	O5'-P-OP1	-9.82	96.86	105.70
33	N	306	U	C2-N3-C4	-9.82	121.11	127.00
33	N	2060	A	O5'-P-OP1	-9.79	96.89	105.70
9	U	27	ARG	NE-CZ-NH1	-9.74	115.43	120.30
33	N	801	G	O5'-P-OP2	-9.62	97.04	105.70
33	N	2726	A	O5'-P-OP1	-9.55	97.11	105.70
33	N	537	G	O5'-P-OP1	-9.54	97.12	105.70
16	b	102	ARG	NE-CZ-NH2	9.52	125.06	120.30
33	N	1809	A	O5'-P-OP1	-9.46	97.19	105.70
33	N	2873	A	C5-C6-N6	9.43	131.25	123.70
35	O	795	C	O5'-P-OP1	-9.42	97.22	105.70
33	N	2776	A	C4-N9-C1'	9.38	143.18	126.30
33	N	2776	A	C8-N9-C1'	-9.37	110.83	127.70
33	N	805	G	O5'-P-OP1	-9.36	97.28	105.70
33	N	2044	C	O5'-P-OP1	-9.29	97.34	105.70
41	6	109	ARG	NE-CZ-NH1	9.29	124.94	120.30
32	r	36	ARG	NE-CZ-NH1	-9.28	115.66	120.30
13	Y	47	ARG	NE-CZ-NH2	9.24	124.92	120.30
33	N	2543	G	O5'-P-OP1	-9.23	97.39	105.70
4	P	258	ARG	NE-CZ-NH1	-9.22	115.69	120.30
25	k	57	ARG	NE-CZ-NH2	9.22	124.91	120.30
33	N	2711	A	O5'-P-OP2	9.20	121.74	110.70
33	N	1190	G	O5'-P-OP2	9.19	121.73	110.70
39	4	111	MET	CG-SD-CE	-9.15	85.56	100.20
33	N	1639	C	O5'-P-OP1	-9.13	97.49	105.70
33	N	2022	U	O5'-P-OP1	-9.10	97.51	105.70
33	N	1253	A	O5'-P-OP1	-9.06	97.54	105.70
36	1	21	ARG	NE-CZ-NH2	-9.01	115.79	120.30
33	N	2513	A	O5'-P-OP2	-9.00	97.60	105.70
33	N	2456	C	O5'-P-OP1	-8.97	97.62	105.70
17	c	72	ARG	NE-CZ-NH2	-8.94	115.83	120.30
47	C	92	ARG	NE-CZ-NH1	8.84	124.72	120.30
35	O	968	A	O5'-P-OP2	-8.83	97.75	105.70
4	P	270	ARG	NE-CZ-NH2	-8.78	115.91	120.30
16	b	30	ARG	NE-CZ-NH2	-8.76	115.92	120.30
16	b	102	ARG	NE-CZ-NH1	-8.74	115.93	120.30
33	N	1798	U	O5'-P-OP2	-8.72	97.85	105.70
13	Y	78	ARG	NE-CZ-NH2	8.69	124.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	E	54	ARG	NE-CZ-NH2	-8.69	115.96	120.30
33	N	2725	A	O5'-P-OP1	-8.65	97.91	105.70
33	N	684	G	O5'-P-OP1	-8.65	97.92	105.70
33	N	2497	A	O5'-P-OP2	8.62	121.04	110.70
15	a	69	ARG	NE-CZ-NH2	8.61	124.61	120.30
33	N	1994	C	O5'-P-OP1	-8.52	98.03	105.70
35	0	816	A	O5'-P-OP1	-8.51	98.04	105.70
3	O	90	C	O5'-P-OP1	-8.49	98.06	105.70
39	4	157	ARG	NE-CZ-NH1	-8.46	116.07	120.30
50	F	70	ARG	NE-CZ-NH1	8.45	124.53	120.30
54	J	10	ARG	CB-CG-CD	-8.44	89.66	111.60
17	c	21	ARG	NE-CZ-NH1	-8.41	116.10	120.30
31	q	8	ARG	NE-CZ-NH1	8.38	124.49	120.30
35	0	726	C	O5'-P-OP1	-8.33	98.21	105.70
33	N	2248	C	O5'-P-OP1	-8.24	98.28	105.70
4	P	221	ARG	CG-CD-NE	-8.24	94.50	111.80
48	D	9	ARG	NE-CZ-NH1	8.23	124.42	120.30
4	P	271	ARG	NE-CZ-NH2	-8.22	116.19	120.30
35	0	1358	U	N3-C4-O4	-8.16	113.69	119.40
11	W	116	ARG	NE-CZ-NH1	8.13	124.36	120.30
16	b	30	ARG	NE-CZ-NH1	8.13	124.36	120.30
33	N	812	C	O5'-P-OP2	-8.10	98.41	105.70
35	0	674	G	O5'-P-OP1	-8.10	98.41	105.70
33	N	2267	A	O5'-P-OP2	-8.08	98.42	105.70
12	X	78	ARG	NE-CZ-NH2	-8.08	116.26	120.30
33	N	234	U	N3-C4-O4	-8.07	113.75	119.40
37	2	156	ARG	NE-CZ-NH1	8.07	124.33	120.30
47	C	92	ARG	NE-CZ-NH2	-8.07	116.26	120.30
33	N	671	C	O5'-P-OP1	-8.06	98.44	105.70
2	M	73	C	OP1-P-O3'	-8.04	87.52	105.20
18	d	51	ARG	NE-CZ-NH1	8.03	124.32	120.30
6	R	69	ARG	NE-CZ-NH2	-8.03	116.28	120.30
33	N	234	U	C5-C4-O4	8.03	130.72	125.90
18	d	51	ARG	NE-CZ-NH2	-8.02	116.29	120.30
6	R	61	ARG	NE-CZ-NH1	8.00	124.30	120.30
28	n	7	LYS	CD-CE-NZ	8.00	130.10	111.70
33	N	1141	U	N3-C4-O4	-8.00	113.80	119.40
33	N	2222	C	O5'-P-OP1	-7.99	98.51	105.70
46	B	12	ARG	NE-CZ-NH1	-7.98	116.31	120.30
39	4	38	VAL	CG1-CB-CG2	-7.97	98.14	110.90
35	0	439	U	C2-N3-C4	-7.96	122.22	127.00
18	d	13	ARG	NE-CZ-NH2	7.94	124.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	N	2847	U	O5'-P-OP1	-7.93	98.56	105.70
33	N	704	G	O5'-P-OP1	-7.91	98.58	105.70
35	0	1191	A	O5'-P-OP1	-7.88	98.61	105.70
35	0	1054	C	O5'-P-OP2	7.87	120.15	110.70
18	d	3	ARG	NE-CZ-NH1	-7.85	116.37	120.30
26	l	52	ARG	NE-CZ-NH1	-7.85	116.37	120.30
6	R	49	ARG	NE-CZ-NH1	-7.85	116.38	120.30
33	N	2061	G	O4'-C1'-N9	7.84	114.47	108.20
33	N	2765	A	C5-C6-N6	7.81	129.94	123.70
33	N	1141	U	C5-C4-O4	7.80	130.58	125.90
40	5	79	ARG	NE-CZ-NH1	7.80	124.20	120.30
33	N	2277	G	O5'-P-OP1	-7.78	98.70	105.70
18	d	58	ARG	NE-CZ-NH2	-7.73	116.43	120.30
33	N	927	A	C6-N1-C2	-7.72	113.97	118.60
33	N	1136	G	P-O5'-C5'	-7.72	108.55	120.90
33	N	581	C	O5'-P-OP1	-7.71	98.76	105.70
33	N	974	G	N9-C1'-C2'	7.70	124.01	114.00
41	6	3	ARG	NE-CZ-NH1	7.69	124.14	120.30
38	3	5	LEU	CA-CB-CG	7.66	132.93	115.30
33	N	1611	C	O5'-P-OP2	-7.66	98.81	105.70
33	N	1255	U	O5'-P-OP2	7.64	119.87	110.70
33	N	2344	U	N3-C4-O4	-7.63	114.06	119.40
33	N	2022	U	OP1-P-OP2	7.63	131.04	119.60
33	N	2544	G	O5'-P-OP2	-7.61	98.85	105.70
33	N	813	U	O5'-P-OP2	-7.61	98.85	105.70
35	0	37	U	N3-C4-O4	-7.60	114.08	119.40
33	N	2729	G	O5'-P-OP1	-7.59	98.87	105.70
33	N	698	C	O5'-P-OP2	-7.59	98.87	105.70
33	N	787	C	O5'-P-OP1	7.58	119.80	110.70
43	8	49	ARG	NE-CZ-NH1	7.58	124.09	120.30
33	N	512	G	P-O3'-C3'	7.56	128.77	119.70
33	N	2447	G	P-O3'-C3'	7.55	128.77	119.70
35	0	368	U	N3-C4-O4	-7.55	114.11	119.40
35	0	567	G	O5'-P-OP1	-7.55	98.91	105.70
35	0	571	U	C2-N3-C4	-7.55	122.47	127.00
33	N	1255	U	O5'-P-OP1	-7.54	98.92	105.70
33	N	2060	A	O5'-P-OP2	7.53	119.73	110.70
33	N	784	G	C2'-C3'-O3'	7.51	126.03	109.50
33	N	430	A	N1-C6-N6	-7.51	114.09	118.60
4	P	177	ARG	NE-CZ-NH1	-7.50	116.55	120.30
33	N	1930	G	O5'-P-OP1	-7.45	99.00	105.70
33	N	1900	A	P-O3'-C3'	7.45	128.64	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l	29	ARG	NE-CZ-NH1	-7.45	116.58	120.30
33	N	1932	A	O5'-P-OP1	-7.42	99.02	105.70
33	N	2542	A	O5'-P-OP2	-7.41	99.03	105.70
35	0	1363	A	N1-C6-N6	-7.41	114.16	118.60
33	N	2693	G	O5'-P-OP1	-7.39	99.05	105.70
33	N	1639	C	O5'-P-OP2	7.39	119.57	110.70
35	0	501	C	O5'-P-OP1	-7.34	99.09	105.70
35	0	1331	G	O5'-P-OP1	-7.34	99.09	105.70
33	N	2256	G	O5'-P-OP1	-7.34	99.10	105.70
33	N	2692	G	O5'-P-OP2	-7.34	99.10	105.70
35	0	498	A	C6-N1-C2	-7.33	114.20	118.60
33	N	784	G	P-O3'-C3'	7.32	128.48	119.70
33	N	2072	C	O5'-P-OP2	7.31	119.48	110.70
35	0	1507	A	O5'-P-OP1	-7.31	99.12	105.70
13	Y	29	LYS	CD-CE-NZ	-7.30	94.92	111.70
33	N	850	U	C2-N3-C4	-7.29	122.62	127.00
33	N	932	U	N3-C4-O4	-7.29	114.30	119.40
33	N	2714	G	O5'-P-OP2	7.27	119.43	110.70
33	N	2497	A	C5'-C4'-C3'	-7.27	104.37	116.00
48	D	85	ARG	NE-CZ-NH1	7.27	123.93	120.30
33	N	795	C	O5'-P-OP1	-7.25	99.18	105.70
42	7	80	ARG	NE-CZ-NH2	-7.20	116.70	120.30
35	0	368	U	C5-C4-O4	7.19	130.21	125.90
33	N	760	G	OP1-P-O3'	7.18	120.99	105.20
24	j	14	ARG	CG-CD-NE	-7.17	96.75	111.80
33	N	510	C	O5'-P-OP2	-7.15	99.26	105.70
33	N	2506[A]	U	OP2-P-O3'	-7.13	89.51	105.20
33	N	2506[B]	U	OP2-P-O3'	-7.13	89.51	105.20
33	N	1145	C	O5'-P-OP1	-7.13	99.28	105.70
33	N	2344	U	C5-C4-O4	7.13	130.18	125.90
33	N	2637	U	O5'-P-OP1	-7.13	99.28	105.70
33	N	1026	G	O5'-P-OP2	-7.12	99.29	105.70
54	J	74	ARG	NE-CZ-NH1	7.12	123.86	120.30
13	Y	82	LEU	CA-CB-CG	7.12	131.66	115.30
6	R	81	GLY	C-N-CA	-7.11	107.36	122.30
13	Y	59	ARG	NE-CZ-NH1	7.08	123.84	120.30
33	N	2344	U	O5'-P-OP1	-7.07	99.34	105.70
52	H	43	ARG	NE-CZ-NH1	7.07	123.83	120.30
53	I	5	LEU	CB-CG-CD1	-7.06	98.99	111.00
33	N	1236	G	P-O3'-C3'	7.05	128.16	119.70
35	0	6	G	O5'-P-OP2	-7.03	99.37	105.70
33	N	1962	C	O5'-P-OP1	-7.02	99.38	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	N	1790	C	O5'-P-OP1	-7.02	99.39	105.70
35	0	24	U	N1-C2-O2	-7.00	117.90	122.80
33	N	740	C	O5'-P-OP1	-6.96	99.43	105.70
33	N	967	U	O5'-P-OP1	-6.96	99.43	105.70
35	0	827	U	N3-C4-O4	-6.95	114.53	119.40
41	6	109	ARG	CG-CD-NE	-6.95	97.20	111.80
33	N	1944	U	O5'-P-OP2	-6.93	99.46	105.70
33	N	2304	G	O5'-P-OP1	-6.92	99.47	105.70
33	N	578	G	O5'-P-OP1	6.91	118.99	110.70
35	0	37	U	C5-C4-O4	6.88	130.03	125.90
33	N	196	A	O5'-P-OP1	-6.88	99.51	105.70
33	N	1607	C	O5'-P-OP1	-6.88	99.51	105.70
33	N	2059	A	O5'-P-OP1	6.88	118.95	110.70
33	N	2272	U	N3-C4-O4	-6.87	114.59	119.40
33	N	2311	A	P-O3'-C3'	6.87	127.94	119.70
33	N	2711	A	O5'-P-OP1	-6.86	99.52	105.70
31	q	13	ARG	NE-CZ-NH1	-6.85	116.87	120.30
35	0	865	A	O5'-P-OP1	-6.85	99.53	105.70
24	j	41	ARG	CD-NE-CZ	6.85	133.19	123.60
6	R	77	ILE	CG1-CB-CG2	-6.85	96.33	111.40
33	N	630	G	O5'-P-OP1	-6.83	99.55	105.70
33	N	1021	A	N1-C6-N6	-6.83	114.50	118.60
33	N	2021	C	O5'-P-OP2	-6.83	99.55	105.70
17	c	93	ARG	CG-CD-NE	-6.83	97.45	111.80
33	N	1836	C	O5'-P-OP1	-6.83	99.56	105.70
35	0	904	U	O5'-P-OP1	-6.83	99.56	105.70
38	3	3	ARG	NE-CZ-NH1	6.82	123.71	120.30
31	q	8	ARG	CD-NE-CZ	-6.82	114.06	123.60
4	P	101	ARG	NE-CZ-NH2	-6.81	116.90	120.30
33	N	2543	G	P-O5'-C5'	-6.79	110.03	120.90
35	0	1358	U	C5-C4-O4	6.79	129.97	125.90
35	0	812	G	P-O3'-C3'	6.76	127.81	119.70
37	2	172	ARG	NE-CZ-NH2	-6.75	116.92	120.30
35	0	1349	A	O5'-P-OP2	6.72	118.77	110.70
48	D	53	ARG	NE-CZ-NH1	-6.72	116.94	120.30
33	N	2576	G	O5'-P-OP2	-6.72	99.65	105.70
33	N	679	C	O5'-P-OP1	-6.72	99.66	105.70
35	0	1343	G	O5'-P-OP1	-6.71	99.66	105.70
21	g	12	ARG	NE-CZ-NH1	6.70	123.65	120.30
5	Q	156	PHE	CB-CG-CD2	-6.70	116.11	120.80
13	Y	59	ARG	NE-CZ-NH2	-6.69	116.95	120.30
33	N	512	G	O4'-C1'-N9	6.69	113.55	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	p	14	ARG	NE-CZ-NH1	-6.69	116.96	120.30
20	f	88	ARG	NE-CZ-NH1	-6.66	116.97	120.30
33	N	932	U	C5-C4-O4	6.66	129.90	125.90
33	N	961	C	O5'-P-OP2	-6.65	99.71	105.70
16	b	25	ARG	NE-CZ-NH1	-6.65	116.98	120.30
35	0	1280	A	O5'-P-OP2	-6.64	99.72	105.70
35	0	738	C	O5'-P-OP1	-6.60	99.76	105.70
35	0	261	U	O5'-P-OP1	-6.60	99.76	105.70
33	N	2060	A	O3'-P-O5'	6.58	116.49	104.00
40	5	24	ARG	NE-CZ-NH1	6.58	123.59	120.30
15	a	4	ARG	NE-CZ-NH2	-6.57	117.02	120.30
33	N	1666	G	O4'-C4'-C3'	-6.55	97.45	104.00
33	N	1648	U	P-O5'-C5'	-6.54	110.43	120.90
8	T	3	ARG	NE-CZ-NH2	6.54	123.57	120.30
33	N	729	G	O5'-P-OP2	-6.53	99.82	105.70
33	N	51	G	O4'-C1'-N9	6.52	113.42	108.20
33	N	2656	U	C2-N1-C1'	6.52	125.52	117.70
33	N	963	U	O5'-P-OP2	6.49	118.49	110.70
35	0	864	A	C6-N1-C2	-6.49	114.71	118.60
47	C	90	ARG	NE-CZ-NH2	-6.49	117.06	120.30
33	N	1902	C	O5'-P-OP1	-6.49	99.86	105.70
33	N	2516	A	O5'-P-OP1	-6.49	99.86	105.70
47	C	3	ARG	NE-CZ-NH1	6.49	123.54	120.30
41	6	95	ARG	NE-CZ-NH1	6.48	123.54	120.30
15	a	69	ARG	NE-CZ-NH1	-6.47	117.07	120.30
35	0	829	G	O5'-P-OP1	-6.46	99.88	105.70
33	N	188	G	O5'-P-OP1	-6.46	99.89	105.70
33	N	1439	A	O5'-P-OP1	-6.45	99.89	105.70
33	N	555	G	O5'-P-OP1	-6.45	99.90	105.70
33	N	1664	A	O5'-P-OP2	6.44	118.43	110.70
46	B	9	ARG	NE-CZ-NH1	6.44	123.52	120.30
33	N	752	A	N9-C1'-C2'	6.43	122.36	114.00
33	N	2048	G	O5'-P-OP1	-6.43	99.91	105.70
11	W	99	ARG	NE-CZ-NH1	6.43	123.52	120.30
32	r	24	ARG	NE-CZ-NH2	6.43	123.52	120.30
46	B	83	ARG	NE-CZ-NH1	6.42	123.51	120.30
33	N	747	U	O5'-P-OP1	-6.41	99.93	105.70
33	N	310	A	O5'-P-OP1	-6.41	99.93	105.70
33	N	204	A	O5'-P-OP2	-6.40	99.94	105.70
33	N	2074	U	O5'-P-OP2	-6.39	99.95	105.70
53	I	37	ARG	NE-CZ-NH1	6.38	123.49	120.30
4	P	87	ARG	NE-CZ-NH2	6.37	123.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	0	397	A	N1-C6-N6	-6.37	114.78	118.60
24	j	41	ARG	NH1-CZ-NH2	-6.37	112.39	119.40
33	N	1313	U	C2-N1-C1'	6.37	125.34	117.70
33	N	1299	G	O5'-P-OP1	-6.36	99.97	105.70
33	N	2725	A	C3'-C2'-O2'	-6.36	94.84	113.30
28	n	17	ARG	NE-CZ-NH2	-6.36	117.12	120.30
35	0	1279	G	N9-C1'-C2'	6.36	122.27	114.00
16	b	13	ARG	NE-CZ-NH1	6.35	123.47	120.30
33	N	1933	G	O5'-P-OP1	-6.35	99.99	105.70
33	N	792	A	O5'-P-OP1	-6.34	99.99	105.70
33	N	1967	C	O5'-P-OP1	-6.34	99.99	105.70
14	Z	40	ARG	NE-CZ-NH2	6.33	123.46	120.30
18	d	48	ARG	NE-CZ-NH2	6.32	123.46	120.30
33	N	2522	U	N1-C2-O2	-6.32	118.38	122.80
35	0	563	A	N1-C6-N6	-6.32	114.81	118.60
35	0	890	G	O4'-C1'-N9	6.32	113.26	108.20
4	P	229	ASP	CB-CG-OD1	-6.32	112.61	118.30
33	N	995	C	C4'-C3'-O3'	-6.31	96.15	109.40
12	X	71	ARG	NE-CZ-NH1	6.31	123.45	120.30
33	N	2423	U	O5'-P-OP2	-6.30	100.03	105.70
33	N	2061	G	O5'-P-OP1	-6.30	100.03	105.70
38	3	3	ARG	NE-CZ-NH2	-6.29	117.16	120.30
33	N	2055	C	O5'-P-OP1	-6.28	100.05	105.70
33	N	2443	C	O4'-C4'-C3'	-6.28	97.72	104.00
28	n	20	ASP	CB-CG-OD2	-6.28	112.65	118.30
33	N	650	C	O5'-P-OP1	-6.28	100.05	105.70
27	m	11	ARG	NE-CZ-NH2	6.27	123.44	120.30
33	N	1205	A	P-O3'-C3'	6.26	127.21	119.70
33	N	1141	U	N3-C2-O2	-6.25	117.82	122.20
35	0	880	C	O5'-P-OP2	-6.25	100.08	105.70
33	N	2364	C	O4'-C4'-C3'	-6.24	97.76	104.00
35	0	131	A	O5'-P-OP1	-6.24	100.09	105.70
35	0	827	U	C5-C4-O4	6.23	129.64	125.90
45	A	122	ARG	NE-CZ-NH2	-6.23	117.19	120.30
33	N	140	C	C2-N1-C1'	6.22	125.64	118.80
33	N	1936	A	C4'-C3'-O3'	-6.22	96.35	109.40
33	N	91	A	O5'-P-OP2	-6.21	100.11	105.70
55	K	34	ARG	NE-CZ-NH1	6.21	123.41	120.30
33	N	1313	U	N1-C1'-C2'	6.19	122.05	114.00
35	0	1054	C	O5'-P-OP1	-6.18	100.14	105.70
35	0	576	C	O5'-P-OP2	-6.17	100.14	105.70
33	N	2243	U	O5'-P-OP2	6.17	118.11	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	229	ASP	CB-CG-OD2	6.17	123.85	118.30
33	N	2258	C	O5'-P-OP1	-6.15	100.16	105.70
33	N	1865	U	O5'-P-OP1	-6.14	100.18	105.70
3	O	94	A	O5'-P-OP1	-6.14	100.18	105.70
33	N	310	A	C6-C5-N7	-6.13	128.01	132.30
33	N	1844	C	O5'-P-OP1	-6.13	100.18	105.70
33	N	2725	A	O5'-P-OP2	6.13	118.06	110.70
31	q	25	LYS	CD-CE-NZ	-6.13	97.61	111.70
33	N	983	A	C5'-C4'-O4'	-6.13	101.75	109.10
4	P	228	VAL	CG1-CB-CG2	-6.12	101.11	110.90
11	W	37	ARG	NE-CZ-NH2	6.11	123.36	120.30
33	N	1264	A	O5'-P-OP1	-6.11	100.20	105.70
33	N	503	A	C4-C5-C6	6.11	120.05	117.00
35	0	540	G	O5'-P-OP1	-6.11	100.20	105.70
35	0	1356	G	O5'-P-OP1	-6.11	100.20	105.70
26	l	6	LEU	CB-CG-CD1	6.09	121.36	111.00
33	N	1501	G	O5'-P-OP1	-6.09	100.22	105.70
35	0	1238	A	C6-C5-N7	-6.08	128.04	132.30
39	4	138	ARG	NE-CZ-NH1	-6.07	117.27	120.30
47	C	107	ARG	NE-CZ-NH2	-6.06	117.27	120.30
33	N	670	A	P-O3'-C3'	6.05	126.95	119.70
52	H	57	ARG	CA-CB-CG	6.04	126.70	113.40
35	0	2	A	O5'-P-OP1	-6.04	100.27	105.70
35	0	762	U	O5'-P-OP1	-6.03	100.27	105.70
35	0	884	U	N3-C4-O4	-6.03	115.18	119.40
8	T	153	ARG	NE-CZ-NH2	6.03	123.31	120.30
15	a	54	LEU	CB-CG-CD1	-6.02	100.77	111.00
35	0	31	G	O5'-P-OP2	-6.02	100.28	105.70
35	0	687	A	O5'-P-OP1	-6.01	100.29	105.70
18	d	28	ARG	NE-CZ-NH1	6.01	123.30	120.30
5	Q	109	VAL	CG1-CB-CG2	-6.00	101.29	110.90
49	E	63	ARG	NE-CZ-NH1	6.00	123.30	120.30
33	N	536	G	O5'-P-OP2	-6.00	100.30	105.70
33	N	2603	G	O5'-P-OP1	-5.99	100.31	105.70
33	N	2699	C	O5'-P-OP1	-5.99	100.31	105.70
35	0	529	G	O5'-P-OP2	-5.99	100.31	105.70
35	0	388	G	P-O3'-C3'	5.98	126.88	119.70
33	N	948	C	O5'-P-OP1	5.98	117.87	110.70
33	N	1328	A	O5'-P-OP1	5.98	117.87	110.70
33	N	2576	G	O5'-P-OP1	5.98	117.87	110.70
14	Z	81	ARG	NE-CZ-NH2	-5.97	117.32	120.30
44	9	60	ASP	CB-CG-OD2	5.96	123.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	N	1795	C	O5'-P-OP1	-5.96	100.34	105.70
15	a	69	ARG	CG-CD-NE	5.96	124.31	111.80
6	R	81	GLY	O-C-N	-5.95	113.08	123.20
33	N	2512	C	O5'-P-OP1	-5.95	100.34	105.70
33	N	2272	U	C5-C4-O4	5.94	129.47	125.90
35	0	59	A	O5'-P-OP1	5.94	117.82	110.70
