



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 04:00 pm GMT

PDB ID : 8QCQ  
EMDB ID : EMD-18332  
Title : B. subtilis ApdA-stalled ribosomal complex  
Authors : Morici, M.; Wilson, D.N.  
Deposited on : 2023-08-28  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

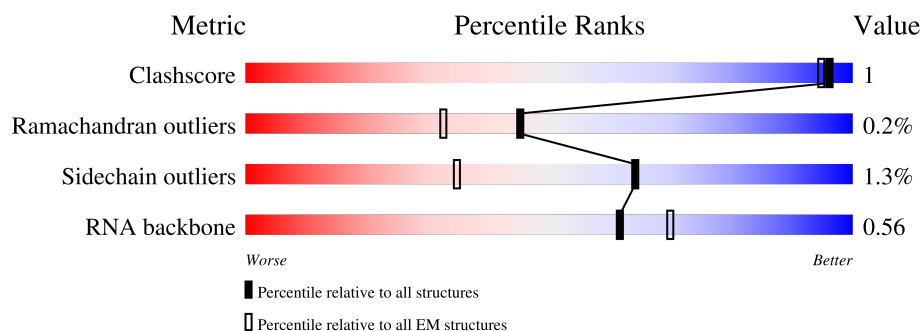
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.30 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.




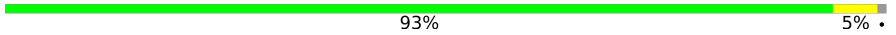
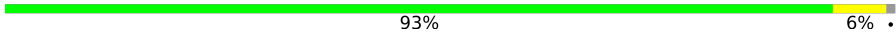
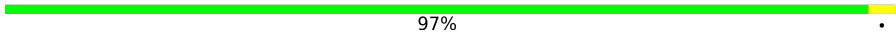
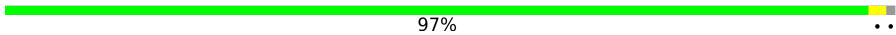
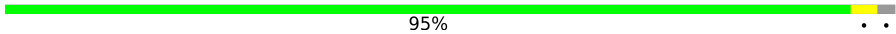
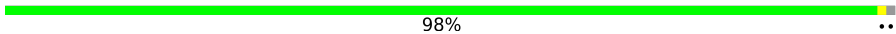
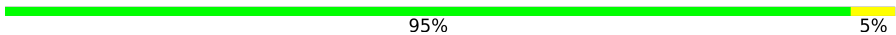
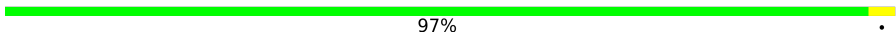

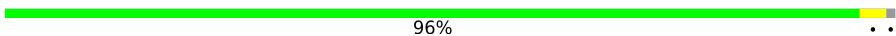
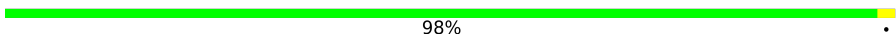


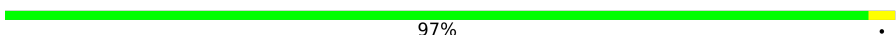
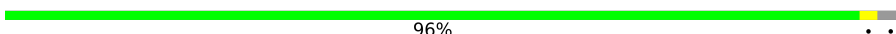
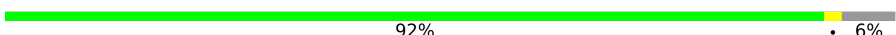
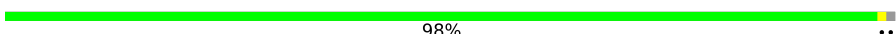


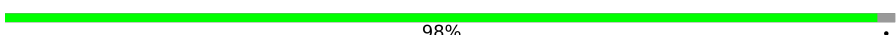
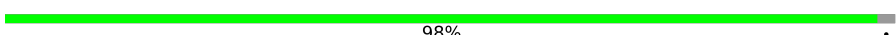



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	0	59	88% 5% 7%
2	1	49	98% .
3	2	44	95% 5%
4	3	66	92% 5% . .
5	4	37	100%
6	6	65	63% 6% . 29%
7	A	2925	72% 18% . 6%

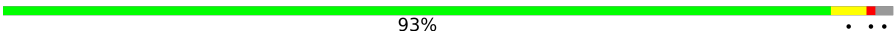
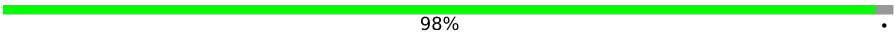

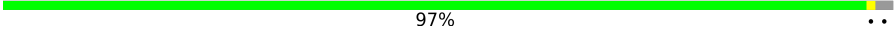



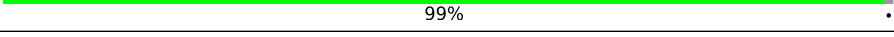
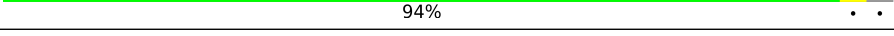
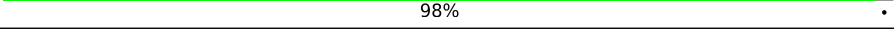
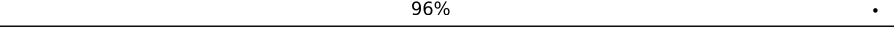
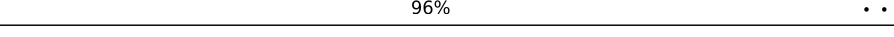
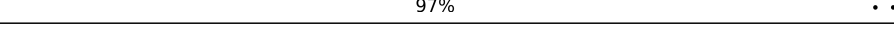
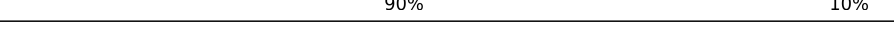


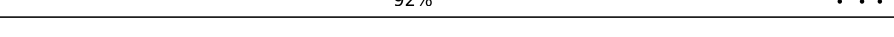
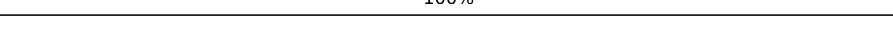
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Mol	Chain	Length	Quality of chain
8	B	119	 75%13%6%6%
9	C	277	 93%5%..
10	D	209	 93%6%..
11	E	207	 97%.
12	F	179	 97%..
13	G	179	 95%..
14	J	145	 98%..
15	K	122	 95%5%
16	L	146	 97%.
17	M	144	 90%..6%
18	N	120	 96%..
19	O	120	 98%.
20	P	115	 94%6%
21	Q	119	 94%5%.
22	R	102	 97%.
23	S	113	 96%..
24	T	95	 92%..6%
25	U	103	 98%..
26	W	94	 90%10%
27	X	62	 89%10%.
28	Y	66	 98%.
29	Z	59	 98%.
30	a	1554	 76%21%..
31	e	166	 90%5%5%
32	k	131	 85%..12%

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Mol	Chain	Length	Quality of chain
33	l	138	 93%
34	o	89	 98%
35	q	87	 92%6%
36	t	88	 97%
37	w	77	 81%18%
37	y	77	 83%17%
38	8	6	 83%17%
39	c	206	 99%
40	g	156	 94%
41	i	130	 98%
42	j	102	 96%
43	m	121	 96%
44	n	61	 97%
45	s	92	 90%10%
46	h	132	 80%11%8%
47	r	79	 81%18%
48	f	95	 92%
49	7	9	 100%

## 2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 136664 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 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	55	Total	C	N	O	S	0	0
			433	267	87	72	7		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	65	Total	C	N	O	S	0	0
			522	327	109	84	2		

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

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

- Molecule 6 is a protein called Large ribosomal subunit protein bL31-A.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	?	-	GLN	deletion	UNP Q03223

- Molecule 7 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	2745	Total	C	N	O	P	0	0
			58964	26308	10911	19002	2743		

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

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

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	273	Total	C	N	O	S	0	0
			2094	1302	412	374	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	115	Total	C	N	O	S	0	0
			945	600	185	159	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	102	Total	C	N	O	S	0	0
			795	506	140	148	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	89	Total	C	N	O	S	0	0
			716	447	133	133	3		

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

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

- Molecule 26 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	W	85	Total	C	N	O	0	0
			650	401	127	122		

- Molecule 27 is a protein called 50S ribosomal protein L28.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	61	Total	C	N	O	S	0	0
			468	289	98	79	2		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	65	Total	C	N	O	S	0	0
			532	329	103	99	1		

- Molecule 29 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 30 is a RNA chain called 16S rRNA.

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

- Molecule 31 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	158	Total	C	N	O	S	0	0
			1170	737	215	216	2		

- Molecule 32 is a protein called 30S ribosomal protein S11.

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

- Molecule 33 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	135	Total	C	N	O	S	0	0
			1047	650	210	185	2		

- Molecule 34 is a protein called 30S ribosomal protein S15.

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

- Molecule 35 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	q	85	Total	C	N	O	S	0	0
			699	441	129	127	2		

- Molecule 36 is a protein called 30S ribosomal protein S20.

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

- Molecule 37 is a RNA chain called Pro-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	y	77	Total	C	N	O	P	0	0
			1645	733	293	542	77		
37	w	77	Total	C	N	O	P	0	0
			1645	733	293	542	77		

- Molecule 38 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	8	6	Total	C	N	O	P	0	0
			120	54	16	44	6		

- Molecule 39 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	204	Total	C	N	O	S	0	0
			1607	1003	302	299	3		

- Molecule 40 is a protein called Small ribosomal subunit protein uS7.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	128	Total	C	N	O	S	0	0
			994	615	198	180	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	98	Total	C	N	O	S	0	0
			788	497	144	145	2		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	118	Total	C	N	O	S	0	0
			942	578	194	170			

- Molecule 44 is a protein called 30S ribosomal protein S14.

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

- Molecule 45 is a protein called 30S ribosomal protein S19.

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

- Molecule 46 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	h	122	Total	C	N	O	S	0	0
			958	601	181	174	2		

- Molecule 47 is a protein called 30S ribosomal protein S18.

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

- Molecule 48 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	f	92	Total	C	N	O	S	0	0
			755	476	132	146	1		

- Molecule 49 is a protein called ApdA nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	7	9	Total	C	N	O	0	0
			67	41	15	11		

- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
50	0	1	Total	Zn	0
			1	1	
50	1	1	Total	Zn	0
			1	1	
50	4	1	Total	Zn	0
			1	1	
50	6	1	Total	Zn	0
			1	1	
50	n	1	Total	Zn	0
			1	1	

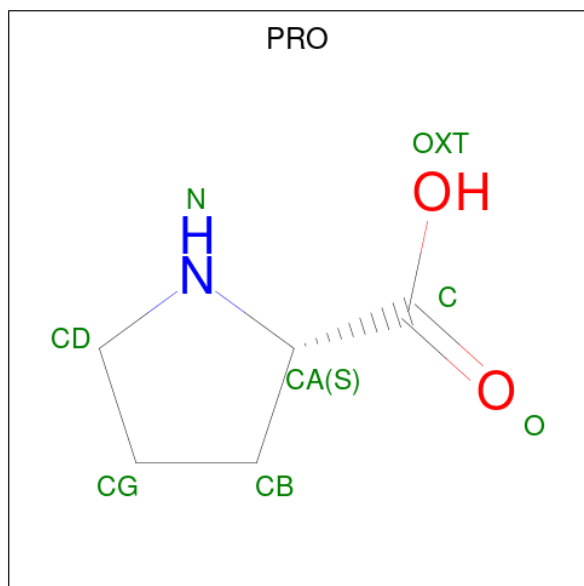
- Molecule 51 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	A	155	Total	Mg	0
			155	155	
51	B	1	Total	Mg	0
			1	1	
51	C	1	Total	Mg	0
			1	1	
51	D	1	Total	Mg	0
			1	1	
51	a	40	Total	Mg	0
			40	40	
51	w	1	Total	Mg	0
			1	1	

- Molecule 52 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
52	A	40	Total	K	0
			40	40	
52	C	2	Total	K	0
			2	2	
52	U	1	Total	K	0
			1	1	

- Molecule 53 is PROLINE (three-letter code: PRO) (formula:  $C_5H_9NO_2$ ).



Mol	Chain	Residues	Atoms				AltConf
53	y	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 54 is water.

Mol	Chain	Residues	Atoms		AltConf
54	3	3	Total	O	0
			3	3	
54	A	811	Total	O	0
			811	811	
54	B	5	Total	O	0
			5	5	
54	C	15	Total	O	0
			15	15	
54	D	1	Total	O	0
			1	1	
54	E	5	Total	O	0
			5	5	

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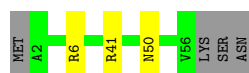
Mol	Chain	Residues	Atoms		AltConf
54	L	5	Total 5	O 5	0
54	N	3	Total 3	O 3	0
54	P	3	Total 3	O 3	0
54	Q	3	Total 3	O 3	0
54	T	1	Total 1	O 1	0
54	a	132	Total 132	O 132	0
54	k	1	Total 1	O 1	0
54	y	3	Total 3	O 3	0
54	w	21	Total 21	O 21	0
54	i	1	Total 1	O 1	0
54	j	1	Total 1	O 1	0
54	7	8	Total 8	O 8	0

### 3 Residue-property plots [i](#)

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

- Molecule 1: 50S ribosomal protein L32

Chain 0: 



- Molecule 2: 50S ribosomal protein L33 1

Chain 1: 



- Molecule 3: 50S ribosomal protein L34

Chain 2: 



- Molecule 4: 50S ribosomal protein L35

Chain 3: 



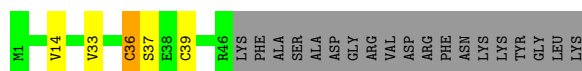
- Molecule 5: 50S ribosomal protein L36

Chain 4: 

There are no outlier residues recorded for this chain.

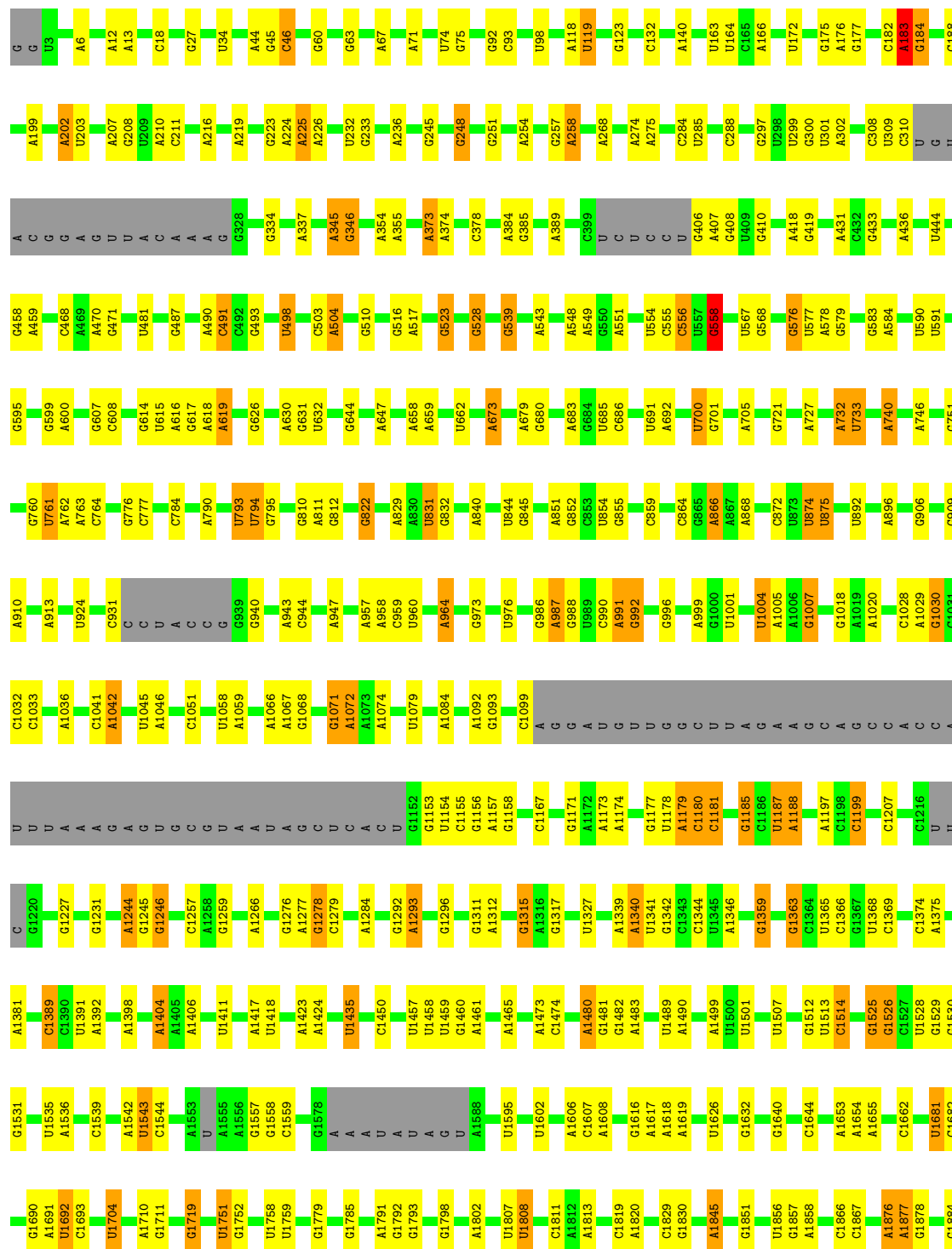
- Molecule 6: Large ribosomal subunit protein bL31-A

Chain 6: 

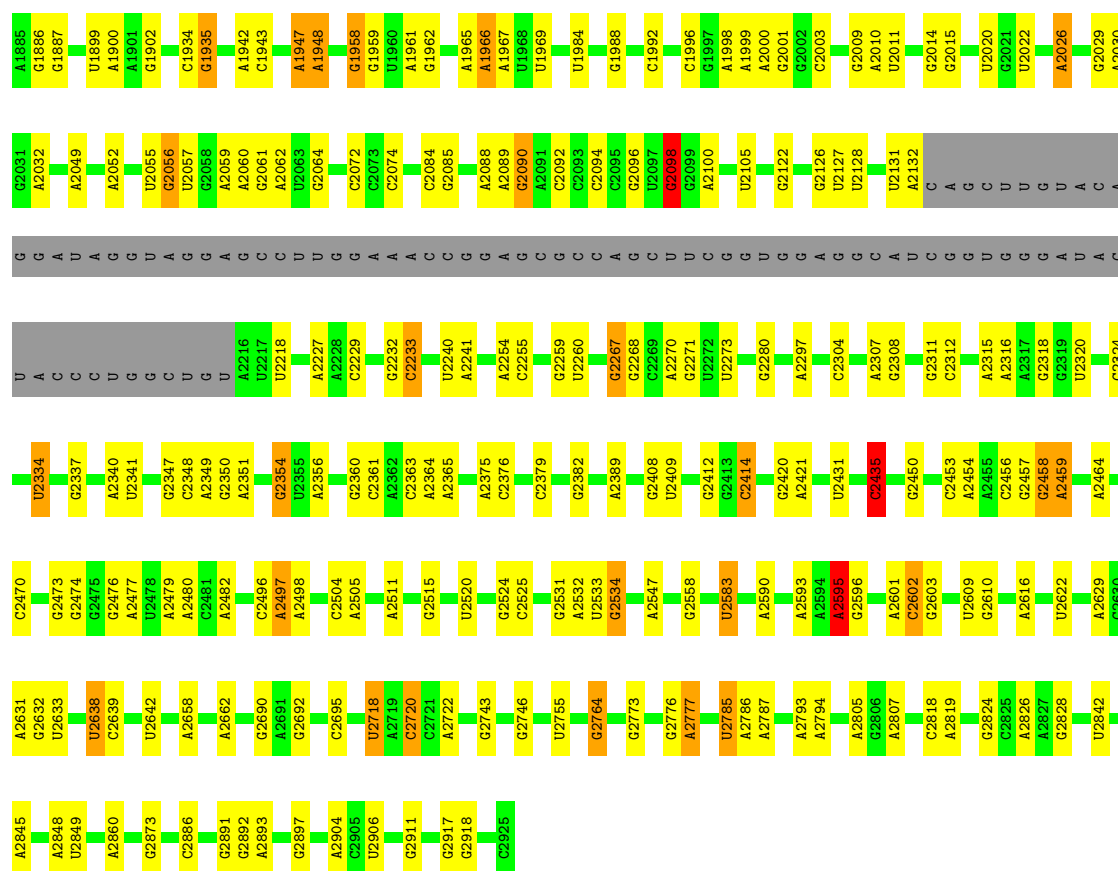


# Molecule 7: 23S rRNA

Chain A: 72% 18% 6%

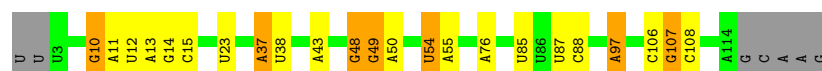






### • Molecule 8: 5S rRNA

Chain B: 75% 13% 6% 6%



### • Molecule 9: 50S ribosomal protein L2

Chain C: 93% 5%



### • Molecule 10: 50S ribosomal protein L3

Chain D: 93% 6%



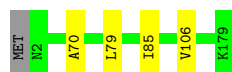
### • Molecule 11: 50S ribosomal protein L4

Chain E: 97%



- Molecule 12: 50S ribosomal protein L5

Chain F: 97% ..



- Molecule 13: Large ribosomal subunit protein uL6

Chain G: 95% ..



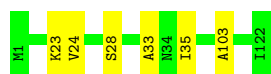
- Molecule 14: 50S ribosomal protein L13

Chain J: 98% ..



- Molecule 15: 50S ribosomal protein L14

Chain K: 95% 5%



- Molecule 16: 50S ribosomal protein L15

Chain L: 97% .



- Molecule 17: 50S ribosomal protein L16

Chain M: 90% . 6%



- Molecule 18: 50S ribosomal protein L17

Chain N: 96% ..