33	N	466	A	O5'-P-OP1	5.93	117.82	110.70
33	N	2246	G	O4'-C4'-C3'	-5.93	98.07	104.00
14	Z	136	MET	CG-SD-CE	5.93	109.69	100.20
33	N	2267	A	N1-C6-N6	-5.93	115.04	118.60
35	0	1301	U	N1-C1'-C2'	5.92	121.69	114.00
31	q	8	ARG	CG-CD-NE	5.92	124.22	111.80
33	N	673	C	O5'-P-OP1	5.91	117.79	110.70
35	0	1347	G	P-O3'-C3'	5.91	126.79	119.70
33	N	2503	A	OP1-P-OP2	-5.91	110.74	119.60
43	8	18	ARG	CB-CG-CD	-5.90	96.25	111.60
31	q	45	ARG	NE-CZ-NH1	5.90	123.25	120.30
4	P	177	ARG	CG-CD-NE	-5.90	99.41	111.80
12	X	23	LYS	CD-CE-NZ	-5.90	98.14	111.70
33	N	2028	U	O5'-P-OP1	-5.89	100.40	105.70
43	8	12	ARG	NE-CZ-NH2	-5.89	117.36	120.30
35	0	1238	A	C4-C5-C6	5.88	119.94	117.00
33	N	27	G	C5'-C4'-O4'	-5.88	102.04	109.10
33	N	404	A	P-O3'-C3'	5.88	126.75	119.70
33	N	2273	A	O5'-P-OP1	-5.88	100.41	105.70
29	o	10	LYS	CD-CE-NZ	5.87	125.21	111.70
38	3	91	LEU	CB-CG-CD1	-5.85	101.05	111.00
6	R	65	THR	C-N-CA	-5.85	110.01	122.30
35	0	1182	G	P-O3'-C3'	5.85	126.72	119.70
38	3	70	ARG	NE-CZ-NH1	5.85	123.22	120.30
28	n	52	ARG	NE-CZ-NH2	5.84	123.22	120.30
33	N	820	A	O4'-C4'-C3'	-5.84	98.16	104.00
33	N	1427	A	O5'-P-OP1	-5.84	100.44	105.70
30	p	12	ARG	CA-CB-CG	5.84	126.24	113.40
33	N	2383	G	O5'-P-OP2	-5.84	100.45	105.70
35	0	9	G	O5'-P-OP1	5.84	117.71	110.70
13	Y	30	THR	N-CA-CB	5.83	121.38	110.30
30	p	12	ARG	NE-CZ-NH1	-5.83	117.39	120.30
33	N	503	A	C6-C5-N7	-5.83	128.22	132.30
33	N	310	A	C4-C5-C6	5.82	119.91	117.00
33	N	578	G	O5'-P-OP2	-5.82	100.47	105.70
33	N	1134	A	P-O3'-C3'	5.81	126.67	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	D	59	ARG	NE-CZ-NH1	5.81	123.20	120.30
33	N	1673	G	O5'-P-OP2	5.81	117.67	110.70
35	O	1201	A	P-O3'-C3'	5.80	126.66	119.70
33	N	1617	C	O5'-P-OP2	-5.79	100.48	105.70
33	N	679	C	OP1-P-OP2	5.78	128.27	119.60
15	a	49	GLU	OE1-CD-OE2	-5.78	116.37	123.30
33	N	2689	U	OP1-P-OP2	5.77	128.26	119.60
33	N	477	A	O5'-P-OP2	-5.77	100.51	105.70
33	N	301	G	C4-N9-C1'	-5.76	119.00	126.50
33	N	1130	U	O5'-P-OP1	-5.76	100.51	105.70
33	N	859	G	P-O3'-C3'	5.75	126.60	119.70
25	k	37	ARG	NE-CZ-NH2	5.75	123.18	120.30
33	N	775	G	O5'-P-OP1	-5.75	100.53	105.70
33	N	783	A	O5'-P-OP2	-5.75	100.53	105.70
5	Q	124	ARG	NE-CZ-NH1	5.75	123.17	120.30
33	N	2682	A	O5'-P-OP2	5.75	117.59	110.70
40	5	90	MET	C-N-CA	5.75	136.06	121.70
43	8	45	ARG	NE-CZ-NH1	5.74	123.17	120.30
33	N	1348	C	O5'-P-OP1	-5.74	100.53	105.70
33	N	504	A	O5'-P-OP2	-5.74	100.53	105.70
33	N	2720	U	N1-C2-O2	-5.74	118.78	122.80
33	N	242	G	C4'-C3'-O3'	5.73	124.46	113.00
19	e	80	ARG	NE-CZ-NH2	-5.73	117.44	120.30
33	N	675	A	O5'-P-OP2	5.73	117.57	110.70
49	E	54	ARG	NE-CZ-NH1	5.73	123.16	120.30
35	O	1254	A	O5'-P-OP1	-5.72	100.55	105.70
39	4	69	ARG	NE-CZ-NH1	5.72	123.16	120.30
33	N	1570	A	O5'-P-OP1	-5.72	100.56	105.70
33	N	2873	A	C3'-C2'-C1'	5.72	106.07	101.50
35	O	176	C	O5'-P-OP1	-5.71	100.56	105.70
46	B	14	ARG	NE-CZ-NH1	5.71	123.15	120.30
49	E	70	LEU	CB-CG-CD2	-5.70	101.31	111.00
33	N	1565	C	C5'-C4'-C3'	-5.68	106.91	116.00
33	N	2688	G	O5'-P-OP1	-5.68	100.59	105.70
33	N	1676	A	O5'-P-OP2	5.68	117.52	110.70
33	N	780	G	O5'-P-OP2	-5.68	100.59	105.70
3	O	44	G	N9-C1'-C2'	5.67	121.38	114.00
35	O	1067	A	O5'-P-OP1	-5.67	100.59	105.70
33	N	1261	C	O4'-C4'-C3'	-5.66	98.34	104.00
33	N	1843	C	O5'-P-OP1	-5.66	100.61	105.70
33	N	860	U	OP1-P-OP2	-5.66	111.11	119.60
33	N	2645	G	C5'-C4'-C3'	-5.65	106.95	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	N	1788	C	OP1-P-O3'	5.65	117.63	105.20
4	P	130	LEU	CA-CB-CG	5.65	128.29	115.30
48	D	61	ARG	NE-CZ-NH2	-5.64	117.48	120.30
4	P	133	ARG	NE-CZ-NH2	5.64	123.12	120.30
33	N	205	G	O4'-C1'-N9	5.64	112.71	108.20
49	E	43	PHE	CB-CG-CD1	-5.63	116.86	120.80
33	N	1688	U	O5'-P-OP1	-5.62	100.64	105.70
39	4	138	ARG	N-CA-CB	5.62	120.72	110.60
35	0	1331	G	O4'-C1'-N9	5.62	112.70	108.20
18	d	28	ARG	NE-CZ-NH2	-5.62	117.49	120.30
4	P	156	ARG	NE-CZ-NH1	5.62	123.11	120.30
33	N	2498	C	OP1-P-OP2	5.61	128.02	119.60
55	K	17	ARG	NE-CZ-NH2	-5.60	117.50	120.30
28	n	16	ARG	NE-CZ-NH1	-5.60	117.50	120.30
4	P	187	ASP	CB-CG-OD1	5.59	123.34	118.30
33	N	2499	C	O5'-P-OP1	5.59	117.41	110.70
33	N	2260	C	O5'-P-OP1	-5.59	100.67	105.70
43	8	123	ARG	NE-CZ-NH1	5.58	123.09	120.30
33	N	2580	U	O5'-P-OP2	-5.58	100.68	105.70
35	0	567	G	OP1-P-OP2	5.57	127.96	119.60
8	T	149	ARG	NE-CZ-NH2	-5.57	117.52	120.30
33	N	528	A	C8-N9-C1'	5.57	137.72	127.70
33	N	1029	A	O5'-P-OP1	-5.57	100.69	105.70
33	N	2725	A	C5'-C4'-O4'	-5.57	102.42	109.10
33	N	2776	A	C2'-C3'-O3'	5.56	122.60	113.70
33	N	1612	C	O5'-P-OP1	-5.56	100.70	105.70
6	R	88	ARG	NE-CZ-NH1	-5.56	117.52	120.30
33	N	1143	A	O5'-P-OP2	-5.55	100.70	105.70
4	P	156	ARG	CG-CD-NE	5.55	123.45	111.80
26	l	48	ARG	NE-CZ-NH2	-5.55	117.53	120.30
33	N	1952	A	O5'-P-OP1	-5.54	100.71	105.70
35	0	1474	U	O5'-P-OP1	-5.54	100.71	105.70
15	a	46	ARG	NE-CZ-NH1	-5.54	117.53	120.30
14	Z	40	ARG	NE-CZ-NH1	-5.54	117.53	120.30
33	N	372	G	P-O3'-C3'	5.54	126.34	119.70
17	c	89	ARG	NE-CZ-NH2	5.53	123.07	120.30
33	N	2543	G	C5'-C4'-C3'	-5.53	107.15	116.00
47	C	109	ARG	NE-CZ-NH2	-5.53	117.53	120.30
33	N	2452	C	O5'-P-OP2	-5.53	100.72	105.70
33	N	1990	C	O5'-P-OP1	-5.52	100.73	105.70
33	N	825	A	O5'-P-OP2	-5.52	100.73	105.70
35	0	653	U	O5'-P-OP1	-5.52	100.73	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	N	871	U	P-O5'-C5'	-5.52	112.07	120.90
33	N	2359	C	O5'-P-OP1	-5.51	100.74	105.70
35	O	734	G	O5'-P-OP1	-5.51	100.74	105.70
33	N	2514	U	O5'-P-OP2	-5.51	100.74	105.70
4	P	239	ASN	N-CA-C	5.51	125.87	111.00
37	2	132	ARG	NE-CZ-NH1	5.50	123.05	120.30
4	P	232	HIS	O-C-N	-5.50	113.84	123.20
35	O	818	G	N9-C1'-C2'	5.50	121.16	114.00
11	W	39	LYS	CD-CE-NZ	-5.50	99.05	111.70
33	N	2872	A	O5'-P-OP1	-5.50	100.75	105.70
33	N	670	A	C2'-C3'-O3'	5.50	122.50	113.70
33	N	573	U	P-O3'-C3'	5.50	126.30	119.70
33	N	463	G	O5'-P-OP2	-5.49	100.76	105.70
33	N	803	U	O5'-P-OP1	-5.49	100.76	105.70
17	c	21	ARG	NH1-CZ-NH2	5.48	125.43	119.40
33	N	301	G	C8-N9-C1'	5.48	134.13	127.00
35	O	330	C	P-O5'-C5'	-5.48	112.14	120.90
33	N	1322	A	O5'-P-OP1	-5.47	100.77	105.70
33	N	790	U	O5'-P-OP2	-5.47	100.78	105.70
33	N	2720	U	N3-C4-C5	5.47	117.88	114.60
33	N	2266	A	C4'-C3'-O3'	-5.46	97.93	109.40
18	d	6	ARG	NE-CZ-NH1	-5.46	117.57	120.30
33	N	2037	A	C5'-C4'-O4'	-5.46	102.55	109.10
33	N	234	U	N3-C2-O2	-5.46	118.38	122.20
35	O	886	G	O5'-P-OP1	-5.45	100.79	105.70
33	N	2873	A	P-O5'-C5'	-5.44	112.19	120.90
13	Y	78	ARG	NE-CZ-NH1	-5.44	117.58	120.30
35	O	37	U	N3-C2-O2	-5.43	118.40	122.20
44	9	92	LEU	CA-CB-CG	5.43	127.79	115.30
33	N	774	G	C1'-C2'-O2'	-5.43	94.31	110.60
16	b	94	ARG	NE-CZ-NH1	-5.42	117.59	120.30
33	N	1695	G	O5'-P-OP2	-5.42	100.82	105.70
35	O	816	A	O5'-P-OP2	5.42	117.20	110.70
11	W	124	VAL	CG1-CB-CG2	-5.41	102.24	110.90
3	O	48	U	O5'-P-OP1	-5.41	100.83	105.70
35	O	976	G	O5'-P-OP2	5.41	117.19	110.70
33	N	2848	G	O4'-C1'-N9	5.41	112.53	108.20
27	m	54	MET	CG-SD-CE	-5.40	91.56	100.20
33	N	1325	U	O5'-P-OP2	-5.39	100.85	105.70
37	2	157	LEU	CA-CB-CG	5.39	127.70	115.30
43	8	99	ARG	NE-CZ-NH2	-5.39	117.61	120.30
33	N	2765	A	C2-N3-C4	-5.39	107.91	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	0	574	A	O5'-P-OP1	-5.39	100.85	105.70
33	N	748	G	O5'-P-OP2	-5.39	100.85	105.70
33	N	1142	A	P-O3'-C3'	5.39	126.16	119.70
49	E	64	ARG	CG-CD-NE	-5.39	100.49	111.80
35	0	880	C	O5'-P-OP1	5.38	117.16	110.70
13	Y	52	GLY	C-N-CA	-5.38	111.00	122.30
33	N	2848	G	O5'-P-OP1	-5.38	100.86	105.70
33	N	514	A	O5'-P-OP1	-5.38	100.86	105.70
33	N	1669	A	C8-N9-C1'	-5.38	118.02	127.70
33	N	1031	G	O5'-P-OP2	-5.38	100.86	105.70
35	0	1301	U	C6-N1-C1'	-5.38	113.67	121.20
33	N	2405	G	P-O3'-C3'	5.37	126.15	119.70
4	P	217	ARG	NE-CZ-NH1	-5.37	117.62	120.30
18	d	92	ARG	NE-CZ-NH2	5.37	122.98	120.30
4	P	195	VAL	CG1-CB-CG2	-5.37	102.31	110.90
16	b	33	ARG	NE-CZ-NH2	-5.37	117.62	120.30
5	Q	146	ILE	CG1-CB-CG2	-5.36	99.61	111.40
33	N	2832	U	P-O3'-C3'	5.35	126.12	119.70
35	0	1504	G	O5'-P-OP2	-5.35	100.88	105.70
46	B	38	TYR	CB-CG-CD1	-5.35	117.79	121.00
35	0	368	U	N3-C2-O2	-5.35	118.46	122.20
35	0	1500	A	O5'-P-OP2	-5.34	100.89	105.70
4	P	84	ASP	CB-CG-OD1	5.34	123.11	118.30
35	0	560	A	O5'-P-OP1	-5.34	100.90	105.70
33	N	1142	A	C3'-C2'-C1'	5.33	105.77	101.50
55	K	16	LEU	CA-CB-CG	5.33	127.57	115.30
33	N	771	G	O5'-P-OP1	-5.33	100.90	105.70
15	a	17	ARG	NE-CZ-NH2	5.33	122.96	120.30
41	6	3	ARG	NE-CZ-NH2	-5.32	117.64	120.30
11	W	99	ARG	NE-CZ-NH2	-5.32	117.64	120.30
33	N	1669	A	C4-N9-C1'	5.32	135.87	126.30
33	N	2613	U	N3-C4-O4	-5.32	115.68	119.40
35	0	96	U	C2'-C3'-O3'	5.32	122.21	113.70
33	N	2394	C	O4'-C4'-C3'	-5.32	98.68	104.00
33	N	2884	U	O4'-C1'-N1	5.32	112.45	108.20
35	0	804	U	O5'-P-OP1	-5.31	100.92	105.70
4	P	14	ARG	NE-CZ-NH1	5.31	122.95	120.30
5	Q	154	LYS	CD-CE-NZ	-5.31	99.50	111.70
17	c	109	ARG	NE-CZ-NH2	5.30	122.95	120.30
28	n	10	ARG	NE-CZ-NH2	5.30	122.95	120.30
33	N	140	C	C6-N1-C1'	-5.30	114.44	120.80
33	N	1256	G	O4'-C1'-N9	-5.29	103.97	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	0	1319	A	O5'-P-OP1	-5.29	100.94	105.70
24	j	41	ARG	CB-CG-CD	5.29	125.35	111.60
33	N	1783	A	O5'-P-OP1	5.29	117.04	110.70
33	N	430	A	C5-C6-N6	5.29	127.93	123.70
33	N	915	C	O5'-P-OP2	-5.29	100.94	105.70
18	d	3	ARG	NE-CZ-NH2	5.28	122.94	120.30
33	N	1021	A	C5-C6-N6	5.28	127.92	123.70
33	N	2286	G	P-O3'-C3'	5.28	126.04	119.70
47	C	98	ARG	CG-CD-NE	5.28	122.89	111.80
42	7	99	LEU	CB-CG-CD1	-5.28	102.03	111.00
35	0	558	G	O5'-P-OP1	5.28	117.03	110.70
32	r	1	MET	CB-CG-SD	-5.28	96.57	112.40
35	0	728	A	O5'-P-OP2	-5.27	100.96	105.70
35	0	890	G	P-O3'-C3'	5.27	126.03	119.70
4	P	221	ARG	N-CA-CB	5.26	120.08	110.60
12	X	23	LYS	N-CA-CB	5.26	120.07	110.60
33	N	1271	G	O5'-P-OP1	5.26	117.01	110.70
25	k	57	ARG	NE-CZ-NH1	-5.26	117.67	120.30
33	N	499	U	N3-C4-C5	5.25	117.75	114.60
35	0	108	G	O4'-C1'-N9	5.25	112.40	108.20
33	N	532	A	O5'-P-OP2	-5.25	100.98	105.70
33	N	2867	G	P-O3'-C3'	5.25	126.00	119.70
35	0	1363	A	C5-C6-N6	5.24	127.89	123.70
32	r	36	ARG	CG-CD-NE	-5.24	100.80	111.80
25	k	28	ARG	NH1-CZ-NH2	5.24	125.16	119.40
35	0	822	U	O5'-P-OP1	-5.24	100.99	105.70
33	N	528	A	C4-N9-C1'	-5.23	116.88	126.30
33	N	1829	A	O5'-P-OP2	-5.23	100.99	105.70
14	Z	18	ARG	NE-CZ-NH2	5.23	122.91	120.30
33	N	611	C	O5'-P-OP1	-5.22	101.00	105.70
32	r	3	VAL	CG1-CB-CG2	-5.22	102.55	110.90
33	N	1800	C	O5'-P-OP2	-5.22	101.00	105.70
46	B	22	PRO	O-C-N	-5.21	114.36	122.70
33	N	1815	A	C5'-C4'-O4'	-5.21	102.85	109.10
33	N	2007	U	O5'-P-OP2	-5.21	101.02	105.70
8	T	149	ARG	NE-CZ-NH1	5.20	122.90	120.30
15	a	2	ARG	NE-CZ-NH1	5.20	122.90	120.30
46	B	61	PHE	CB-CG-CD1	5.20	124.44	120.80
35	0	595	A	P-O3'-C3'	5.20	125.94	119.70
33	N	2243	U	O5'-P-OP1	-5.20	101.02	105.70
5	Q	124	ARG	NE-CZ-NH2	-5.19	117.70	120.30
13	Y	132	ARG	NE-CZ-NH2	-5.19	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	N	1313	U	C6-N1-C1'	-5.19	113.93	121.20
33	N	825	A	OP1-P-O3'	5.19	116.61	105.20
33	N	2831	G	O5'-P-OP1	-5.18	101.03	105.70
15	a	86	ARG	NE-CZ-NH2	-5.18	117.71	120.30
18	d	33	ARG	CB-CG-CD	-5.17	98.15	111.60
33	N	932	U	N3-C2-O2	-5.17	118.58	122.20
36	l	103	ASN	N-CA-CB	5.17	119.91	110.60
33	N	1950	G	O5'-P-OP1	-5.17	101.05	105.70
33	N	1606	C	O5'-P-OP2	-5.16	101.05	105.70
19	e	79	ARG	CD-NE-CZ	-5.16	116.38	123.60
33	N	1270	C	O5'-P-OP1	-5.16	101.06	105.70
35	0	1125	U	C2-N1-C1'	5.16	123.89	117.70
48	D	13	ARG	NE-CZ-NH2	-5.15	117.72	120.30
33	N	2874	C	O5'-P-OP2	-5.15	101.07	105.70
33	N	2645	G	P-O5'-C5'	-5.14	112.67	120.90
4	P	156	ARG	CB-CG-CD	-5.14	98.24	111.60
33	N	752	A	O4'-C1'-N9	5.14	112.31	108.20
35	0	1358	U	N3-C2-O2	-5.14	118.60	122.20
50	F	70	ARG	CG-CD-NE	5.14	122.59	111.80
49	E	58	ARG	NE-CZ-NH1	5.13	122.87	120.30
33	N	830	G	O4'-C1'-N9	-5.13	104.09	108.20
33	N	997	G	O5'-P-OP1	-5.13	101.08	105.70
35	0	163	C	O5'-P-OP1	-5.13	101.08	105.70
33	N	953	G	OP1-P-OP2	5.12	127.28	119.60
33	N	2093	G	O5'-P-OP1	-5.12	101.09	105.70
33	N	1236	G	C5'-C4'-O4'	-5.12	102.96	109.10
40	5	24	ARG	NE-CZ-NH2	-5.12	117.74	120.30
33	N	1998	A	O4'-C4'-C3'	-5.12	98.88	104.00
33	N	1288	G	C4-N9-C1'	5.11	133.15	126.50
33	N	2049	G	O4'-C4'-C3'	-5.11	98.89	104.00
4	P	217	ARG	CG-CD-NE	-5.11	101.07	111.80
33	N	651	G	O5'-P-OP2	-5.11	101.10	105.70
45	A	126	LYS	CB-CA-C	5.11	120.61	110.40
33	N	704	G	O4'-C1'-N9	5.10	112.28	108.20
47	C	3	ARG	CD-NE-CZ	5.10	130.74	123.60
50	F	14	ARG	NE-CZ-NH2	-5.09	117.75	120.30
50	F	51	ARG	NE-CZ-NH1	5.09	122.85	120.30
5	Q	114	LYS	CA-CB-CG	5.09	124.60	113.40
33	N	1020	A	P-O3'-C3'	5.09	125.81	119.70
33	N	1667	G	O5'-P-OP2	5.09	116.81	110.70
33	N	658	U	O5'-P-OP2	-5.09	101.12	105.70
33	N	2656	U	C6-N1-C1'	-5.09	114.08	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	N	1997	C	O4'-C4'-C3'	-5.09	98.91	104.00
3	O	52	A	P-O3'-C3'	5.08	125.80	119.70
33	N	278	A	C4-N9-C1'	5.08	135.45	126.30
33	N	2049	G	OP1-P-OP2	-5.08	111.98	119.60
33	N	578	G	OP1-P-OP2	-5.08	111.99	119.60
17	c	53	ARG	CB-CG-CD	-5.07	98.41	111.60
33	N	2267	A	N9-C1'-C2'	5.07	120.59	114.00
33	N	2720	U	N1-C2-N3	5.07	117.94	114.90
33	N	2215	C	O5'-P-OP1	-5.07	101.14	105.70
35	0	887	G	O5'-P-OP2	-5.07	101.14	105.70
43	8	85	ARG	NE-CZ-NH2	-5.07	117.77	120.30
49	E	66	LEU	CB-CG-CD2	-5.07	102.39	111.00
6	R	65	THR	O-C-N	-5.07	114.59	123.20
35	0	578	C	O5'-P-OP1	5.06	116.78	110.70
33	N	1764	C	O5'-P-OP1	-5.06	101.14	105.70
33	N	2496	C	O5'-P-OP2	-5.06	101.14	105.70
4	P	24	LEU	CB-CG-CD1	-5.06	102.40	111.00
33	N	555	G	P-O3'-C3'	5.05	125.76	119.70
19	e	81	LYS	CD-CE-NZ	5.05	123.32	111.70
1	s	153	LEU	CA-CB-CG	5.05	126.92	115.30
12	X	71	ARG	NE-CZ-NH2	-5.05	117.78	120.30
33	N	140	C	N1-C1'-C2'	5.05	120.56	114.00
33	N	1026	G	O5'-P-OP1	5.05	116.76	110.70
33	N	1784	A	O5'-P-OP1	-5.05	101.16	105.70
35	0	1300	G	P-O3'-C3'	5.04	125.75	119.70
38	3	13	ARG	NE-CZ-NH1	5.04	122.82	120.30
3	O	15	A	O4'-C1'-N9	5.04	112.23	108.20
33	N	2765	A	C4-N9-C1'	5.03	135.35	126.30
35	0	502	A	O5'-P-OP2	-5.03	101.17	105.70
56	t	465	U	O4'-C1'-N1	5.03	112.22	108.20
21	g	7	LEU	CA-CB-CG	5.03	126.86	115.30
35	0	85	U	P-O3'-C3'	5.03	125.73	119.70
35	0	578	C	O5'-P-OP2	-5.03	101.18	105.70
33	N	1968	G	O4'-C4'-C3'	-5.02	98.98	104.00
44	9	17	LEU	CB-CG-CD2	-5.02	102.47	111.00
13	Y	2	ARG	NE-CZ-NH1	5.01	122.81	120.30
14	Z	38	ARG	NE-CZ-NH2	-5.01	117.80	120.30
33	N	918	A	O5'-P-OP1	-5.01	101.19	105.70
54	J	69	LYS	N-CA-C	5.01	124.53	111.00
24	j	79	PHE	CB-CG-CD1	5.01	124.31	120.80
48	D	85	ARG	NE-CZ-NH2	-5.01	117.80	120.30
13	Y	3	LEU	CB-CG-CD1	-5.00	102.49	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	k	72	ARG	NE-CZ-NH1	5.00	122.80	120.30
35	0	103	U	O5'-P-OP1	-5.00	101.19	105.70
33	N	962	G	OP1-P-OP2	-5.00	112.09	119.60
33	N	2778	A	O5'-P-OP2	-5.00	101.20	105.70
50	F	8	ARG	NE-CZ-NH1	5.00	122.80	120.30
33	N	556	A	O5'-P-OP1	-5.00	101.20	105.70