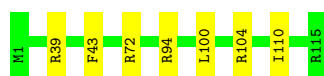
- Molecule 19: 50S ribosomal protein L18

Chain O: 98%



- Molecule 20: 50S ribosomal protein L19

Chain P: 94%



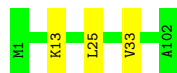
- Molecule 21: Large ribosomal subunit protein bL20

Chain Q: 94%



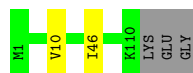
- Molecule 22: 50S ribosomal protein L21

Chain R: 97%



- Molecule 23: 50S ribosomal protein L22

Chain S: 96%



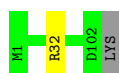
- Molecule 24: Large ribosomal subunit protein uL23

Chain T: 92%



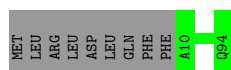
- Molecule 25: 50S ribosomal protein L24

Chain U: 98%



- Molecule 26: Large ribosomal subunit protein bL27

Chain W: 90% 10%



- Molecule 27: 50S ribosomal protein L28

Chain X: 89% 10%



- Molecule 28: 50S ribosomal protein L29

Chain Y: 98%



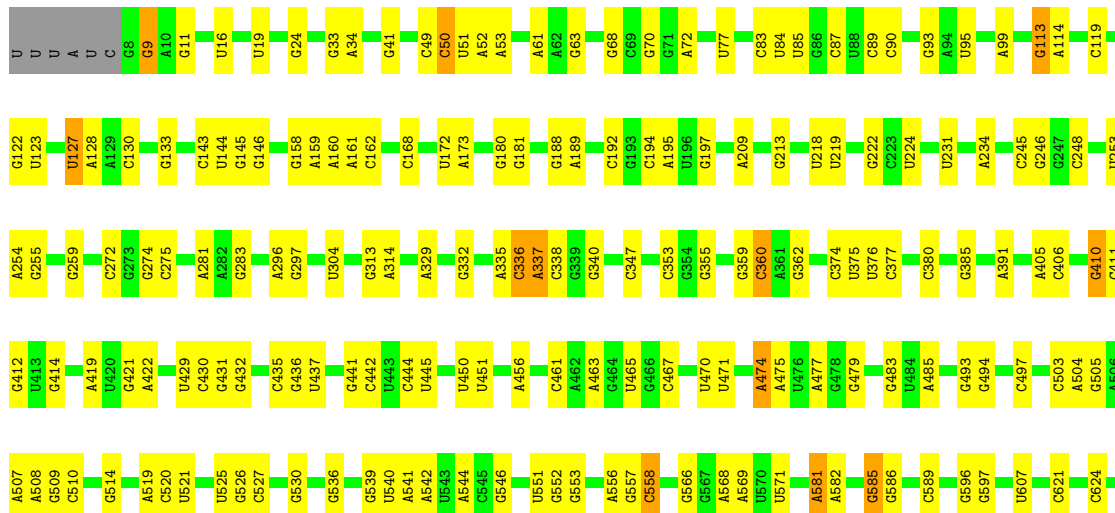
- Molecule 29: Large ribosomal subunit protein uL30

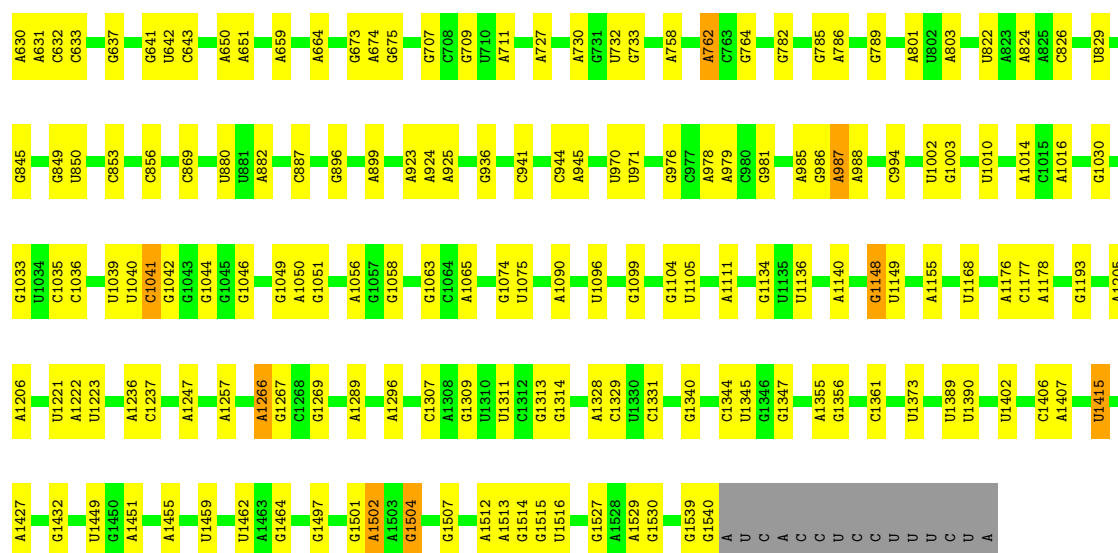
Chain Z: 98%



- Molecule 30: 16S rRNA

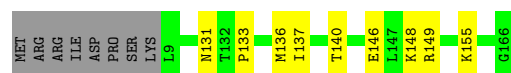
Chain a: 76% 21%





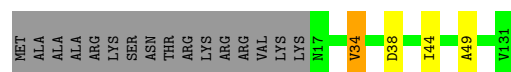
• Molecule 31: 30S ribosomal protein S5

Chain e: 90% 5% 5%



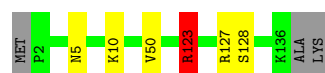
• Molecule 32: 30S ribosomal protein S11

Chain k: 85% 12%



• Molecule 33: 30S ribosomal protein S12

Chain l: 93%



• Molecule 34: 30S ribosomal protein S15

Chain o: 98%



• Molecule 35: 30S ribosomal protein S17

Chain q: 92% 6%



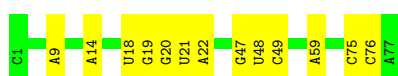
- Molecule 36: 30S ribosomal protein S20

Chain t: 97%



- Molecule 37: Pro-tRNA

Chain y: 83%



- Molecule 37: Pro-tRNA

Chain w: 81%



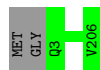
- Molecule 38: mRNA

Chain 8: 83%



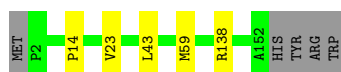
- Molecule 39: Small ribosomal subunit protein uS3

Chain c: 99%



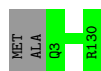
- Molecule 40: Small ribosomal subunit protein uS7

Chain g: 94%



- Molecule 41: 30S ribosomal protein S9

Chain i: 98%



- Molecule 42: 30S ribosomal protein S10



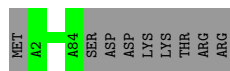
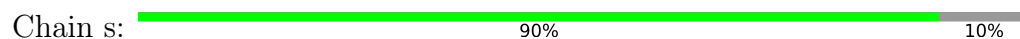
- Molecule 43: 30S ribosomal protein S13



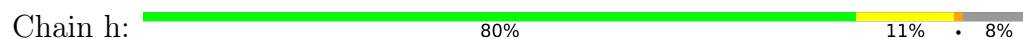
- Molecule 44: 30S ribosomal protein S14



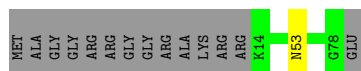
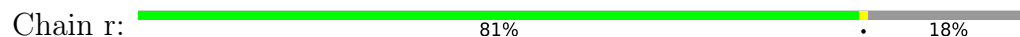
- Molecule 45: 30S ribosomal protein S19



- Molecule 46: 30S ribosomal protein S8



- Molecule 47: 30S ribosomal protein S18



- Molecule 48: 30S ribosomal protein S6





- Molecule 49: ApdA nascent chain

Chain 7:  100%

There are no outlier residues recorded for this chain.



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	142978	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	75.6	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, PSU, OMG, 2MA, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	0	0.42	0/440	0.84	0/584
2	1	0.30	0/408	0.65	0/541
3	2	0.44	0/371	0.79	0/483
4	3	0.47	0/529	0.74	0/691
5	4	0.38	0/300	0.75	0/393
6	6	0.33	0/363	0.67	0/485
7	A	0.60	1/65970 (0.0%)	1.29	312/102904 (0.3%)
8	B	0.50	0/2675	1.21	10/4170 (0.2%)
9	C	0.39	0/2131	0.73	0/2859
10	D	0.39	0/1597	0.72	0/2140
11	E	0.38	0/1586	0.66	0/2139
12	F	0.28	0/1424	0.62	0/1910
13	G	0.30	0/1360	0.65	0/1832
14	J	0.36	0/1165	0.67	0/1566
15	K	0.36	0/928	0.73	0/1245
16	L	0.37	0/1094	0.69	0/1457
17	M	0.38	0/1099	0.72	0/1468
18	N	0.35	0/961	0.67	0/1284
19	O	0.30	0/922	0.62	0/1236
20	P	0.33	0/958	0.75	0/1279
21	Q	0.41	0/962	0.73	0/1277
22	R	0.34	0/806	0.68	0/1080
23	S	0.39	0/859	0.73	0/1156
24	T	0.32	0/722	0.68	0/962
25	U	0.32	0/780	0.65	0/1043
26	W	0.40	0/658	0.71	0/873
27	X	0.42	0/472	0.68	0/627
28	Y	0.27	0/533	0.55	0/708
29	Z	0.32	0/458	0.65	0/613
30	a	0.55	0/36826	1.17	64/57450 (0.1%)
31	e	0.35	0/1181	0.74	0/1588
32	k	0.36	0/861	0.72	0/1164

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	l	0.31	0/1064	0.75	1/1428 (0.1%)
34	o	0.29	0/738	0.62	0/985
35	q	0.28	0/707	0.69	0/944
36	t	0.27	0/661	0.62	0/882
37	w	0.59	0/1838	1.14	3/2864 (0.1%)
37	y	0.57	0/1838	1.13	1/2864 (0.0%)
38	8	0.73	0/131	1.05	0/200
39	c	0.29	0/1629	0.61	0/2192
40	g	0.35	0/1215	0.62	0/1629
41	i	0.32	0/1007	0.66	0/1351
42	j	0.29	0/800	0.65	0/1077
43	m	0.31	0/948	0.67	0/1267
44	n	0.30	0/508	0.72	2/672 (0.3%)
45	s	0.32	0/685	0.61	0/920
46	h	0.33	0/966	0.80	2/1292 (0.2%)
47	r	0.28	0/530	0.66	0/710
48	f	0.27	0/766	0.65	0/1031
49	7	0.42	0/67	0.85	0/89
All	All	0.53	1/147497 (0.0%)	1.14	395/221604 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	2
3	2	0	1
4	3	0	1
7	A	0	5
9	C	0	10
10	D	0	3
11	E	0	2
16	L	0	1
19	O	0	1
20	P	0	2
21	Q	0	1
25	U	0	1
27	X	0	2
33	l	0	1
35	q	0	1
40	g	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
46	h	0	2
48	f	0	2
All	All	0	40

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2090	G	C8-N7	6.26	1.34	1.30

All (395) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	619	A	O5'-P-OP1	-26.46	78.95	110.70
7	A	2090	G	O5'-P-OP2	-21.68	84.68	110.70
7	A	1199	C	O5'-P-OP2	-19.86	86.87	110.70
7	A	1681	U	O5'-P-OP2	-19.42	87.40	110.70
7	A	1315	G	O5'-P-OP2	-15.09	92.12	105.70
7	A	733	U	O5'-P-OP1	14.57	128.19	110.70
7	A	866	A	O5'-P-OP1	-14.27	92.86	105.70
7	A	1185	G	O5'-P-OP2	-14.02	93.08	105.70
7	A	1007	G	O5'-P-OP2	-13.93	93.17	105.70
7	A	46	C	O5'-P-OP2	-13.18	93.83	105.70
7	A	732	A	O3'-P-O5'	-13.01	79.28	104.00
30	a	1432	G	O5'-P-OP2	-12.92	94.07	105.70
7	A	1042	A	O5'-P-OP1	-12.78	94.19	105.70
7	A	1199	C	O5'-P-OP1	12.73	125.97	110.70
7	A	991	A	O5'-P-OP1	-12.35	94.59	105.70
7	A	2583	U	O5'-P-OP1	-12.29	94.64	105.70
7	A	225	A	O3'-P-O5'	-11.91	81.38	104.00
7	A	258	A	O5'-P-OP1	-11.84	95.04	105.70
7	A	1375	A	O3'-P-O5'	-11.58	82.00	104.00
7	A	992	G	O5'-P-OP1	-11.28	95.55	105.70
7	A	491	C	O5'-P-OP1	11.15	124.08	110.70
7	A	1819	C	O5'-P-OP2	-11.08	95.73	105.70
7	A	1278	G	O5'-P-OP2	-10.70	96.07	105.70
7	A	346	G	O5'-P-OP1	-10.67	96.09	105.70
7	A	2090	G	O5'-P-OP1	10.56	123.37	110.70
7	A	490	A	O3'-P-O5'	-10.34	84.35	104.00
30	a	1507	G	O5'-P-OP2	-10.29	96.44	105.70
7	A	864	C	O5'-P-OP2	-10.26	96.47	105.70
7	A	2233	C	O5'-P-OP1	-10.11	96.60	105.70
7	A	1278	G	O5'-P-OP1	9.74	122.39	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	987	A	O5'-P-OP1	-9.73	96.94	105.70
7	A	1867	C	O5'-P-OP1	-9.67	97.00	105.70
7	A	558	G	O4'-C1'-N9	9.61	115.88	108.20
7	A	556	C	O5'-P-OP2	-9.60	97.06	105.70
7	A	183	A	C1'-O4'-C4'	-9.43	102.35	109.90
7	A	794	U	O5'-P-OP1	-9.28	97.35	105.70
7	A	2616	A	O5'-P-OP2	-8.92	97.67	105.70
30	a	1313	G	O3'-P-O5'	-8.91	87.06	104.00
7	A	2382	G	O3'-P-O5'	-8.77	87.34	104.00
7	A	1277	A	O3'-P-O5'	-8.59	87.67	104.00
7	A	874	U	O5'-P-OP1	8.52	120.92	110.70
7	A	2026	A	O5'-P-OP1	8.29	120.65	110.70
7	A	1340	A	O3'-P-O5'	-8.22	88.38	104.00
7	A	2308	G	O3'-P-O5'	-8.15	88.50	104.00
7	A	2764	G	O3'-P-O5'	-8.11	88.60	104.00
7	A	2873	G	O4'-C1'-N9	7.98	114.58	108.20
7	A	2375	A	O5'-P-OP1	-7.95	98.55	105.70
7	A	2525	C	O5'-P-OP2	-7.94	98.56	105.70
30	a	899	A	O3'-P-O5'	-7.92	88.96	104.00
7	A	2603	G	O5'-P-OP2	-7.83	98.66	105.70
7	A	2260	U	O5'-P-OP2	-7.70	98.78	105.70
7	A	2534	G	O5'-P-OP2	-7.66	98.81	105.70
7	A	2026	A	O5'-P-OP2	-7.66	98.81	105.70
7	A	2435	C	O5'-P-OP1	-7.62	98.84	105.70
7	A	1389	C	O5'-P-OP2	-7.58	98.88	105.70
7	A	2324	C	O5'-P-OP2	-7.56	98.89	105.70
7	A	2482	A	O4'-C1'-N9	7.54	114.23	108.20
30	a	585	G	O5'-P-OP1	7.52	119.72	110.70
7	A	1606	A	O3'-P-O5'	-7.51	89.73	104.00
7	A	2015	G	O5'-P-OP2	-7.47	98.97	105.70
7	A	1244	A	O4'-C1'-N9	7.43	114.14	108.20
7	A	1845	A	O5'-P-OP1	-7.39	99.05	105.70
7	A	986	G	O3'-P-O5'	7.36	117.98	104.00
7	A	795	G	C1'-O4'-C4'	-7.33	104.03	109.90
7	A	1988	G	O5'-P-OP2	-7.33	99.10	105.70
7	A	274	A	O3'-P-O5'	-7.33	90.08	104.00
7	A	1398	A	O3'-P-O5'	-7.30	90.12	104.00
7	A	1340	A	O5'-P-OP1	-7.29	99.14	105.70
7	A	844	U	O5'-P-OP2	-7.26	99.17	105.70
7	A	2420	G	O4'-C1'-N9	7.25	114.00	108.20
7	A	988	G	O5'-P-OP2	-7.25	99.18	105.70
7	A	1032	C	O5'-P-OP2	-7.22	99.20	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	1501	G	O3'-P-O5'	-7.21	90.31	104.00
7	A	1363	G	O4'-C1'-N9	7.20	113.96	108.20
7	A	1751	U	P-O3'-C3'	7.15	128.28	119.70
8	B	54	U	O3'-P-O5'	-7.15	90.42	104.00
7	A	1998	A	O3'-P-O5'	-7.14	90.42	104.00
7	A	1317	G	O5'-P-OP2	-7.13	99.28	105.70
7	A	207	A	O3'-P-O5'	-7.12	90.48	104.00
30	a	1504	G	O5'-P-OP2	-7.12	99.30	105.70
7	A	1798	G	O5'-P-OP2	-7.10	99.31	105.70
7	A	373	A	O3'-P-O5'	-7.10	90.51	104.00
8	B	48	G	C2'-C3'-O3'	7.05	125.01	109.50
7	A	2340	A	O3'-P-O5'	-6.99	90.72	104.00
7	A	964	A	O5'-P-OP1	-6.98	99.42	105.70
7	A	1018	G	O5'-P-OP2	-6.95	99.44	105.70
8	B	13	A	O4'-C1'-N9	6.93	113.74	108.20
7	A	874	U	OP1-P-OP2	-6.91	109.23	119.60
7	A	1374	C	O3'-P-O5'	-6.88	90.92	104.00
7	A	2090	G	C5-N7-C8	-6.87	100.87	104.30
7	A	2090	G	C8-N9-C4	-6.85	103.66	106.40
7	A	2307	A	O3'-P-O5'	-6.84	91.00	104.00
7	A	2361	C	O3'-P-O5'	-6.82	91.05	104.00
7	A	2032	A	O3'-P-O5'	-6.80	91.07	104.00
7	A	119	U	O3'-P-O5'	-6.78	91.12	104.00
30	a	245	C	O3'-P-O5'	-6.77	91.14	104.00
7	A	373	A	O5'-P-OP2	-6.76	99.62	105.70
7	A	202	A	C1'-O4'-C4'	-6.73	104.52	109.90
7	A	608	C	O5'-P-OP2	-6.68	99.69	105.70
30	a	566	G	O3'-P-O5'	-6.65	91.36	104.00
30	a	1148	G	P-O3'-C3'	6.65	127.68	119.70
30	a	923	A	O3'-P-O5'	-6.64	91.38	104.00
30	a	1361	C	O3'-P-O5'	-6.64	91.39	104.00
7	A	2633	U	O5'-P-OP2	-6.62	99.74	105.70
30	a	782	G	O5'-P-OP2	-6.62	99.74	105.70
7	A	2347	G	O3'-P-O5'	-6.62	91.42	104.00
7	A	1857	G	C5-C6-O6	-6.62	124.63	128.60
7	A	618	A	OP1-P-O3'	6.59	119.71	105.20
7	A	567	U	O4'-C1'-N1	6.59	113.47	108.20
7	A	1884	G	O3'-P-O5'	-6.58	91.49	104.00
7	A	1245	G	C5-N7-C8	-6.55	101.03	104.30
46	h	66	TYR	CB-CG-CD2	6.54	124.92	121.00
7	A	182	C	C4'-C3'-O3'	6.53	126.07	113.00
7	A	1934	C	O3'-P-O5'	-6.52	91.61	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1655	A	O5'-P-OP2	-6.49	99.86	105.70
7	A	1417	A	O3'-P-O5'	-6.44	91.76	104.00
7	A	644	G	O5'-P-OP2	-6.43	99.91	105.70
30	a	558	C	O4'-C1'-N1	6.36	113.29	108.20
30	a	246	G	O3'-P-O5'	-6.34	91.95	104.00
7	A	2480	A	O5'-P-OP2	-6.29	100.03	105.70
30	a	801	A	O4'-C1'-N9	6.29	113.23	108.20
7	A	958	A	O3'-P-O5'	-6.28	92.07	104.00
7	A	2026	A	C5'-C4'-O4'	6.27	116.63	109.10
7	A	2818	C	O4'-C1'-N1	6.27	113.22	108.20
7	A	1886	G	O3'-P-O5'	-6.27	92.09	104.00
7	A	746	A	O3'-P-O5'	-6.23	92.16	104.00
7	A	2105	U	O4'-C1'-N1	6.22	113.17	108.20
30	a	581	A	O3'-P-O5'	-6.21	92.20	104.00
30	a	589	C	O3'-P-O5'	-6.21	92.21	104.00
7	A	1966	A	O3'-P-O5'	-6.19	92.24	104.00
30	a	1504	G	O3'-P-O5'	-6.17	92.27	104.00
30	a	336	C	C1'-O4'-C4'	-6.17	104.96	109.90
7	A	1525	G	C2'-C3'-O3'	6.15	123.54	113.70
30	a	1502	A	O5'-P-OP1	6.15	118.08	110.70
7	A	794	U	O5'-P-OP2	6.14	118.06	110.70
7	A	1244	A	C5-N7-C8	-6.12	100.84	103.90
7	A	2088	A	O5'-P-OP2	-6.12	100.20	105.70
7	A	2029	G	O5'-P-OP2	-6.11	100.20	105.70
8	B	37	A	P-O3'-C3'	6.11	127.03	119.70
7	A	470	A	O3'-P-O5'	-6.11	92.39	104.00
7	A	1616	G	O5'-P-OP2	-6.11	100.20	105.70
7	A	784	C	O5'-P-OP1	6.11	118.03	110.70
30	a	1266	A	P-O3'-C3'	6.09	127.01	119.70
7	A	1179	A	C1'-O4'-C4'	-6.06	105.05	109.90
7	A	1276	G	O4'-C1'-N9	6.05	113.04	108.20
7	A	851	A	O5'-P-OP2	-6.05	100.26	105.70
7	A	2474	G	C2-N3-C4	6.04	114.92	111.90
7	A	1359	G	C5-C6-O6	-6.03	124.98	128.60
7	A	1543	U	P-O3'-C3'	6.02	126.93	119.70
30	a	607	U	O3'-P-O5'	-6.02	92.56	104.00
7	A	1692	U	O5'-P-OP1	-6.01	100.29	105.70
7	A	517	A	O5'-P-OP1	6.01	117.91	110.70
7	A	183	A	N9-C1'-C2'	6.00	121.81	114.00
8	B	10	G	O3'-P-O5'	-5.99	92.62	104.00
7	A	2456	C	O3'-P-O5'	-5.97	92.65	104.00
7	A	182	C	C3'-C2'-C1'	-5.95	96.74	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2511	A	O5'-P-OP1	5.95	117.84	110.70
7	A	1071	G	N3-C2-N2	-5.95	115.74	119.90
7	A	1246	G	O4'-C1'-N9	5.94	112.95	108.20
7	A	1435	U	O4'-C1'-N1	5.94	112.95	108.20
30	a	1340	G	O4'-C1'-N9	5.92	112.94	108.20
30	a	557	G	O3'-P-O5'	-5.91	92.77	104.00
7	A	2496	C	O5'-P-OP2	-5.90	100.39	105.70
7	A	2658	A	O5'-P-OP1	-5.90	100.39	105.70
7	A	498	U	C1'-O4'-C4'	-5.90	105.18	109.90
7	A	2891	G	O3'-P-O5'	-5.88	92.84	104.00
7	A	1045	U	O5'-P-OP2	5.86	117.74	110.70
7	A	1381	A	O5'-P-OP2	-5.85	100.43	105.70
7	A	793	U	OP1-P-O3'	5.85	118.06	105.20
7	A	2842	U	O3'-P-O5'	-5.84	92.91	104.00
7	A	1244	A	O5'-P-OP2	-5.83	100.45	105.70
7	A	2911	G	C5-N7-C8	-5.83	101.38	104.30
7	A	673	A	O3'-P-O5'	-5.83	92.92	104.00
7	A	1244	A	N7-C8-N9	5.83	116.71	113.80
30	a	296	A	O3'-P-O5'	-5.83	92.93	104.00
30	a	673	G	O3'-P-O5'	-5.82	92.94	104.00
7	A	700	U	C1'-O4'-C4'	-5.81	105.25	109.90
7	A	1856	U	O5'-P-OP2	-5.81	100.47	105.70
7	A	1071	G	N9-C4-C5	5.80	107.72	105.40
30	a	1090	A	O3'-P-O5'	-5.77	93.04	104.00
7	A	2525	C	P-O5'-C5'	-5.75	111.69	120.90
7	A	721	G	O5'-P-OP2	-5.75	100.53	105.70
7	A	123	G	O3'-P-O5'	-5.75	93.08	104.00
7	A	2414	C	O3'-P-O5'	-5.75	93.08	104.00
30	a	50	C	O3'-P-O5'	-5.74	93.09	104.00
7	A	1004	U	O3'-P-O5'	-5.74	93.09	104.00
7	A	44	A	O3'-P-O5'	-5.74	93.10	104.00
7	A	539	G	O3'-P-O5'	-5.74	93.10	104.00
8	B	11	A	O4'-C1'-N9	5.74	112.79	108.20
7	A	132	C	O3'-P-O5'	-5.74	93.10	104.00
7	A	2524	G	O3'-P-O5'	5.73	114.88	104.00
7	A	1246	G	O4'-C4'-C3'	-5.71	98.29	104.00
30	a	1356	G	C3'-C2'-C1'	-5.71	96.93	101.50
7	A	1662	C	O5'-P-OP2	-5.70	100.57	105.70
7	A	516	G	O3'-P-O5'	-5.69	93.19	104.00
30	a	896	G	O3'-P-O5'	-5.69	93.19	104.00
7	A	2267	G	O5'-P-OP1	-5.68	100.58	105.70