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	0	24	U	Sidechain
35	0	368	U	Sidechain
35	0	559	A	Sidechain
35	0	571	U	Sidechain
35	0	864	A	Sidechain
36	1	10	LEU	Peptide
36	1	102	THR	Peptide
36	1	14	VAL	Peptide
37	2	79	LYS	Peptide
37	2	80	LYS	Peptide
39	4	102	GLY	Peptide
39	4	136	VAL	Peptide
39	4	137	VAL	Peptide
39	4	142	ASP	Peptide
39	4	89	HIS	Peptide
40	5	52	ASN	Peptide
40	5	93	LYS	Peptide
43	8	128	SER	Peptide
43	8	53	GLU	Peptide
43	8	54	LEU	Peptide
43	8	55	VAL	Peptide
45	A	125	LYS	Peptide
46	B	22	PRO	Peptide
46	B	77	HIS	Peptide
51	G	17	MET	Peptide
51	G	69	LYS	Peptide
53	I	37	ARG	Peptide
54	J	3	ASN	Peptide
55	K	34	ARG	Peptide
33	N	1802	A	Sidechain
33	N	2105	U	Sidechain

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Mol	Chain	Res	Type	Group
33	N	2522	U	Sidechain
33	N	2765	A	Sidechain
33	N	586	A	Sidechain
33	N	850	U	Sidechain
33	N	927	A	Sidechain
4	P	195	VAL	Peptide
4	P	234	GLY	Peptide
4	P	238	ARG	Peptide
5	Q	151	THR	Peptide
7	S	174	ASP	Peptide
7	S	175	PHE	Peptide
9	U	34	GLY	Peptide
10	V	11	LEU	Peptide
13	Y	114	GLY	Peptide
13	Y	82	LEU	Peptide
14	Z	57	VAL	Mainchain,Peptide
22	h	52	LEU	Peptide
31	q	31	HIS	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	s	35/179 (20%)	32 (91%)	3 (9%)	0	100	100
4	P	269/273 (98%)	247 (92%)	18 (7%)	4 (2%)	8	29
5	Q	207/209 (99%)	195 (94%)	11 (5%)	1 (0%)	25	56
6	R	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
7	S	175/179 (98%)	163 (93%)	11 (6%)	1 (1%)	22	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	T	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
9	U	45/149 (30%)	35 (78%)	9 (20%)	1 (2%)	5	21
10	V	139/142 (98%)	112 (81%)	27 (19%)	0	100	100
11	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
12	X	120/123 (98%)	109 (91%)	9 (8%)	2 (2%)	7	27
13	Y	141/144 (98%)	121 (86%)	16 (11%)	4 (3%)	4	16
14	Z	134/136 (98%)	118 (88%)	11 (8%)	5 (4%)	2	11
15	a	118/127 (93%)	102 (86%)	14 (12%)	2 (2%)	7	27
16	b	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
17	c	112/115 (97%)	104 (93%)	8 (7%)	0	100	100
18	d	115/118 (98%)	115 (100%)	0	0	100	100
19	e	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	13	40
20	f	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	14	43
21	g	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	5	21
22	h	100/104 (96%)	84 (84%)	14 (14%)	2 (2%)	6	23
23	i	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
24	j	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
25	k	75/78 (96%)	71 (95%)	3 (4%)	1 (1%)	10	33
26	l	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
27	m	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
28	n	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	6	24
29	o	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
30	p	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
31	q	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	8	28
32	r	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
34	L	64/70 (91%)	56 (88%)	7 (11%)	1 (2%)	8	28
36	1	216/233 (93%)	187 (87%)	28 (13%)	1 (0%)	25	56
37	2	204/233 (88%)	186 (91%)	16 (8%)	2 (1%)	13	40
38	3	203/206 (98%)	182 (90%)	21 (10%)	0	100	100
39	4	148/166 (89%)	116 (78%)	30 (20%)	2 (1%)	9	31
40	5	98/131 (75%)	81 (83%)	11 (11%)	6 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	6	149/156 (96%)	139 (93%)	10 (7%)	0	100	100
42	7	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
43	8	125/130 (96%)	103 (82%)	20 (16%)	2 (2%)	8	28
44	9	96/103 (93%)	84 (88%)	9 (9%)	3 (3%)	3	14
45	A	115/129 (89%)	102 (89%)	13 (11%)	0	100	100
46	B	121/124 (98%)	104 (86%)	15 (12%)	2 (2%)	7	27
47	C	112/118 (95%)	103 (92%)	8 (7%)	1 (1%)	14	43
48	D	92/101 (91%)	77 (84%)	14 (15%)	1 (1%)	12	37
49	E	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
50	F	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	10	33
51	G	78/84 (93%)	66 (85%)	9 (12%)	3 (4%)	2	11
52	H	53/75 (71%)	49 (92%)	3 (6%)	1 (2%)	6	24
53	I	77/92 (84%)	73 (95%)	4 (5%)	0	100	100
54	J	83/87 (95%)	78 (94%)	4 (5%)	1 (1%)	11	35
55	K	49/71 (69%)	40 (82%)	9 (18%)	0	100	100
All	All	5614/6198 (91%)	5069 (90%)	489 (9%)	56 (1%)	16	40