7	A	1876	A	O3'-P-O5'	-5.68	93.21	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	831	U	O3'-P-O5'	-5.68	93.21	104.00
7	A	700	U	O4'-C1'-N1	5.67	112.74	108.20
7	A	822	G	O4'-C1'-N9	5.67	112.73	108.20
7	A	1181	C	OP2-P-O3'	-5.67	92.73	105.20
7	A	1227	G	O5'-P-OP1	-5.65	100.61	105.70
30	a	127	U	C2'-C3'-O3'	5.65	122.74	113.70
30	a	337	A	O3'-P-O5'	-5.64	93.29	104.00
7	A	257	G	OP2-P-O3'	5.64	117.60	105.20
7	A	1180	C	OP2-P-O3'	5.63	117.58	105.20
7	A	378	C	O3'-P-O5'	-5.62	93.31	104.00
7	A	872	C	O5'-P-OP2	-5.62	100.64	105.70
7	A	1369	C	P-O5'-C5'	-5.62	111.91	120.90
7	A	2009	G	O5'-P-OP2	-5.61	100.65	105.70
7	A	468	C	O3'-P-O5'	-5.61	93.34	104.00
7	A	2497	A	O4'-C1'-N9	5.61	112.69	108.20
44	n	49	TYR	CB-CG-CD1	5.60	124.36	121.00
46	h	66	TYR	CB-CG-CD1	-5.60	117.64	121.00
7	A	2056	G	O5'-P-OP2	-5.60	100.66	105.70
7	A	2746	G	O3'-P-O5'	-5.58	93.40	104.00
30	a	360	C	O3'-P-O5'	-5.58	93.41	104.00
7	A	1526	G	O3'-P-O5'	-5.57	93.41	104.00
7	A	1751	U	OP1-P-O3'	5.57	117.44	105.20
7	A	2776	G	OP2-P-O3'	5.57	117.44	105.20
8	B	37	A	C4'-C3'-C2'	-5.57	97.03	102.60
30	a	664	A	O3'-P-O5'	-5.57	93.43	104.00
7	A	1704	U	O3'-P-O5'	-5.56	93.44	104.00
7	A	1808	U	C5-C6-N1	-5.56	119.92	122.70
7	A	1424	A	O3'-P-O5'	-5.55	93.44	104.00
33	l	123	ARG	CG-CD-NE	5.55	123.46	111.80
7	A	1866	C	O3'-P-O5'	-5.55	93.46	104.00
7	A	1867	C	O5'-P-OP2	5.55	117.36	110.70
7	A	1958	G	O3'-P-O5'	-5.54	93.47	104.00
8	B	37	A	C2'-C3'-O3'	5.54	122.57	113.70
30	a	988	A	OP1-P-O3'	5.54	117.38	105.20
7	A	2849	U	O5'-P-OP2	-5.53	100.72	105.70
30	a	789	G	O3'-P-O5'	-5.52	93.50	104.00
7	A	1969	U	O5'-P-OP2	-5.52	100.73	105.70
7	A	1359	G	O3'-P-O5'	-5.52	93.51	104.00
7	A	1036	A	O3'-P-O5'	-5.51	93.52	104.00
7	A	1173	A	O3'-P-O5'	-5.51	93.52	104.00
7	A	2609	U	O5'-P-OP2	-5.51	100.74	105.70
7	A	831	U	P-O3'-C3'	5.51	126.31	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	113	G	O5'-P-OP2	-5.50	100.75	105.70
7	A	1935	G	O3'-P-O5'	-5.50	93.56	104.00
7	A	2520	U	O5'-P-OP1	-5.48	100.77	105.70
7	A	2595	A	O3'-P-O5'	-5.48	93.59	104.00
7	A	1246	G	C5'-C4'-O4'	5.47	115.66	109.10
7	A	2722	A	O5'-P-OP2	-5.47	100.78	105.70
7	A	2777	A	O5'-P-OP2	-5.47	100.78	105.70
7	A	2904	A	O3'-P-O5'	-5.46	93.62	104.00
7	A	810	G	O3'-P-O5'	-5.46	93.63	104.00
7	A	1177	G	O3'-P-O5'	-5.46	93.63	104.00
7	A	590	U	O3'-P-O5'	-5.45	93.64	104.00
7	A	740	A	O5'-P-OP2	-5.45	100.80	105.70
7	A	2459	A	C1'-O4'-C4'	-5.45	105.54	109.90
7	A	2805	A	OP1-P-O3'	5.43	117.15	105.20
30	a	338	C	OP2-P-O3'	5.42	117.14	105.20
7	A	1188	A	O4'-C1'-N9	5.42	112.53	108.20
30	a	882	A	O3'-P-O5'	-5.42	93.70	104.00
30	a	887	C	O3'-P-O5'	-5.42	93.71	104.00
7	A	2917	G	O4'-C1'-N9	5.41	112.53	108.20
7	A	2911	G	N7-C8-N9	5.40	115.80	113.10
7	A	868	A	O5'-P-OP2	-5.39	100.84	105.70
7	A	2354	G	O5'-P-OP1	5.39	117.17	110.70
7	A	2098	G	O3'-P-O5'	-5.38	93.77	104.00
7	A	2074	C	O3'-P-O5'	-5.38	93.78	104.00
7	A	2273	U	O5'-P-OP1	-5.38	100.86	105.70
7	A	354	A	O3'-P-O5'	-5.38	93.79	104.00
7	A	2639	C	O3'-P-O5'	-5.38	93.79	104.00
7	A	2094	C	OP2-P-O3'	5.37	117.02	105.20
7	A	1965	A	C1'-O4'-C4'	-5.37	105.61	109.90
30	a	1041	C	P-O3'-C3'	5.36	126.14	119.70
30	a	1090	A	OP1-P-O3'	5.36	117.00	105.20
7	A	845	G	O5'-P-OP2	-5.36	100.88	105.70
30	a	304	U	O5'-P-OP2	-5.35	100.88	105.70
7	A	2049	A	O3'-P-O5'	-5.35	93.83	104.00
30	a	785	G	O3'-P-O5'	-5.35	93.83	104.00
30	a	1402	U	O5'-P-OP2	-5.34	100.89	105.70
7	A	504	A	O4'-C1'-N9	5.34	112.47	108.20
7	A	1417	A	OP1-P-O3'	5.34	116.94	105.20
7	A	875	U	O4'-C1'-N1	-5.33	103.94	108.20
30	a	1313	G	OP2-P-O3'	5.33	116.93	105.20
7	A	245	G	O5'-P-OP1	5.32	117.08	110.70
7	A	751	G	O4'-C1'-N9	5.31	112.45	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1257	C	O5'-P-OP1	5.31	117.07	110.70
7	A	2602	C	OP2-P-O3'	5.31	116.87	105.20
7	A	2662	A	O3'-P-O5'	-5.30	93.92	104.00
37	w	46	G	O3'-P-O5'	-5.30	93.92	104.00
7	A	183	A	C4-N9-C1'	5.30	135.84	126.30
7	A	1167	C	O3'-P-O5'	-5.29	93.95	104.00
7	A	2629	A	O3'-P-O5'	-5.29	93.95	104.00
37	y	76	C	OP2-P-O3'	5.28	116.82	105.20
7	A	2030	A	O3'-P-O5'	-5.28	93.97	104.00
7	A	1231	G	C4'-C3'-C2'	-5.28	97.32	102.60
30	a	9	G	C1'-O4'-C4'	-5.28	105.68	109.90
7	A	632	U	OP2-P-O3'	5.28	116.81	105.20
7	A	1480	A	O3'-P-O5'	-5.28	93.98	104.00
7	A	2473	G	O3'-P-O5'	-5.27	93.98	104.00
7	A	2334	U	O4'-C1'-N1	5.27	112.42	108.20
7	A	2003	C	O5'-P-OP2	-5.27	100.96	105.70
7	A	2270	A	O5'-P-OP2	-5.26	100.96	105.70
7	A	208	G	O5'-P-OP1	5.26	117.01	110.70
7	A	2029	G	C3'-C2'-C1'	-5.26	97.29	101.50
7	A	864	C	C4'-C3'-C2'	-5.26	97.34	102.60
7	A	2793	A	O3'-P-O5'	-5.26	94.01	104.00
7	A	1966	A	OP2-P-O3'	5.25	116.74	105.20
8	B	49	G	C2'-C3'-O3'	5.24	122.09	113.70
7	A	1245	G	C4-C5-N7	5.24	112.90	110.80
7	A	1276	G	O5'-P-OP1	-5.24	100.98	105.70
30	a	1415	U	O5'-P-OP2	-5.23	100.99	105.70
7	A	27	G	O4'-C1'-N9	5.23	112.38	108.20
7	A	2389	A	O3'-P-O5'	-5.22	94.09	104.00
7	A	188	C	O3'-P-O5'	-5.21	94.10	104.00
7	A	987	A	OP2-P-O3'	5.21	116.66	105.20
7	A	1785	G	O5'-P-OP2	-5.21	101.01	105.70
37	w	77	A	C1'-O4'-C4'	-5.21	105.73	109.90
7	A	1284	A	O5'-P-OP2	-5.21	101.01	105.70
7	A	960	U	O3'-P-O5'	-5.20	94.12	104.00
7	A	2504	C	O3'-P-O5'	-5.20	94.12	104.00
7	A	2090	G	N7-C8-N9	5.20	115.70	113.10
7	A	1719	G	C3'-C2'-C1'	5.19	105.66	101.50
7	A	523	G	OP2-P-O3'	5.19	116.61	105.20
7	A	2270	A	OP2-P-O3'	5.19	116.61	105.20
7	A	18	C	O5'-P-OP2	-5.18	101.04	105.70
7	A	1644	C	O3'-P-O5'	-5.18	94.16	104.00
7	A	1690	G	O3'-P-O5'	-5.18	94.16	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	n	49	TYR	CB-CG-CD2	-5.18	117.89	121.00
7	A	2911	G	O4'-C1'-N9	5.17	112.34	108.20
7	A	2638	U	O5'-P-OP2	-5.17	101.04	105.70
7	A	183	A	C8-N9-C1'	-5.17	118.39	127.70
7	A	1958	G	O5'-P-OP1	5.17	116.90	110.70
7	A	776	G	C1'-O4'-C4'	-5.17	105.77	109.90
7	A	254	A	O3'-P-O5'	-5.17	94.19	104.00
7	A	854	U	C4'-C3'-C2'	-5.17	97.44	102.60
8	B	107	G	O4'-C1'-N9	5.16	112.33	108.20
7	A	1245	G	O5'-P-OP2	5.16	116.89	110.70
7	A	2014	G	O5'-P-OP2	-5.16	101.06	105.70
7	A	2304	C	C6-N1-C2	-5.15	118.24	120.30
7	A	1480	A	O4'-C1'-N9	5.15	112.32	108.20
7	A	1246	G	C4'-C3'-C2'	-5.15	97.45	102.60
37	w	75	C	O3'-P-O5'	-5.15	94.22	104.00
30	a	822	U	O5'-P-OP2	-5.14	101.07	105.70
30	a	1313	G	C2'-C3'-O3'	5.14	121.92	113.70
7	A	2601	A	C2'-C3'-O3'	-5.14	98.20	109.50
7	A	2886	C	O5'-P-OP2	-5.13	101.08	105.70
30	a	1512	A	O4'-C1'-N9	5.13	112.30	108.20
30	a	1514	G	O3'-P-O5'	-5.13	94.25	104.00
7	A	436	A	O3'-P-O5'	-5.13	94.26	104.00
7	A	123	G	OP2-P-O3'	5.12	116.47	105.20
7	A	1406	A	O3'-P-O5'	-5.12	94.27	104.00
30	a	987	A	O3'-P-O5'	-5.12	94.27	104.00
7	A	223	G	OP2-P-O3'	5.11	116.45	105.20
7	A	2457	G	P-O3'-C3'	5.11	125.83	119.70
7	A	2695	C	O4'-C1'-N1	5.11	112.29	108.20
7	A	1207	C	OP2-P-O3'	5.11	116.44	105.20
7	A	1559	C	O3'-P-O5'	-5.11	94.30	104.00
30	a	829	U	OP2-P-O3'	5.10	116.43	105.20
7	A	297	G	O3'-P-O5'	-5.10	94.31	104.00
7	A	2458	G	O3'-P-O5'	-5.10	94.31	104.00
7	A	2601	A	C1'-O4'-C4'	-5.10	105.82	109.90
7	A	1030	G	O4'-C1'-N9	5.09	112.28	108.20
7	A	2720	C	O5'-P-OP1	-5.09	101.12	105.70
30	a	410	G	C3'-C2'-C1'	5.09	105.57	101.50
30	a	650	A	C3'-C2'-C1'	5.09	105.57	101.50
30	a	254	A	O3'-P-O5'	-5.08	94.34	104.00
7	A	481	U	O3'-P-O5'	-5.08	94.35	104.00
7	A	543	A	O3'-P-O5'	-5.08	94.35	104.00
7	A	1197	A	O3'-P-O5'	-5.07	94.36	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2638	U	O4'-C1'-N1	5.07	112.26	108.20
7	A	679	A	O3'-P-O5'	5.07	113.63	104.00
7	A	1293	A	O4'-C1'-N9	-5.07	104.15	108.20
7	A	2259	G	OP2-P-O3'	5.07	116.35	105.20
7	A	996	G	OP2-P-O3'	5.06	116.33	105.20
7	A	1279	C	O3'-P-O5'	-5.06	94.39	104.00
7	A	2457	G	OP2-P-O3'	5.06	116.33	105.20
7	A	1514	C	C1'-O4'-C4'	-5.05	105.86	109.90
7	A	583	G	O3'-P-O5'	-5.05	94.41	104.00
30	a	762	A	C3'-C2'-C1'	-5.05	97.46	101.50
7	A	2271	G	O3'-P-O5'	-5.04	94.42	104.00
30	a	122	G	O5'-P-OP2	-5.04	101.16	105.70
7	A	626	G	O5'-P-OP2	-5.04	101.17	105.70
7	A	345	A	OP1-P-O3'	5.04	116.28	105.20
7	A	1501	U	O3'-P-O5'	-5.04	94.43	104.00
30	a	707	G	O3'-P-O5'	-5.04	94.43	104.00
7	A	2057	U	O3'-P-O5'	-5.03	94.44	104.00
7	A	208	G	C3'-C2'-C1'	-5.03	97.47	101.50
30	a	474	A	C3'-C2'-C1'	5.03	105.53	101.50
7	A	2622	U	O3'-P-O5'	-5.03	94.44	104.00
7	A	1072	A	OP2-P-O3'	5.03	116.26	105.20
7	A	528	G	O4'-C1'-N9	5.02	112.22	108.20
7	A	1018	G	O3'-P-O5'	-5.02	94.47	104.00
7	A	1067	A	O3'-P-O5'	-5.01	94.47	104.00
30	a	19	U	C4'-C3'-C2'	-5.01	97.59	102.60
7	A	705	A	O5'-P-OP2	-5.01	101.19	105.70
7	A	896	A	OP2-P-O3'	5.01	116.22	105.20
30	a	16	U	O4'-C1'-N1	5.01	112.21	108.20
7	A	1851	G	O5'-P-OP1	5.00	116.71	110.70