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	P	239	ASN
13	Y	36	LYS
14	Z	58	LYS
19	e	53	PHE
28	n	55	ILE
31	q	32	ILE
40	5	53	LYS
44	9	58	ASN
50	F	44	SER
51	G	70	THR
14	Z	59	ARG
15	a	3	HIS
37	2	81	GLY
40	5	56	LYS
40	5	91	ARG
43	8	55	VAL
46	B	23	ALA

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Mol	Chain	Res	Type
51	G	18	GLU
54	J	69	LYS
4	P	235	GLY
14	Z	39	GLY
21	g	77	ARG
21	g	78	SER
22	h	99	ASN
25	k	3	ARG
37	2	80	LYS
40	5	54	LEU
40	5	94	HIS
44	9	43	PRO
46	B	78	SER
51	G	71	LYS
52	H	48	ARG
4	P	10	SER
4	P	238	ARG
5	Q	149	ASN
7	S	175	PHE
9	U	35	LYS
12	X	93	GLN
13	Y	29	LYS
13	Y	30	THR
13	Y	31	GLY
14	Z	69	PRO
34	L	3	LYS
39	4	51	GLY
40	5	86	ARG
47	C	66	GLU
15	a	88	ALA
20	f	64	ALA
22	h	53	ASN
36	1	194	ASP
39	4	90	THR
48	D	4	GLN
44	9	42	LEU
14	Z	87	GLY
43	8	10	GLY
12	X	119	ALA