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	41	ARG	Sidechain
1	0	6	ARG	Sidechain
3	2	36	ARG	Sidechain
4	3	13	ARG	Sidechain
7	A	1363	G	Sidechain
7	A	2497	A	Sidechain
7	A	2593	A	Sidechain
7	A	510	G	Sidechain

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Mol	Chain	Res	Type	Group
7	A	558	G	Sidechain
9	C	13	ARG	Sidechain
9	C	14	ARG	Sidechain
9	C	156	ARG	Sidechain
9	C	189	ARG	Sidechain
9	C	212	ARG	Sidechain
9	C	217	ARG	Sidechain
9	C	238	ARG	Sidechain
9	C	274	ARG	Sidechain
9	C	43	ARG	Sidechain
9	C	87	ARG	Sidechain
10	D	130	ARG	Sidechain
10	D	57	ARG	Sidechain
10	D	8	ARG	Sidechain
11	E	106	ARG	Sidechain
11	E	107	ARG	Sidechain
16	L	60	ARG	Sidechain
19	O	17	ARG	Sidechain
20	P	104	ARG	Sidechain
20	P	94	ARG	Sidechain
21	Q	51	ARG	Sidechain
25	U	32	ARG	Sidechain
27	X	16	ASN	Peptide
27	X	3	ARG	Sidechain
48	f	77	ARG	Sidechain
48	f	87	ARG	Sidechain
40	g	138	ARG	Sidechain
40	g	14	PRO	Peptide
46	h	42	ARG	Sidechain
46	h	79	ARG	Sidechain
33	l	123	ARG	Sidechain
35	q	4	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	433	0	450	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1	403	0	411	0	0
3	2	368	0	410	0	0
4	3	522	0	577	4	0
5	4	297	0	339	0	0
6	6	356	0	346	3	0
7	A	58964	0	29662	59	0
8	B	2392	0	1213	1	0
9	C	2094	0	2181	2	0
10	D	1575	0	1642	5	0
11	E	1567	0	1652	2	0
12	F	1405	0	1467	4	0
13	G	1342	0	1388	1	0
14	J	1142	0	1182	1	0
15	K	921	0	977	4	0
16	L	1082	0	1132	2	0
17	M	1076	0	1145	3	0
18	N	954	0	983	3	0
19	O	913	0	947	1	0
20	P	945	0	1020	2	0
21	Q	950	0	1018	4	0
22	R	795	0	838	2	0
23	S	850	0	911	1	0
24	T	716	0	764	1	0
25	U	770	0	824	0	0
26	W	650	0	662	0	0
27	X	468	0	514	3	0
28	Y	532	0	569	0	0
29	Z	456	0	491	0	0
30	a	32891	0	16559	0	0
31	e	1170	0	1247	0	0
32	k	847	0	860	0	0
33	l	1047	0	1107	0	0
34	o	730	0	759	0	0
35	q	699	0	739	0	0
36	t	658	0	715	0	0
37	w	1645	0	829	0	0
37	y	1645	0	829	0	0
38	8	120	0	65	0	0
39	c	1607	0	1644	0	0
40	g	1199	0	1256	0	0
41	i	994	0	1035	0	0
42	j	788	0	832	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	m	942	0	1006	0	0
44	n	498	0	529	0	0
45	s	668	0	682	0	0
46	h	958	0	1020	0	0
47	r	522	0	558	0	0
48	f	755	0	746	0	0
49	7	67	0	71	0	0
50	0	1	0	0	0	0
50	1	1	0	0	0	0
50	4	1	0	0	0	0
50	6	1	0	0	0	0
50	n	1	0	0	0	0
51	A	155	0	0	0	0
51	B	1	0	0	0	0
51	C	1	0	0	0	0
51	D	1	0	0	0	0
51	a	40	0	0	0	0
51	w	1	0	0	0	0
52	A	40	0	0	0	0
52	C	2	0	0	0	0
52	U	1	0	0	0	0
53	y	7	0	7	0	0
54	3	3	0	0	0	0
54	7	8	0	0	0	0
54	A	811	0	0	0	0
54	B	5	0	0	0	0
54	C	15	0	0	0	0
54	D	1	0	0	0	0
54	E	5	0	0	0	0
54	L	5	0	0	0	0
54	N	3	0	0	0	0
54	P	3	0	0	0	0
54	Q	3	0	0	0	0
54	T	1	0	0	0	0
54	a	132	0	0	0	0
54	i	1	0	0	0	0
54	j	1	0	0	0	0
54	k	1	0	0	0	0
54	w	21	0	0	0	0
54	y	3	0	0	0	0
All	All	136664	0	88810	91	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including



hydrogen atoms). The all-atom clashscore for this structure is 1.

All (91) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1808:U:H5	7:A:1813:A:N7	1.91	0.69
7:A:790:A:O2'	7:A:1704:U:OP1	2.13	0.63
7:A:1411:U:HO2'	7:A:2241:A:H8	1.46	0.63
11:E:32:VAL:HG21	11:E:108:LEU:HD23	1.82	0.61
7:A:761:U:H2'	7:A:763:A:H2	1.66	0.61
17:M:77:LYS:NZ	17:M:86:GLY:O	2.34	0.60
7:A:2435:C:C6	16:L:69:ILE:HD13	2.37	0.59
7:A:2906:U:O2	18:N:41:ARG:NH2	2.36	0.58
7:A:1327:U:H5	7:A:1365:U:O2	1.87	0.57
27:X:6:VAL:HG21	27:X:47:VAL:HB	1.88	0.55
7:A:2590:A:N3	15:K:23:LYS:NZ	2.55	0.54
13:G:51:LEU:HD21	13:G:73:LEU:HD13	1.92	0.51
7:A:761:U:H2'	7:A:763:A:C2	2.46	0.49
7:A:840:A:OP2	7:A:2100:A:O2'	2.28	0.49
7:A:2595:A:N1	15:K:28:SER:OG	2.39	0.49
4:3:31:HIS:HD2	7:A:2450:G:N7	2.10	0.49
6:6:33:VAL:HG11	12:F:106:VAL:HG13	1.95	0.49
7:A:1028:C:O2	7:A:1028:C:O5'	2.30	0.49
7:A:1947:A:H8	7:A:1948:A:H62	1.62	0.48
7:A:1066:A:N1	7:A:1187:U:O2'	2.40	0.47
7:A:2785:U:H5	7:A:2787:A:N7	2.13	0.47
16:L:17:ASN:HD21	16:L:27:ASN:HD22	1.61	0.47
9:C:144:ILE:HG21	9:C:184:ILE:HD13	1.97	0.47
24:T:58:ASN:ND2	24:T:77:ARG:HH11	2.12	0.47
7:A:2320:U:OP1	7:A:2409:U:O2'	2.30	0.47
23:S:10:VAL:HG11	23:S:46:ILE:HG21	1.97	0.47
7:A:1681:U:H2'	7:A:1682:C:C6	2.50	0.47
10:D:110:VAL:HG13	10:D:200:ILE:HG23	1.97	0.46
7:A:140:A:N1	7:A:1640:G:O2'	2.44	0.46
7:A:1074:A:N3	7:A:2515:G:O2'	2.39	0.46
10:D:28:ILE:HD13	10:D:188:ILE:HD12	1.96	0.46
7:A:2229:C:O2	7:A:2255:C:N4	2.48	0.46
7:A:999:A:OP2	17:M:18:ARG:NH2	2.49	0.46
7:A:2498:A:H4'	17:M:56:ARG:HD2	1.98	0.45
10:D:126:HIS:CD2	10:D:159:LEU:HB3	2.51	0.45
22:R:25:LEU:HD13	22:R:33:VAL:HG21	1.98	0.45
7:A:1292:G:H1	21:Q:37:GLN:HE21	1.64	0.45
7:A:183:A:OP1	7:A:184:G:H5''	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1074:A:N6	7:A:1171:G:H2'	2.32	0.45
6:6:14:VAL:HG11	12:F:106:VAL:HG21	1.98	0.45
7:A:909:G:H2'	7:A:910:A:O4'	2.17	0.45
7:A:1359:G:C2	7:A:1368:U:H5''	2.51	0.45
7:A:1480:A:H2'	7:A:1481:G:O4'	2.17	0.45
7:A:2096:G:O2'	7:A:2098:G:H5'	2.17	0.45
7:A:760:G:H2'	7:A:761:U:C6	2.51	0.45
9:C:29:PRO:HG2	9:C:34:LEU:HD11	1.99	0.45
7:A:2092:C:O2	7:A:2479:A:N1	2.49	0.44
7:A:1618:A:H2'	7:A:1619:A:C8	2.52	0.44
10:D:17:ALA:HB2	10:D:23:ILE:HD13	1.98	0.44
4:3:31:HIS:HE1	7:A:2421:A:OP2	1.99	0.44
7:A:2055:U:H2'	7:A:2056:G:O4'	2.17	0.44
20:P:100:LEU:HD11	20:P:110:ILE:HD11	2.00	0.44
18:N:59:ARG:HA	18:N:84:PHE:CZ	2.52	0.44
7:A:210:A:H2'	7:A:211:C:O4'	2.18	0.44
7:A:1710:A:H2'	7:A:1711:G:O4'	2.17	0.44
12:F:79:LEU:HD13	12:F:85:ILE:HG21	2.00	0.44
7:A:248:G:O2'	7:A:431:A:N1	2.45	0.43
7:A:614:G:H2'	7:A:2059:A:N7	2.33	0.43
4:3:26:HIS:CD2	4:3:46:LYS:O	2.71	0.43
6:6:36:CYS:SG	6:6:37:SER:N	2.91	0.43
7:A:6:A:O2'	14:J:136:GLN:NE2	2.52	0.43
7:A:1259:G:OP1	21:Q:22:LYS:NZ	2.41	0.43
15:K:24:VAL:HG13	15:K:33:ALA:HB2	2.00	0.43
4:3:26:HIS:HD2	4:3:46:LYS:O	2.02	0.43
7:A:1482:G:H2'	7:A:1483:A:O4'	2.19	0.43
7:A:2360:G:O2'	7:A:2365:A:N1	2.43	0.43
7:A:1512:G:H2'	7:A:1513:U:O4'	2.19	0.42
7:A:539:G:H2'	7:A:539:G:N3	3.22	0.42
7:A:1411:U:O2'	7:A:2241:A:H8	2.00	0.42
7:A:1066:A:C2	7:A:1187:U:C2	3.07	0.42
8:B:76:A:C2	8:B:97:A:C4	3.07	0.42
7:A:384:A:H2'	7:A:385:G:O4'	2.20	0.42
7:A:444:U:H5''	27:X:32:ASN:HB2	2.02	0.42
7:A:1961:A:H2'	7:A:1962:G:O4'	2.20	0.42
21:Q:94:MET:HE1	22:R:13:LYS:HB2	2.01	0.42
7:A:523:G:H4'	7:A:548:A:N1	2.35	0.42
7:A:576:G:N3	7:A:576:G:H2'	2.35	0.41
7:A:1807:U:H2'	7:A:1813:A:N6	2.35	0.41
21:Q:58:ARG:HA	21:Q:61:TRP:CE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:131:LEU:HD21	11:E:142:ILE:HD12	2.03	0.41
7:A:740:A:O2'	7:A:1392:A:N3	2.45	0.41
7:A:1404:A:OP1	27:X:12:THR:HG21	2.21	0.41
19:O:11:ARG:HD2	19:O:100:TYR:CZ	2.56	0.41
20:P:43:PHE:CE2	20:P:72:ARG:HG3	2.56	0.41
7:A:1366:C:O3'	18:N:108:ARG:NH2	2.48	0.41
10:D:49:ILE:HG23	10:D:88:MET:HE1	2.03	0.41
15:K:35:ILE:HG21	15:K:103:ALA:HB3	2.03	0.41
7:A:685:U:H2'	7:A:686:C:C6	2.56	0.40
7:A:1033:C:O2'	7:A:1046:A:N3	2.46	0.40
7:A:1877:A:H2'	7:A:1878:G:O4'	2.20	0.40
12:F:70:ALA:HB2	12:F:79:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	53/59 (90%)	50 (94%)	3 (6%)	0	100	100
2	1	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
3	2	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
4	3	63/66 (96%)	63 (100%)	0	0	100	100
5	4	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
6	6	44/65 (68%)	39 (89%)	5 (11%)	0	100	100
9	C	271/277 (98%)	263 (97%)	8 (3%)	0	100	100
10	D	205/209 (98%)	200 (98%)	5 (2%)	0	100	100
11	E	204/207 (99%)	200 (98%)	4 (2%)	0	100	100
12	F	176/179 (98%)	167 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	G	173/179 (97%)	162 (94%)	10 (6%)	1 (1%)	22	27
14	J	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
15	K	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
16	L	144/146 (99%)	139 (96%)	4 (3%)	1 (1%)	19	23
17	M	133/144 (92%)	131 (98%)	2 (2%)	0	100	100
18	N	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
19	O	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
20	P	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
21	Q	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
22	R	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
23	S	108/113 (96%)	107 (99%)	1 (1%)	0	100	100
24	T	87/95 (92%)	86 (99%)	1 (1%)	0	100	100
25	U	100/103 (97%)	99 (99%)	1 (1%)	0	100	100
26	W	83/94 (88%)	80 (96%)	3 (4%)	0	100	100
27	X	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
28	Y	63/66 (96%)	63 (100%)	0	0	100	100
29	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
31	e	156/166 (94%)	140 (90%)	14 (9%)	2 (1%)	10	11
32	k	113/131 (86%)	95 (84%)	16 (14%)	2 (2%)	7	6
33	l	133/138 (96%)	125 (94%)	8 (6%)	0	100	100
34	o	85/89 (96%)	78 (92%)	7 (8%)	0	100	100
35	q	83/87 (95%)	75 (90%)	8 (10%)	0	100	100
36	t	84/88 (96%)	80 (95%)	4 (5%)	0	100	100
39	c	202/206 (98%)	185 (92%)	17 (8%)	0	100	100
40	g	149/156 (96%)	140 (94%)	9 (6%)	0	100	100
41	i	126/130 (97%)	118 (94%)	8 (6%)	0	100	100
42	j	96/102 (94%)	91 (95%)	5 (5%)	0	100	100
43	m	116/121 (96%)	115 (99%)	1 (1%)	0	100	100
44	n	58/61 (95%)	58 (100%)	0	0	100	100
45	s	81/92 (88%)	77 (95%)	4 (5%)	0	100	100
46	h	120/132 (91%)	95 (79%)	20 (17%)	5 (4%)	2	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	r	63/79 (80%)	61 (97%)	2 (3%)	0	100	100
48	f	90/95 (95%)	85 (94%)	5 (6%)	0	100	100
49	7	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
All	All	4733/4978 (95%)	4503 (95%)	219 (5%)	11 (0%)	45	55

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	e	131	ASN
32	k	34	VAL
46	h	113	LEU
46	h	122	GLN
46	h	44	GLY
46	h	46	ILE
16	L	29	LYS
31	e	149	ARG
32	k	49	ALA
46	h	80	ILE
13	G	127	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	49/53 (92%)	48 (98%)	1 (2%)	50	68
2	1	46/47 (98%)	46 (100%)	0	100	100
3	2	39/39 (100%)	38 (97%)	1 (3%)	41	58
4	3	55/56 (98%)	54 (98%)	1 (2%)	54	71
5	4	35/35 (100%)	35 (100%)	0	100	100
6	6	39/54 (72%)	37 (95%)	2 (5%)	20	29
9	C	221/225 (98%)	218 (99%)	3 (1%)	62	77
10	D	168/170 (99%)	168 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	E	169/170 (99%)	169 (100%)	0	100	100
12	F	153/154 (99%)	153 (100%)	0	100	100
13	G	148/151 (98%)	146 (99%)	2 (1%)	62	77
14	J	122/123 (99%)	121 (99%)	1 (1%)	79	89
15	K	101/101 (100%)	101 (100%)	0	100	100
16	L	110/110 (100%)	110 (100%)	0	100	100
17	M	109/116 (94%)	108 (99%)	1 (1%)	75	87
18	N	99/100 (99%)	99 (100%)	0	100	100
19	O	93/93 (100%)	93 (100%)	0	100	100
20	P	100/100 (100%)	99 (99%)	1 (1%)	73	85
21	Q	97/98 (99%)	97 (100%)	0	100	100
22	R	84/84 (100%)	84 (100%)	0	100	100
23	S	91/93 (98%)	91 (100%)	0	100	100
24	T	80/85 (94%)	80 (100%)	0	100	100
25	U	86/87 (99%)	86 (100%)	0	100	100
26	W	65/74 (88%)	65 (100%)	0	100	100
27	X	49/50 (98%)	49 (100%)	0	100	100
28	Y	56/57 (98%)	56 (100%)	0	100	100
29	Z	52/53 (98%)	52 (100%)	0	100	100
31	e	122/130 (94%)	115 (94%)	7 (6%)	17	25
32	k	87/100 (87%)	84 (97%)	3 (3%)	32	47
33	l	114/116 (98%)	108 (95%)	6 (5%)	19	28
34	o	82/83 (99%)	82 (100%)	0	100	100
35	q	78/80 (98%)	74 (95%)	4 (5%)	20	29
36	t	69/70 (99%)	68 (99%)	1 (1%)	62	77
39	c	167/168 (99%)	167 (100%)	0	100	100
40	g	127/132 (96%)	124 (98%)	3 (2%)	44	61
41	i	101/102 (99%)	101 (100%)	0	100	100
42	j	89/92 (97%)	89 (100%)	0	100	100
43	m	101/104 (97%)	99 (98%)	2 (2%)	50	68
44	n	53/54 (98%)	53 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	s	72/81 (89%)	72 (100%)	0	100	100
46	h	102/112 (91%)	93 (91%)	9 (9%)	8	10
47	r	56/64 (88%)	55 (98%)	1 (2%)	54	71
48	f	81/84 (96%)	77 (95%)	4 (5%)	21	31
49	7	6/6 (100%)	6 (100%)	0	100	100
All	All	4023/4156 (97%)	3970 (99%)	53 (1%)	64	79