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	s	34/158 (22%)	34 (100%)	0	100	100
4	P	216/218 (99%)	215 (100%)	1 (0%)	86	96
5	Q	164/164 (100%)	161 (98%)	3 (2%)	54	82
6	R	165/165 (100%)	161 (98%)	4 (2%)	44	76
7	S	148/150 (99%)	148 (100%)	0	100	100
8	T	137/138 (99%)	137 (100%)	0	100	100
9	U	38/114 (33%)	37 (97%)	1 (3%)	41	74
10	V	109/110 (99%)	108 (99%)	1 (1%)	75	92
11	W	116/116 (100%)	116 (100%)	0	100	100
12	X	103/104 (99%)	103 (100%)	0	100	100
13	Y	102/103 (99%)	102 (100%)	0	100	100
14	Z	109/109 (100%)	108 (99%)	1 (1%)	75	92
15	a	100/103 (97%)	97 (97%)	3 (3%)	36	71
16	b	86/87 (99%)	86 (100%)	0	100	100
17	c	98/100 (98%)	95 (97%)	3 (3%)	35	70
18	d	89/90 (99%)	88 (99%)	1 (1%)	70	90
19	e	84/84 (100%)	82 (98%)	2 (2%)	44	76
20	f	93/93 (100%)	93 (100%)	0	100	100
21	g	80/84 (95%)	80 (100%)	0	100	100
22	h	83/85 (98%)	82 (99%)	1 (1%)	67	89
23	i	78/78 (100%)	78 (100%)	0	100	100
24	j	56/63 (89%)	55 (98%)	1 (2%)	54	82
25	k	67/68 (98%)	67 (100%)	0	100	100
26	l	55/55 (100%)	55 (100%)	0	100	100
27	m	48/49 (98%)	48 (100%)	0	100	100
28	n	47/48 (98%)	46 (98%)	1 (2%)	48	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	o	45/49 (92%)	45 (100%)	0	100	100
30	p	38/38 (100%)	38 (100%)	0	100	100
31	q	51/52 (98%)	49 (96%)	2 (4%)	27	62
32	r	34/34 (100%)	34 (100%)	0	100	100
34	L	59/62 (95%)	58 (98%)	1 (2%)	56	83
36	1	180/192 (94%)	179 (99%)	1 (1%)	84	95
37	2	170/190 (90%)	169 (99%)	1 (1%)	84	95
38	3	172/173 (99%)	171 (99%)	1 (1%)	84	95
39	4	113/125 (90%)	110 (97%)	3 (3%)	40	73
40	5	87/112 (78%)	86 (99%)	1 (1%)	70	90
41	6	124/129 (96%)	123 (99%)	1 (1%)	79	93
42	7	104/105 (99%)	104 (100%)	0	100	100
43	8	105/107 (98%)	104 (99%)	1 (1%)	73	91
44	9	86/90 (96%)	85 (99%)	1 (1%)	67	89
45	A	90/99 (91%)	89 (99%)	1 (1%)	70	90
46	B	103/104 (99%)	103 (100%)	0	100	100
47	C	92/96 (96%)	91 (99%)	1 (1%)	70	90
48	D	79/84 (94%)	79 (100%)	0	100	100
49	E	75/77 (97%)	74 (99%)	1 (1%)	65	88
50	F	65/65 (100%)	65 (100%)	0	100	100
51	G	74/78 (95%)	73 (99%)	1 (1%)	62	86
52	H	48/65 (74%)	48 (100%)	0	100	100
53	I	70/79 (89%)	68 (97%)	2 (3%)	37	72
54	J	65/66 (98%)	65 (100%)	0	100	100
55	K	44/61 (72%)	43 (98%)	1 (2%)	45	77
All	All	4678/5068 (92%)	4635 (99%)	43 (1%)	74	92

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	P	218	PRO
5	Q	73	VAL
5	Q	105	LYS

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Mol	Chain	Res	Type
5	Q	205	PRO
6	R	61	ARG
6	R	69	ARG
6	R	149	ILE
6	R	163	ASN
9	U	27	ARG
10	V	65	ARG
14	Z	128	THR
15	a	2	ARG
15	a	50	PRO
15	a	70	THR
17	c	53	ARG
17	c	73	VAL
17	c	93	ARG
18	d	33	ARG
19	e	49	ILE
19	e	53	PHE
22	h	68	SER
24	j	41	ARG
28	n	28	LEU
31	q	2	PRO
31	q	32	ILE
34	L	59	ARG
36	1	207	ILE
37	2	55	ILE
38	3	5	LEU
39	4	15	LEU
39	4	115	LEU
39	4	157	ARG
40	5	9	MET
41	6	25	LYS
43	8	120	LYS
44	9	17	LEU
45	A	93	ARG
47	C	98	ARG
49	E	70	LEU
51	G	61	ILE
53	I	5	LEU
53	I	49	ILE
55	K	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	s	126	HIS
4	P	53	HIS
4	P	86	ASN
4	P	134	ASN
4	P	260	ASN
5	Q	49	GLN
5	Q	149	ASN
5	Q	150	GLN
6	R	163	ASN
6	R	165	HIS
8	T	22	GLN
8	T	143	GLN
9	U	11	ASN
10	V	12	GLN
11	W	40	HIS
16	b	38	GLN
17	c	12	GLN
18	d	37	GLN
18	d	44	GLN
20	f	15	GLN
26	l	27	ASN
26	l	58	ASN
28	n	6	ASN
29	o	19	HIS
34	L	20	ASN
39	4	89	HIS
40	5	3	HIS
40	5	11	HIS
40	5	55	HIS
41	6	28	ASN
43	8	32	GLN
45	A	118	HIS
47	C	8	ASN
48	D	49	GLN
50	F	63	GLN
51	G	31	HIS
52	H	52	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	M	74/75 (98%)	11 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	O	117/120 (97%)	21 (17%)	1 (0%)
33	N	2894/2903 (99%)	536 (18%)	34 (1%)
35	0	1538/1539 (99%)	279 (18%)	22 (1%)
56	t	3/4 (75%)	1 (33%)	0
All	All	4626/4641 (99%)	848 (18%)	57 (1%)

All (848) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	M	9	C
2	M	10	G
2	M	15	G
2	M	16	C
2	M	17	G
2	M	19	U
2	M	20	A
2	M	42	G
2	M	47	C
2	M	74	C
2	M	75	A
3	O	13	G
3	O	25	U
3	O	31	C
3	O	35	C
3	O	41	G
3	O	44	G
3	O	45	A
3	O	51	G
3	O	53	A
3	O	56	G
3	O	57	A
3	O	64	G
3	O	66	A
3	O	67	G
3	O	88	C
3	O	89	U
3	O	90	C
3	O	91	C
3	O	99	A
3	O	108	A
3	O	109	A
33	N	10	A

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Mol	Chain	Res	Type
33	N	23	G
33	N	28	A
33	N	35	G
33	N	36	G
33	N	42	A
33	N	46	G
33	N	51	G
33	N	55	G
33	N	60	G
33	N	63	A
33	N	71	A
33	N	74	A
33	N	75	G
33	N	84	A
33	N	96	C
33	N	101	A
33	N	102	U
33	N	103	A
33	N	118	A
33	N	119	A
33	N	120	U
33	N	125	A
33	N	138	U
33	N	139	U
33	N	140	C
33	N	141	G
33	N	142	A
33	N	162	U
33	N	163	C
33	N	165	A
33	N	166	U
33	N	188	G
33	N	196	A
33	N	199	A
33	N	201	C
33	N	215	G
33	N	216	A
33	N	221	A
33	N	222	A
33	N	223	A
33	N	224	U
33	N	228	C

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Mol	Chain	Res	Type
33	N	241	A
33	N	242	G
33	N	243	U
33	N	248	G
33	N	255	A
33	N	265	A
33	N	266	G
33	N	267	C
33	N	271	G
33	N	272	A
33	N	276	U
33	N	278	A
33	N	281	C
33	N	284	U
33	N	294	A
33	N	301	G
33	N	311	A
33	N	323	C
33	N	329	G
33	N	330	A
33	N	332	A
33	N	346	A
33	N	361	G
33	N	362	A
33	N	371	A
33	N	372	G
33	N	373	U
33	N	386	G
33	N	396	G
33	N	399	U
33	N	403	U
33	N	404	A
33	N	405	U
33	N	406	G
33	N	411	G
33	N	412	A
33	N	421	C
33	N	422	A
33	N	424	G
33	N	435	C
33	N	447	A
33	N	455	C

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Mol	Chain	Res	Type
33	N	456	C
33	N	457	A
33	N	467	G
33	N	471	A
33	N	473	G
33	N	481	G
33	N	491	G
33	N	501	A
33	N	504	A
33	N	505	A
33	N	509	C
33	N	513	A
33	N	529	A
33	N	531	C
33	N	532	A
33	N	543	G
33	N	544	C
33	N	546	U
33	N	548	G
33	N	549	G
33	N	550	C
33	N	556	A
33	N	563	A
33	N	573	U
33	N	575	A
33	N	578	G
33	N	586	A
33	N	603	A
33	N	613	A
33	N	614	A
33	N	616	A
33	N	622	G
33	N	627	A
33	N	637	A
33	N	645	C
33	N	646	U
33	N	647	G
33	N	648	G
33	N	654	A
33	N	655	A
33	N	669	G
33	N	670	A

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Mol	Chain	Res	Type
33	N	671	C
33	N	677	A
33	N	686	U
33	N	695	G
33	N	696	G
33	N	717	C
33	N	729	G
33	N	730	A
33	N	738	G
33	N	747	U
33	N	764	A
33	N	765	C
33	N	775	G
33	N	776	G
33	N	782	A
33	N	783	A
33	N	784	G
33	N	785	G
33	N	792	A
33	N	800	A
33	N	805	G
33	N	806	C
33	N	812	C
33	N	819	A
33	N	827	U
33	N	828	U
33	N	829	A
33	N	845	A
33	N	846	U
33	N	858	G
33	N	860	U
33	N	866	A
33	N	869	G
33	N	878	A
33	N	885	C
33	N	896	A
33	N	897	C
33	N	907	G
33	N	910	A
33	N	914	G
33	N	919	U
33	N	932	U

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Mol	Chain	Res	Type
33	N	941	A
33	N	945	A
33	N	946	C
33	N	953	G
33	N	961	C
33	N	973	A
33	N	974	G
33	N	983	A
33	N	985	C
33	N	989	G
33	N	995	C
33	N	996	A
33	N	997	G
33	N	1004	U
33	N	1012	U
33	N	1013	C
33	N	1020	A
33	N	1021	A
33	N	1022	G
33	N	1023	U
33	N	1025	G
33	N	1026	G
33	N	1033	U
33	N	1046	A
33	N	1047	G
33	N	1057	A
33	N	1060	U
33	N	1062	G
33	N	1064	C
33	N	1066	U
33	N	1067	A
33	N	1068	G
33	N	1070	A
33	N	1077	A
33	N	1082	U
33	N	1083	U
33	N	1088	A
33	N	1089	A
33	N	1090	A
33	N	1094	U
33	N	1096	A
33	N	1097	U

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Mol	Chain	Res	Type
33	N	1100	C
33	N	1104	C
33	N	1110	G
33	N	1111	A
33	N	1112	G
33	N	1119	U
33	N	1122	G
33	N	1130	U
33	N	1132	U
33	N	1133	A
33	N	1135	C
33	N	1136	G
33	N	1141	U
33	N	1142	A
33	N	1143	A
33	N	1155	A
33	N	1168	G
33	N	1171	G
33	N	1173	U
33	N	1174	U
33	N	1175	A
33	N	1180	U
33	N	1186	G
33	N	1195	G
33	N	1204	A
33	N	1205	A
33	N	1206	G
33	N	1210	G
33	N	1212	G
33	N	1237	A
33	N	1238	G
33	N	1250	G
33	N	1251	C
33	N	1253	A
33	N	1256	G
33	N	1257	C
33	N	1265	A
33	N	1266	G
33	N	1268	A
33	N	1271	G
33	N	1272	A
33	N	1275	A

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Mol	Chain	Res	Type
33	N	1300	G
33	N	1301	A
33	N	1321	A
33	N	1329	U
33	N	1332	G
33	N	1345	C
33	N	1352	U
33	N	1365	A
33	N	1368	G
33	N	1376	C
33	N	1379	U
33	N	1383	A
33	N	1386	C
33	N	1395	A
33	N	1403	A
33	N	1416	G
33	N	1419	A
33	N	1420	A
33	N	1421	G
33	N	1427	A
33	N	1428	C
33	N	1434	A
33	N	1437	C
33	N	1453	A
33	N	1458	U
33	N	1461	C
33	N	1478	G
33	N	1482	G
33	N	1504	A
33	N	1508	A
33	N	1509	A
33	N	1515	A
33	N	1524	G
33	N	1529	G
33	N	1535	A
33	N	1536	C
33	N	1537	G
33	N	1538	G
33	N	1554	U
33	N	1565	C
33	N	1566	A
33	N	1569	A

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Mol	Chain	Res	Type
33	N	1578	U
33	N	1583	A
33	N	1584	U
33	N	1585	C
33	N	1587	G
33	N	1607	C
33	N	1608	A
33	N	1610	A
33	N	1613	G
33	N	1622	G
33	N	1647	U
33	N	1648	U
33	N	1651	G
33	N	1674	G
33	N	1675	C
33	N	1676	A
33	N	1698	A
33	N	1699	G
33	N	1713	A
33	N	1715	G
33	N	1728	C
33	N	1729	U
33	N	1730	C
33	N	1733	G
33	N	1738	G
33	N	1757	A
33	N	1758	U
33	N	1760	C
33	N	1764	C
33	N	1773	A
33	N	1784	A
33	N	1787	A
33	N	1800	C
33	N	1801	A
33	N	1802	A
33	N	1808	A
33	N	1811	G
33	N	1816	C
33	N	1829	A
33	N	1833	C
33	N	1835	G
33	N	1857	G

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Mol	Chain	Res	Type
33	N	1869	G
33	N	1870	C
33	N	1900	A
33	N	1901	A
33	N	1905	C
33	N	1906	G
33	N	1913	A
33	N	1919	A
33	N	1927	A
33	N	1929	G
33	N	1930	G
33	N	1931	U
33	N	1938	A
33	N	1955	U
33	N	1964	G
33	N	1967	C
33	N	1970	A
33	N	1971	U
33	N	1972	G
33	N	1991	U
33	N	1993	U
33	N	1997	C
33	N	2004	G
33	N	2006	C
33	N	2020	A
33	N	2022	U
33	N	2023	C
33	N	2031	A
33	N	2033	A
33	N	2043	C
33	N	2046	G
33	N	2055	C
33	N	2056	G
33	N	2060	A
33	N	2061	G
33	N	2062	A
33	N	2063	C
33	N	2069	G
33	N	2072	C
33	N	2077	A
33	N	2092	U
33	N	2093	G

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Mol	Chain	Res	Type
33	N	2097	A
33	N	2098	U
33	N	2102	G
33	N	2106	U
33	N	2110	G
33	N	2111	U
33	N	2112	G
33	N	2113	U
33	N	2118	U
33	N	2119	A
33	N	2121	G
33	N	2123	G
33	N	2125	G
33	N	2128	G
33	N	2131	U
33	N	2132	U
33	N	2133	G
33	N	2137	U
33	N	2139	U
33	N	2146	C
33	N	2149	U
33	N	2158	A
33	N	2159	G
33	N	2161	C
33	N	2162	G
33	N	2163	A
33	N	2164	C
33	N	2165	C
33	N	2170	A
33	N	2172	U
33	N	2173	A
33	N	2174	C
33	N	2178	C
33	N	2186	G
33	N	2189	U
33	N	2198	A
33	N	2203	U
33	N	2204	G
33	N	2211	A
33	N	2212	A
33	N	2214	C
33	N	2225	A

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Mol	Chain	Res	Type
33	N	2226	C
33	N	2238	G
33	N	2239	G
33	N	2266	A
33	N	2278	A
33	N	2279	G
33	N	2283	C
33	N	2286	G
33	N	2287	A
33	N	2288	A
33	N	2297	A
33	N	2305	U
33	N	2307	G
33	N	2309	A
33	N	2312	U
33	N	2325	G
33	N	2333	A
33	N	2334	U
33	N	2345	G
33	N	2347	C
33	N	2350	C
33	N	2354	C
33	N	2357	G
33	N	2361	G
33	N	2383	G
33	N	2385	C
33	N	2391	G
33	N	2402	U
33	N	2403	C
33	N	2406	A
33	N	2407	A
33	N	2422	C
33	N	2423	U
33	N	2425	A
33	N	2426	A
33	N	2427	C
33	N	2429	G
33	N	2430	A
33	N	2431	U
33	N	2435	A
33	N	2441	U
33	N	2448	A

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Mol	Chain	Res	Type
33	N	2470	G
33	N	2476	A
33	N	2498	C
33	N	2502	G
33	N	2503	A
33	N	2504	U
33	N	2505	G
33	N	2507	C
33	N	2518	A
33	N	2520	C
33	N	2529	G
33	N	2535	G
33	N	2547	A
33	N	2554	U
33	N	2566	A
33	N	2567	G
33	N	2572	A
33	N	2573	C
33	N	2574	G
33	N	2578	G
33	N	2585	U
33	N	2602	A
33	N	2603	G
33	N	2609	U
33	N	2613	U
33	N	2615	U
33	N	2629	U
33	N	2630	G
33	N	2636	C
33	N	2645	G
33	N	2646	C
33	N	2655	G
33	N	2656	U
33	N	2661	G
33	N	2663	G
33	N	2682	A
33	N	2689	U
33	N	2690	U
33	N	2714	G
33	N	2716	C
33	N	2718	G
33	N	2724	U

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Mol	Chain	Res	Type
33	N	2727	A
33	N	2733	A
33	N	2748	A
33	N	2751	G
33	N	2752	C
33	N	2765	A
33	N	2776	A
33	N	2777	G
33	N	2778	A
33	N	2779	U
33	N	2791	G
33	N	2792	A
33	N	2798	U
33	N	2801	G
33	N	2818	U
33	N	2820	A
33	N	2833	U
33	N	2834	G
33	N	2836	U
33	N	2849	U
33	N	2850	A
33	N	2859	G
33	N	2867	G
33	N	2868	A
33	N	2872	A
33	N	2873	A
33	N	2880	C
33	N	2884	U
33	N	2887	A
33	N	2891	U
33	N	2903	U
35	0	4	U
35	0	6	G
35	0	9	G
35	0	32	A
35	0	39	G
35	0	44	A
35	0	47	C
35	0	48	C
35	0	50	A
35	0	51	A
35	0	52	C

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Mol	Chain	Res	Type
35	0	58	C
35	0	65	A
35	0	69	G
35	0	71	A
35	0	72	A
35	0	83	C
35	0	84	U
35	0	85	U
35	0	86	G
35	0	87	C
35	0	92	U
35	0	97	G
35	0	108	G
35	0	115	G
35	0	116	A
35	0	122	G
35	0	130	A
35	0	141	G
35	0	143	A
35	0	144	G
35	0	149	A
35	0	156	C
35	0	163	C
35	0	174	A
35	0	177	G
35	0	182	A
35	0	183	C
35	0	184	G
35	0	197	A
35	0	209	U
35	0	210	C
35	0	211	G
35	0	226	G
35	0	245	U
35	0	247	G
35	0	251	G
35	0	266	G
35	0	267	C
35	0	280	C
35	0	281	G
35	0	289	G
35	0	298	A

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Mol	Chain	Res	Type
35	0	306	A
35	0	321	A
35	0	328	C
35	0	332	G
35	0	347	G
35	0	351	G
35	0	352	C
35	0	354	G
35	0	358	U
35	0	367	U
35	0	372	C
35	0	375	U
35	0	384	G
35	0	389	A
35	0	397	A
35	0	398	U
35	0	406	G
35	0	412	A
35	0	413	G
35	0	421	U
35	0	422	C
35	0	423	G
35	0	424	G
35	0	429	U
35	0	430	A
35	0	439	U
35	0	451	A
35	0	458	U
35	0	459	A
35	0	467	U
35	0	468	A
35	0	474	G
35	0	478	A
35	0	479	U
35	0	481	G
35	0	484	G
35	0	485	U
35	0	486	U
35	0	495	A
35	0	497	G
35	0	511	C
35	0	518	C

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Mol	Chain	Res	Type
35	0	519	C
35	0	521	G
35	0	527	G
35	0	531	U
35	0	532	A
35	0	533	A
35	0	547	A
35	0	559	A
35	0	562	U
35	0	572	A
35	0	573	A
35	0	576	C
35	0	596	A
35	0	607	A
35	0	633	G
35	0	639	G
35	0	650	G
35	0	652	U
35	0	665	A
35	0	675	A
35	0	688	G
35	0	695	A
35	0	701	U
35	0	702	A
35	0	703	G
35	0	718	A
35	0	721	G
35	0	723	U
35	0	724	G
35	0	731	G
35	0	734	G
35	0	747	A
35	0	755	G
35	0	777	A
35	0	793	U
35	0	794	A
35	0	813	U
35	0	815	A
35	0	817	C
35	0	818	G
35	0	819	A
35	0	821	G

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Mol	Chain	Res	Type
35	0	828	U
35	0	832	G
35	0	836	G
35	0	841	C
35	0	843	U
35	0	844	G
35	0	846	G
35	0	849	G
35	0	859	G
35	0	864	A
35	0	885	G
35	0	889	A
35	0	890	G
35	0	891	U
35	0	902	G
35	0	914	A
35	0	922	G
35	0	926	G
35	0	934	C
35	0	935	A
35	0	960	U
35	0	965	U
35	0	966	G
35	0	969	A
35	0	971	G
35	0	972	C
35	0	975	A
35	0	976	G
35	0	977	A
35	0	989	U
35	0	993	G
35	0	996	A
35	0	999	C
35	0	1000	A
35	0	1004	A
35	0	1008	U
35	0	1009	U
35	0	1017	U
35	0	1018	G
35	0	1020	G
35	0	1022	A
35	0	1024	G

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Mol	Chain	Res	Type
35	0	1025	U
35	0	1026	G
35	0	1027	C
35	0	1030	U
35	0	1031	C
35	0	1032	G
35	0	1043	G
35	0	1044	A
35	0	1053	G
35	0	1056	U
35	0	1065	U
35	0	1085	U
35	0	1092	A
35	0	1094	G
35	0	1095	U
35	0	1101	A
35	0	1125	U
35	0	1130	A
35	0	1132	C
35	0	1136	C
35	0	1137	C
35	0	1138	G
35	0	1139	G
35	0	1140	C
35	0	1146	A
35	0	1158	C
35	0	1159	U
35	0	1168	U
35	0	1171	A
35	0	1182	G
35	0	1183	U
35	0	1184	G
35	0	1190	G
35	0	1196	A
35	0	1200	C
35	0	1201	A
35	0	1202	U
35	0	1212	U
35	0	1213	A
35	0	1227	A
35	0	1238	A
35	0	1253	G

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Mol	Chain	Res	Type
35	0	1256	A
35	0	1257	A
35	0	1258	G
35	0	1260	G
35	0	1261	A
35	0	1274	A
35	0	1275	A
35	0	1278	G
35	0	1280	A
35	0	1281	C
35	0	1287	A
35	0	1297	G
35	0	1298	U
35	0	1300	G
35	0	1301	U
35	0	1302	C
35	0	1305	G
35	0	1317	C
35	0	1318	A
35	0	1319	A
35	0	1320	C
35	0	1322	C
35	0	1323	G
35	0	1331	G
35	0	1332	A
35	0	1340	A
35	0	1346	A
35	0	1347	G
35	0	1348	U
35	0	1353	G
35	0	1363	A
35	0	1364	U
35	0	1370	G
35	0	1379	G
35	0	1383	C
35	0	1394	A
35	0	1400	C
35	0	1419	G
35	0	1422	G
35	0	1433	A
35	0	1441	A
35	0	1446	A

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Mol	Chain	Res	Type
35	0	1451	U
35	0	1452	C
35	0	1487	G
35	0	1492	A
35	0	1494	G
35	0	1497	G
35	0	1503	A
35	0	1506	U
35	0	1517	G
35	0	1519	A
35	0	1529	G
35	0	1530	G
35	0	1531	A
35	0	1534	A
35	0	1535	C
35	0	1537	U
56	t	466	C

All (57) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	O	52	A
33	N	60	G
33	N	227	A
33	N	242	G
33	N	249	C
33	N	372	G
33	N	404	A
33	N	421	C
33	N	446	G
33	N	456	C
33	N	474	G
33	N	503	A
33	N	512	G
33	N	555	G
33	N	670	A
33	N	774	G
33	N	784	G
33	N	859	G
33	N	995	C
33	N	1020	A
33	N	1134	A

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Mol	Chain	Res	Type
33	N	1141	U
33	N	1142	A
33	N	1236	G
33	N	1900	A
33	N	2062	A
33	N	2225	A
33	N	2282	G
33	N	2286	G
33	N	2311	A
33	N	2405	G
33	N	2655	G
33	N	2776	A
33	N	2867	G
33	N	2873	A
35	0	64	G
35	0	85	U
35	0	96	U
35	0	115	G
35	0	388	G
35	0	429	U
35	0	518	C
35	0	595	A
35	0	812	G
35	0	890	G
35	0	965	U
35	0	1124	G
35	0	1145	A
35	0	1182	G
35	0	1190	G
35	0	1201	A
35	0	1300	G
35	0	1345	U
35	0	1347	G
35	0	1491	G
35	0	1493	A
35	0	1528	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

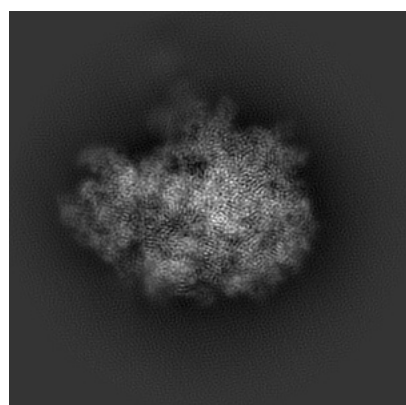
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3713. These allow visual inspection of the internal detail of the map and identification of artifacts.

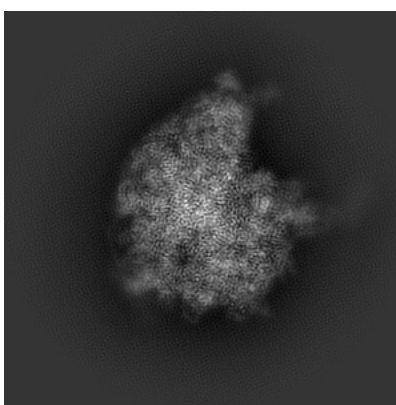
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

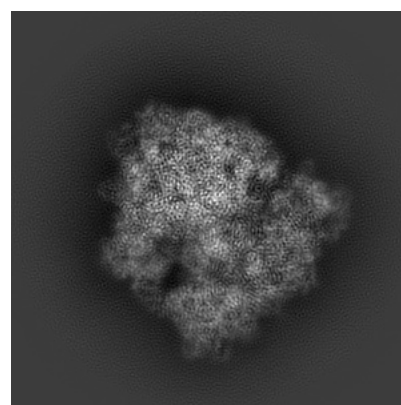
6.1.1 Primary map



X



Y

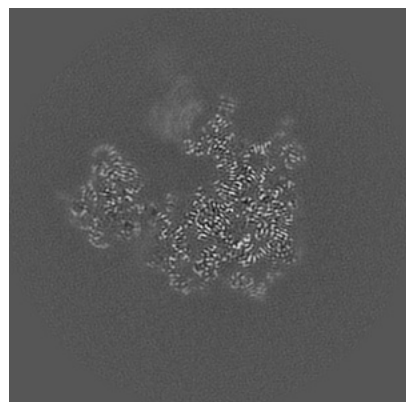


Z

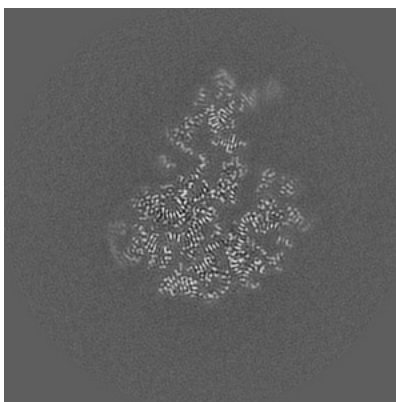
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

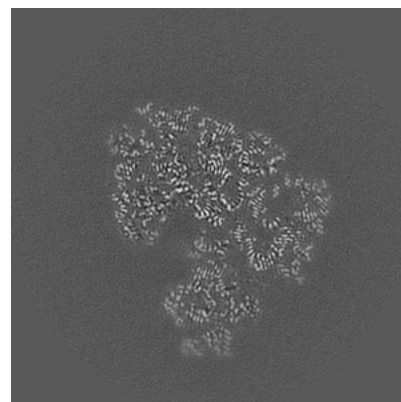
6.2.1 Primary map



X Index: 184



Y Index: 184

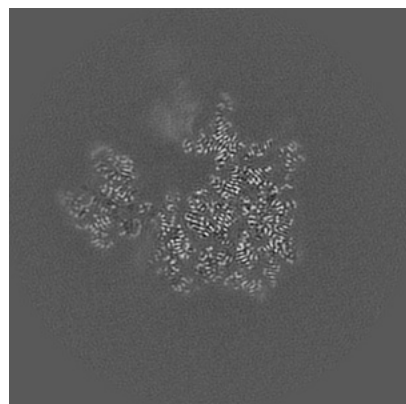


Z Index: 184

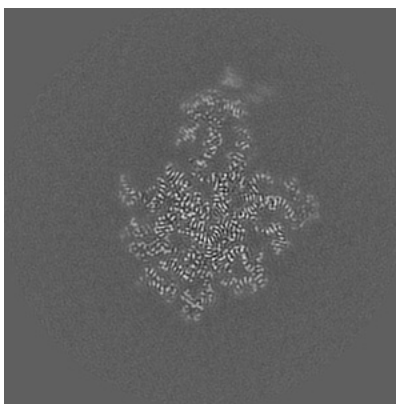
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

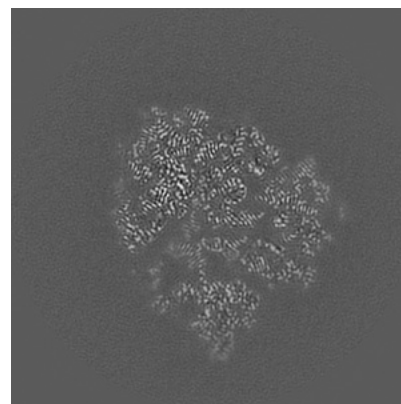
6.3.1 Primary map



X Index: 187



Y Index: 199

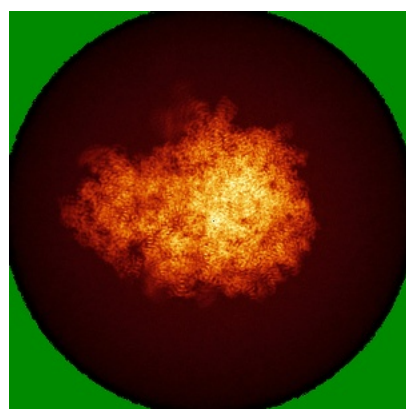


Z Index: 193

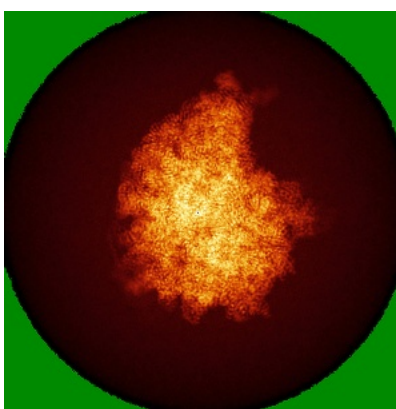
The images above show the largest variance slices of the map in three orthogonal directions.

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

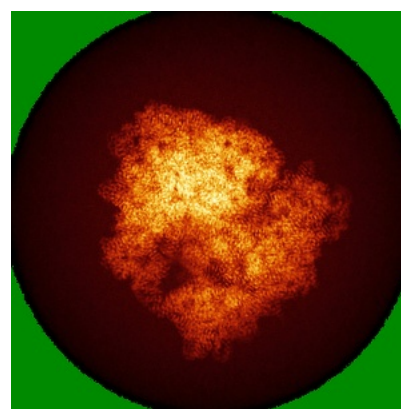
6.4.1 Primary map



X



Y



Z

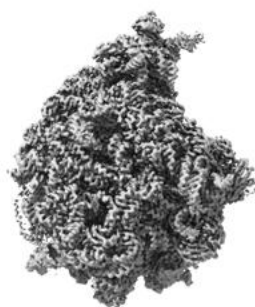
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

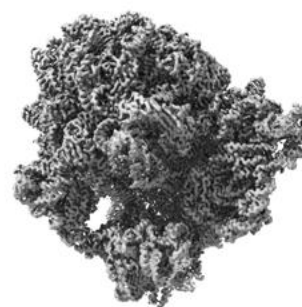
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

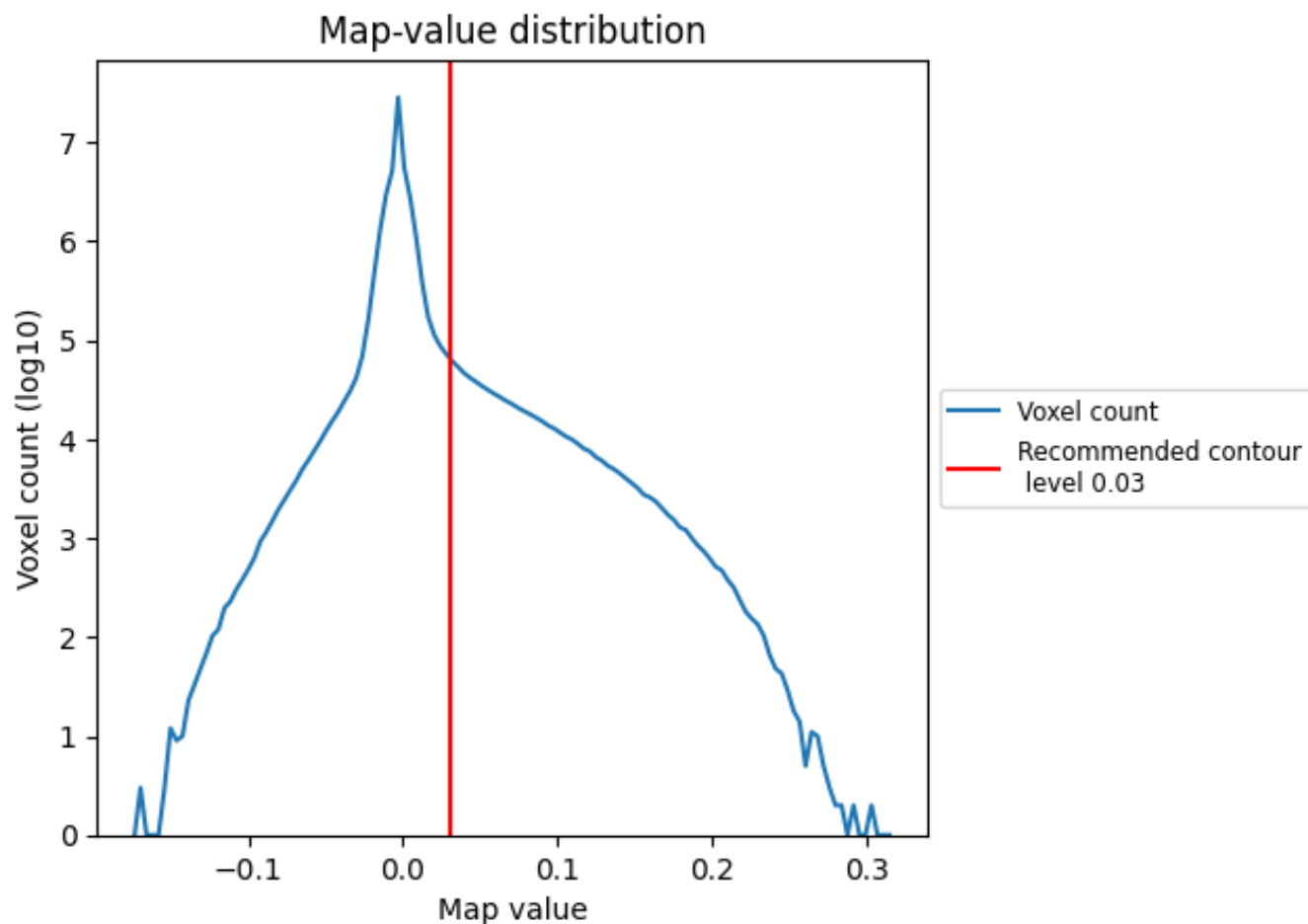
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

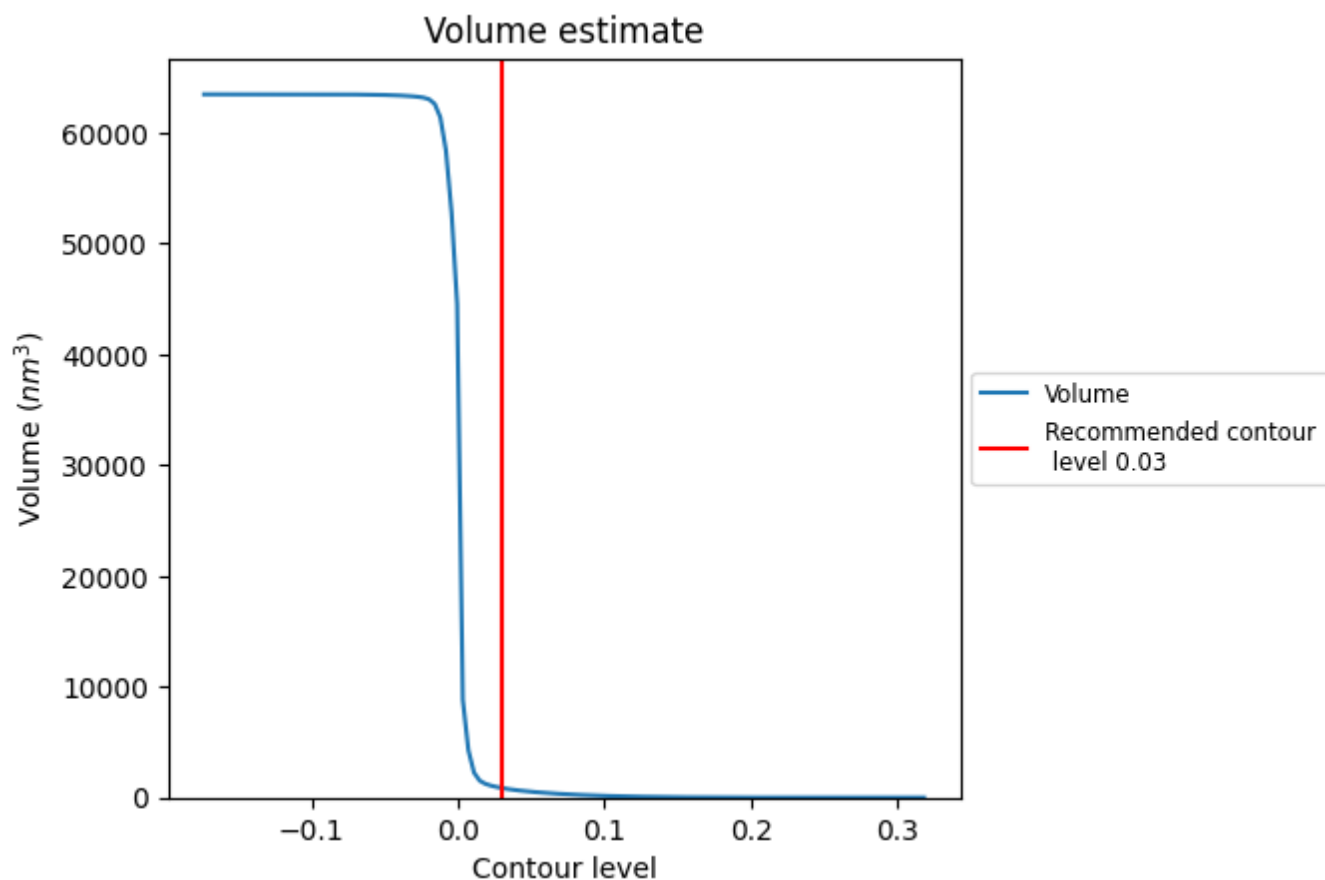
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

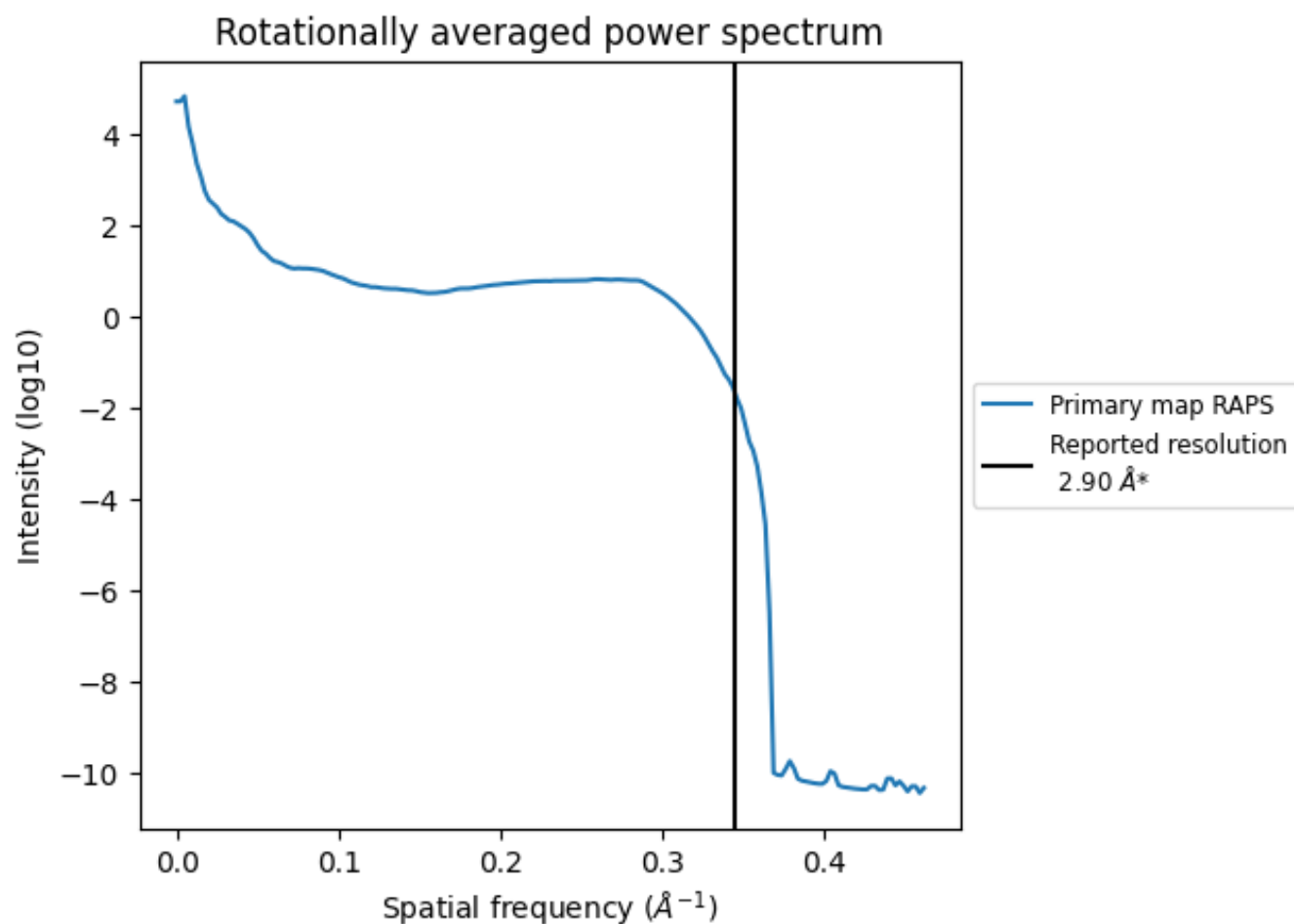
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 859 nm^3 ; this corresponds to an approximate mass of 776 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 ⓘ

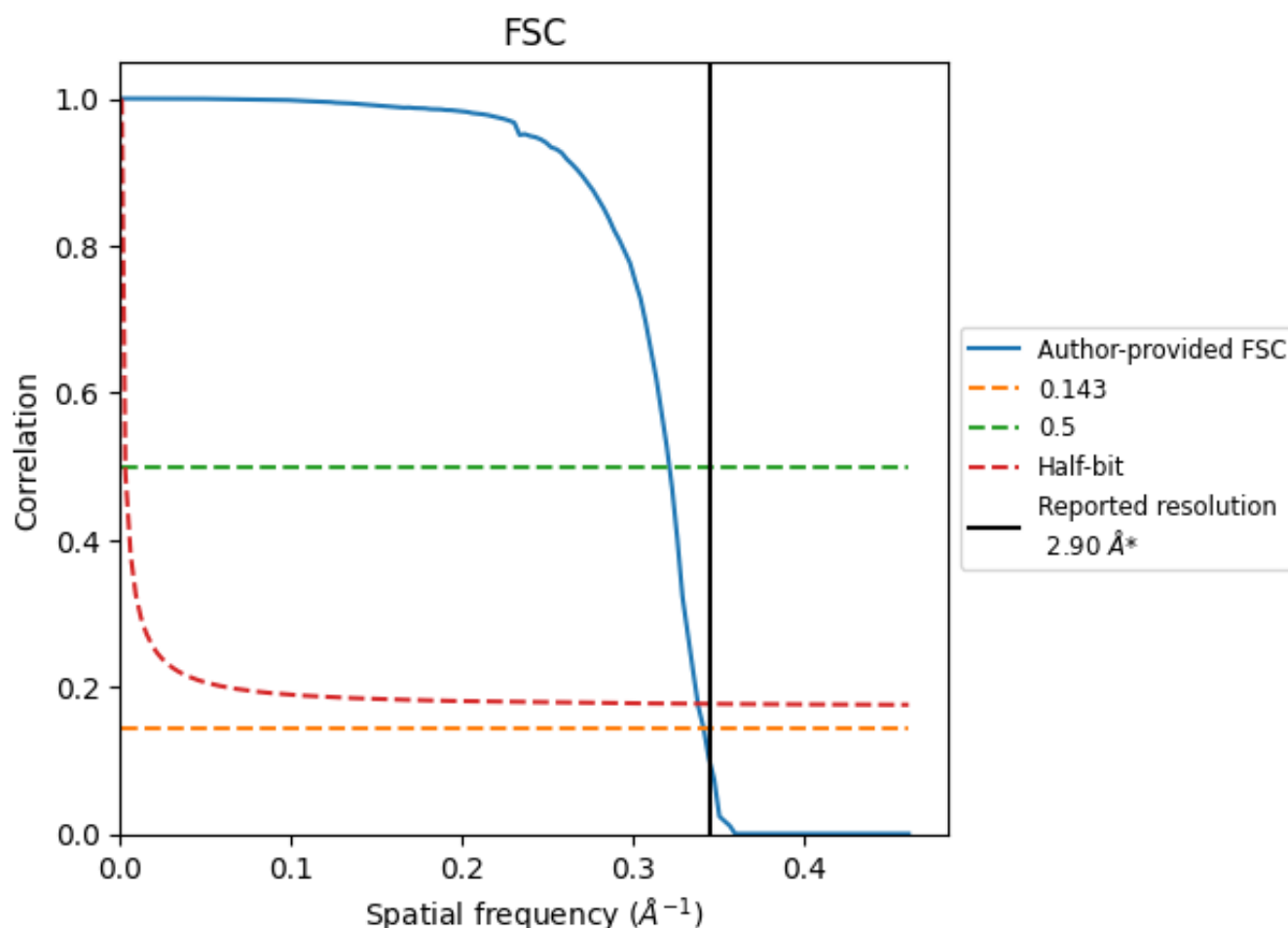


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

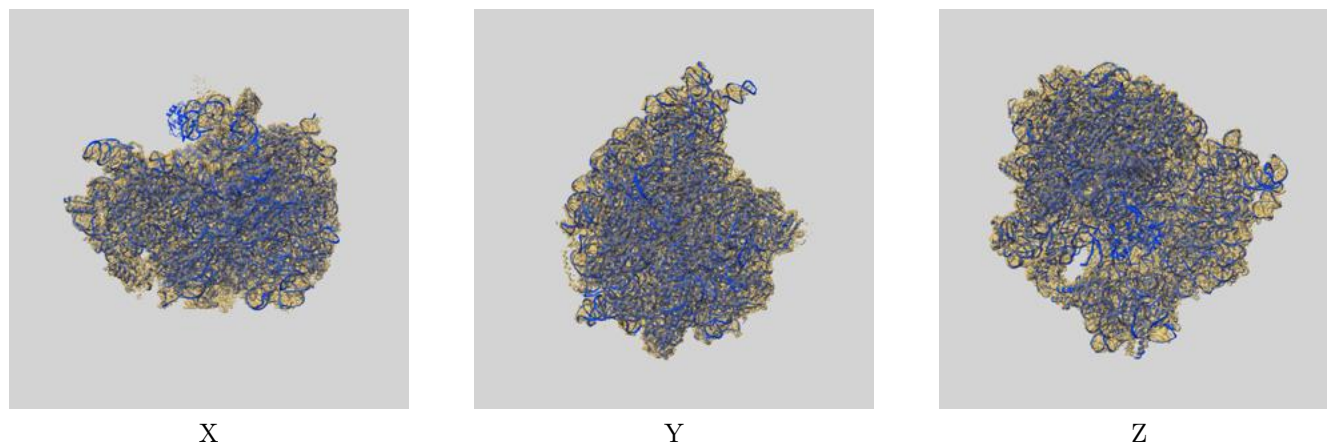
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.93	3.11	2.96
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

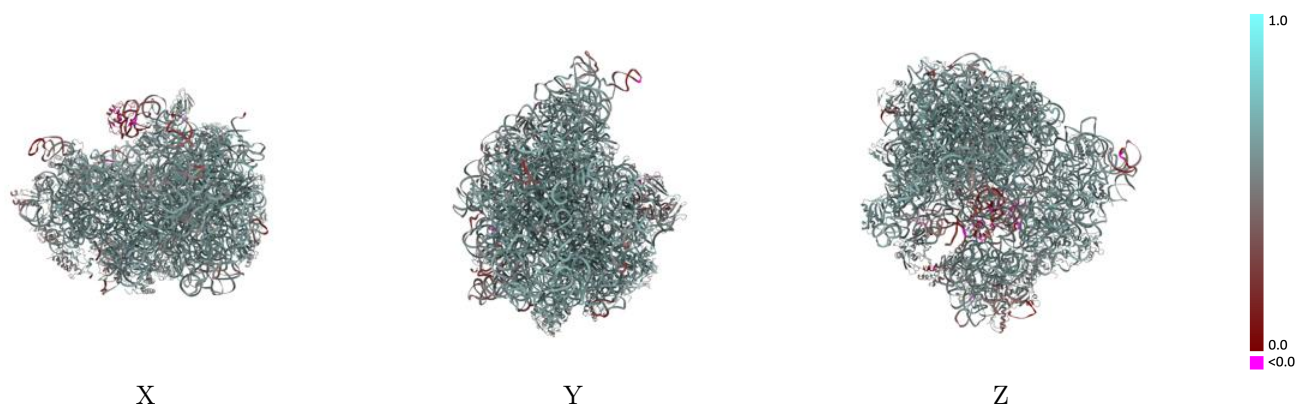
This section contains information regarding the fit between EMDB map EMD-3713 and PDB model 5NWY. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



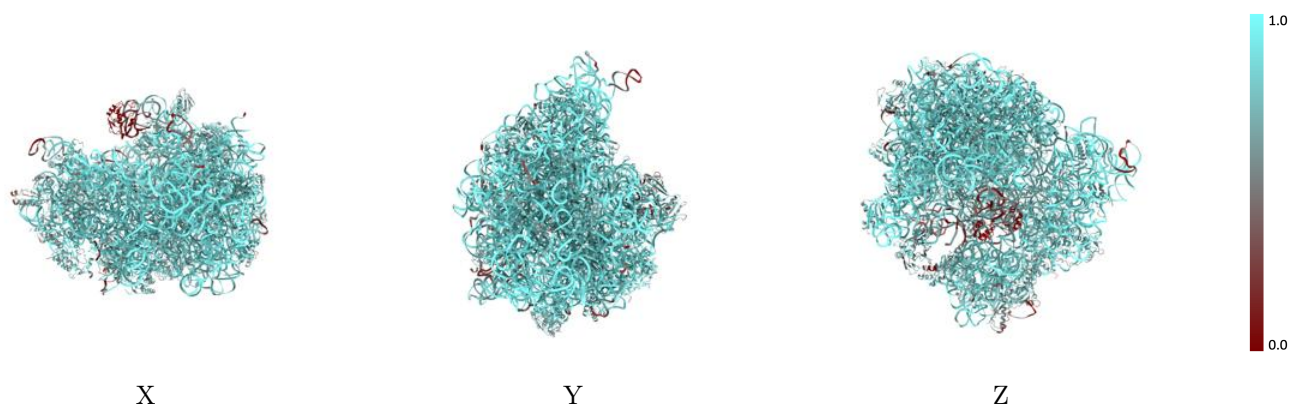
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



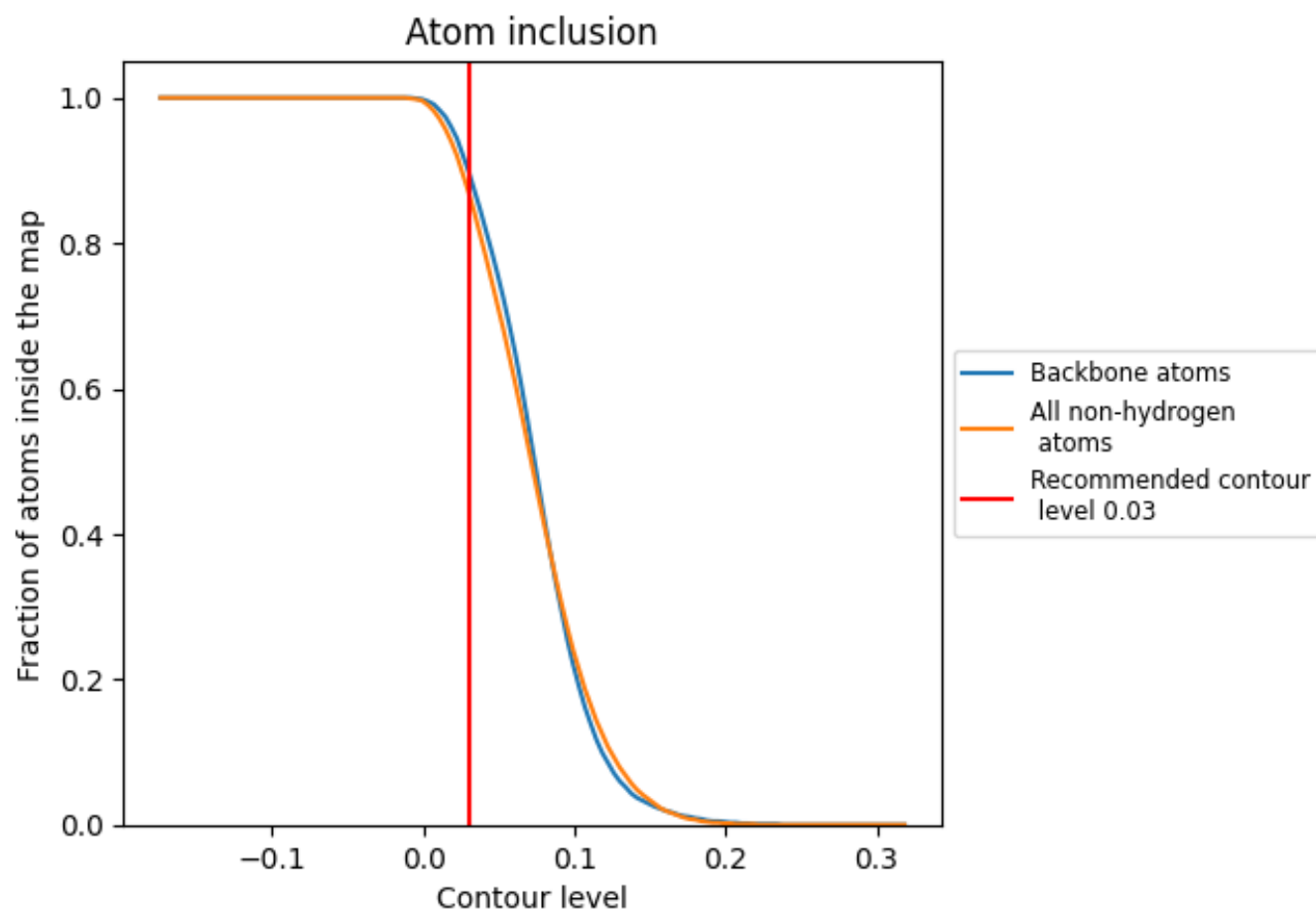
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8710	 0.5580
0	 0.9260	 0.5680
1	 0.6770	 0.4790
2	 0.7490	 0.5300
3	 0.7430	 0.5250
4	 0.8200	 0.5570
5	 0.7300	 0.4990
6	 0.6570	 0.4860
7	 0.8110	 0.5570
8	 0.7380	 0.4890
9	 0.6350	 0.4720
A	 0.7680	 0.5310
B	 0.8060	 0.5630
C	 0.7390	 0.4970
D	 0.7880	 0.5180
E	 0.8010	 0.5410
F	 0.7870	 0.5270
G	 0.7500	 0.5280
H	 0.8140	 0.5480
I	 0.7540	 0.5100
J	 0.7640	 0.5280
K	 0.4680	 0.3800
L	 0.5520	 0.4100
M	 0.8000	 0.5240
N	 0.9140	 0.5700
O	 0.9450	 0.5730
P	 0.8810	 0.5940
Q	 0.8750	 0.5870
R	 0.7840	 0.5620
S	 0.7230	 0.5120
T	 0.7240	 0.5210
U	 0.6660	 0.4780
V	 0.0110	 0.1470
W	 0.8600	 0.5820
X	 0.8470	 0.5720



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Chain	Atom inclusion	Q-score
Y	 0.8440	 0.5730
Z	 0.8430	 0.5760
a	 0.8770	 0.5890
b	 0.8230	 0.5640
c	 0.8320	 0.5770
d	 0.8830	 0.6000
e	 0.8250	 0.5570
f	 0.8330	 0.5790
g	 0.7840	 0.5470
h	 0.7500	 0.5340
i	 0.7960	 0.5550
j	 0.8840	 0.5970
k	 0.8580	 0.5790
l	 0.7320	 0.5080
m	 0.8100	 0.5710
n	 0.8480	 0.5720
o	 0.7710	 0.5490
p	 0.8840	 0.6010
q	 0.9080	 0.6130
r	 0.8660	 0.5800
s	 0.6490	 0.5340
t	 0.8940	 0.5800