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	50	ASN
3	2	25	LYS
4	3	31	HIS
6	6	36	CYS
6	6	39	CYS
9	C	63	ARG
9	C	87	ARG
9	C	262	LYS
13	G	8	LEU
13	G	18	THR
14	J	61	GLU
17	M	6	ARG
20	P	39	ARG
31	e	133	PRO
31	e	136	MET
31	e	137	ILE
31	e	140	THR
31	e	146	GLU
31	e	148	LYS
31	e	155	LYS
32	k	34	VAL
32	k	38	ASP
32	k	44	ILE
33	l	5	ASN
33	l	10	LYS
33	l	50	VAL
33	l	123	ARG
33	l	127	ARG
33	l	128	SER
35	q	8	LYS

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Mol	Chain	Res	Type
35	q	13	ARG
35	q	56	LYS
35	q	59	ASP
36	t	59	ASP
40	g	23	VAL
40	g	43	LEU
40	g	59	MET
43	m	107	ARG
43	m	114	ARG
46	h	9	ASP
46	h	26	GLU
46	h	34	ARG
46	h	45	PHE
46	h	66	TYR
46	h	71	GLU
46	h	74	ILE
46	h	110	GLN
46	h	112	VAL
47	r	53	ASN
48	f	11	ARG
48	f	33	ASN
48	f	52	ILE
48	f	77	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	40	HIS
1	0	50	ASN
1	0	55	ASN
4	3	26	HIS
4	3	31	HIS
4	3	35	ASN
4	3	60	GLN
11	E	10	ASN
11	E	46	GLN
13	G	129	GLN
14	J	136	GLN
15	K	3	GLN
16	L	27	ASN
18	N	76	ASN
21	Q	37	GLN

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Mol	Chain	Res	Type
23	S	95	GLN
24	T	58	ASN
27	X	17	ASN
27	X	23	ASN
29	Z	59	GLN
32	k	121	ASN
33	l	59	ASN
33	l	86	ASN
34	o	51	HIS
39	c	133	GLN
42	j	56	HIS
42	j	78	ASN
43	m	118	ASN
46	h	122	GLN
47	r	21	ASN
47	r	69	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	a	1532/1554 (98%)	306 (19%)	0
37	w	76/77 (98%)	13 (17%)	0
37	y	76/77 (98%)	12 (15%)	0
38	8	5/6 (83%)	1 (20%)	0
7	A	2736/2925 (93%)	341 (12%)	82 (2%)
8	B	111/119 (93%)	16 (14%)	5 (4%)
All	All	4536/4758 (95%)	689 (15%)	87 (1%)

All (689) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	12	A
7	A	13	A
7	A	34	U
7	A	45	G
7	A	46	C
7	A	60	G
7	A	63	G
7	A	71	A
7	A	74	U
7	A	75	G

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Mol	Chain	Res	Type
7	A	93	C
7	A	118	A
7	A	119	U
7	A	163	U
7	A	164	U
7	A	166	A
7	A	175	G
7	A	176	A
7	A	177	G
7	A	183	A
7	A	184	G
7	A	199	A
7	A	202	A
7	A	203	U
7	A	216	A
7	A	219	A
7	A	224	A
7	A	225	A
7	A	226	A
7	A	232	U
7	A	233	G
7	A	236	A
7	A	248	G
7	A	251	G
7	A	258	A
7	A	268	A
7	A	275	A
7	A	284	C
7	A	285	U
7	A	288	C
7	A	300	G
7	A	301	U
7	A	302	A
7	A	308	C
7	A	309	U
7	A	310	C
7	A	334	G
7	A	345	A
7	A	346	G
7	A	355	A
7	A	373	A
7	A	374	A

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Mol	Chain	Res	Type
7	A	407	A
7	A	408	G
7	A	410	G
7	A	418	A
7	A	419	G
7	A	433	G
7	A	458	G
7	A	459	A
7	A	471	G
7	A	487	G
7	A	491	C
7	A	498	U
7	A	503	C
7	A	504	A
7	A	528	G
7	A	551	A
7	A	554	U
7	A	555	C
7	A	556	C
7	A	568	G
7	A	576	G
7	A	577	U
7	A	578	A
7	A	579	G
7	A	584	A
7	A	591	U
7	A	595	G
7	A	600	A
7	A	607	G
7	A	615	U
7	A	616	A
7	A	617	G
7	A	619	A
7	A	630	A
7	A	631	G
7	A	647	A
7	A	658	A
7	A	659	A
7	A	673	A
7	A	680	G
7	A	683	A
7	A	691	U

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Mol	Chain	Res	Type
7	A	692	A
7	A	700	U
7	A	701	G
7	A	732	A
7	A	733	U
7	A	761	U
7	A	762	A
7	A	764	C
7	A	777	C
7	A	793	U
7	A	794	U
7	A	811	A
7	A	812	G
7	A	822	G
7	A	829	A
7	A	831	U
7	A	832	G
7	A	852	G
7	A	859	C
7	A	866	A
7	A	874	U
7	A	875	U
7	A	892	U
7	A	906	G
7	A	913	A
7	A	924	U
7	A	931	C
7	A	940	G
7	A	943	A
7	A	944	C
7	A	947	A
7	A	957	A
7	A	959	C
7	A	964	A
7	A	973	G
7	A	976	U
7	A	987	A
7	A	991	A
7	A	992	G
7	A	1005	A
7	A	1007	G
7	A	1020	A

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Mol	Chain	Res	Type
7	A	1029	A
7	A	1042	A
7	A	1051	C
7	A	1058	U
7	A	1059	A
7	A	1068	G
7	A	1072	A
7	A	1079	U
7	A	1084	A
7	A	1093	G
7	A	1099	C
7	A	1153	G
7	A	1154	U
7	A	1155	C
7	A	1156	G
7	A	1157	A
7	A	1158	G
7	A	1174	A
7	A	1178	U
7	A	1179	A
7	A	1180	C
7	A	1181	C
7	A	1185	G
7	A	1188	A
7	A	1199	C
7	A	1278	G
7	A	1293	A
7	A	1296	G
7	A	1311	G
7	A	1312	A
7	A	1315	G
7	A	1339	A
7	A	1340	A
7	A	1341	U
7	A	1342	G
7	A	1346	A
7	A	1389	C
7	A	1391	U
7	A	1404	A
7	A	1418	U
7	A	1423	A
7	A	1435	U

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Mol	Chain	Res	Type
7	A	1450	C
7	A	1457	U
7	A	1458	U
7	A	1459	U
7	A	1460	G
7	A	1461	A
7	A	1465	A
7	A	1473	A
7	A	1474	C
7	A	1489	U
7	A	1490	A
7	A	1499	A
7	A	1507	U
7	A	1514	C
7	A	1525	G
7	A	1526	G
7	A	1528	U
7	A	1529	G
7	A	1531	G
7	A	1536	A
7	A	1539	C
7	A	1542	A
7	A	1543	U
7	A	1544	C
7	A	1557	G
7	A	1558	G
7	A	1595	U
7	A	1607	C
7	A	1608	A
7	A	1617	A
7	A	1626	U
7	A	1632	G
7	A	1653	A
7	A	1654	A
7	A	1691	A
7	A	1692	U
7	A	1693	C
7	A	1719	G
7	A	1752	G
7	A	1758	U
7	A	1759	U
7	A	1779	G

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Mol	Chain	Res	Type
7	A	1791	A
7	A	1792	G
7	A	1793	G
7	A	1802	A
7	A	1811	C
7	A	1820	A
7	A	1829	C
7	A	1830	G
7	A	1845	A
7	A	1858	A
7	A	1877	A
7	A	1887	G
7	A	1899	U
7	A	1900	A
7	A	1902	G
7	A	1935	G
7	A	1943	C
7	A	1948	A
7	A	1958	G
7	A	1959	G
7	A	1966	A
7	A	1967	A
7	A	1984	U
7	A	1992	C
7	A	1996	C
7	A	1999	A
7	A	2000	A
7	A	2001	G
7	A	2011	U
7	A	2020	U
7	A	2022	U
7	A	2026	A
7	A	2052	A
7	A	2060	A
7	A	2061	G
7	A	2062	A
7	A	2072	C
7	A	2084	C
7	A	2085	G
7	A	2089	A
7	A	2090	G
7	A	2098	G

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Mol	Chain	Res	Type
7	A	2122	G
7	A	2126	G
7	A	2128	U
7	A	2131	U
7	A	2132	A
7	A	2218	U
7	A	2227	A
7	A	2232	G
7	A	2233	C
7	A	2240	U
7	A	2254	A
7	A	2267	G
7	A	2268	G
7	A	2297	A
7	A	2312	C
7	A	2316	A
7	A	2318	G
7	A	2334	U
7	A	2337	G
7	A	2341	U
7	A	2348	C
7	A	2349	A
7	A	2350	G
7	A	2351	A
7	A	2354	G
7	A	2356	A
7	A	2363	C
7	A	2364	A
7	A	2376	C
7	A	2379	C
7	A	2408	G
7	A	2412	G
7	A	2414	C
7	A	2431	U
7	A	2435	C
7	A	2453	C
7	A	2454	A
7	A	2458	G
7	A	2459	A
7	A	2464	A
7	A	2470	C
7	A	2476	G

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Mol	Chain	Res	Type
7	A	2477	A
7	A	2505	A
7	A	2531	G
7	A	2534	G
7	A	2547	A
7	A	2558	G
7	A	2583	U
7	A	2595	A
7	A	2596	G
7	A	2602	C
7	A	2631	A
7	A	2632	G
7	A	2638	U
7	A	2642	U
7	A	2690	G
7	A	2692	G
7	A	2718	PSU
7	A	2720	C
7	A	2743	G
7	A	2755	U
7	A	2764	G
7	A	2773	G
7	A	2777	A
7	A	2786	A
7	A	2794	A
7	A	2807	A
7	A	2819	A
7	A	2824	G
7	A	2826	A
7	A	2828	G
7	A	2845	A
7	A	2848	A
7	A	2860	A
7	A	2892	G
7	A	2893	A
7	A	2897	G
7	A	2918	G
8	B	10	G
8	B	12	U
8	B	14	G
8	B	15	C
8	B	23	U

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Mol	Chain	Res	Type
8	B	38	U
8	B	43	A
8	B	49	G
8	B	50	A
8	B	54	U
8	B	55	A
8	B	87	U
8	B	88	C
8	B	97	A
8	B	107	G
8	B	108	C
30	a	9	G
30	a	11	G
30	a	24	G
30	a	33	G
30	a	34	A
30	a	41	G
30	a	49	C
30	a	50	C
30	a	51	U
30	a	52	A
30	a	53	A
30	a	61	A
30	a	63	G
30	a	68	G
30	a	70	G
30	a	72	A
30	a	77	U
30	a	83	C
30	a	84	U
30	a	85	U
30	a	87	C
30	a	89	C
30	a	90	C
30	a	93	G
30	a	95	U
30	a	99	A
30	a	113	G
30	a	114	A
30	a	119	C
30	a	123	U
30	a	127	U

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Mol	Chain	Res	Type
30	a	128	A
30	a	130	C
30	a	133	G
30	a	143	C
30	a	144	U
30	a	145	G
30	a	146	G
30	a	158	G
30	a	159	A
30	a	160	A
30	a	161	A
30	a	162	C
30	a	168	C
30	a	172	U
30	a	173	A
30	a	180	G
30	a	181	G
30	a	188	G
30	a	189	A
30	a	192	C
30	a	194	C
30	a	195	A
30	a	197	G
30	a	209	A
30	a	213	G
30	a	218	U
30	a	219	U
30	a	222	G
30	a	224	U
30	a	231	U
30	a	234	A
30	a	248	C
30	a	253	U
30	a	255	G
30	a	259	G
30	a	272	C
30	a	274	G
30	a	275	C
30	a	281	A
30	a	283	G
30	a	297	G
30	a	313	G

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Mol	Chain	Res	Type
30	a	314	A
30	a	329	A
30	a	332	G
30	a	335	A
30	a	336	C
30	a	337	A
30	a	340	G
30	a	347	C
30	a	353	C
30	a	355	G
30	a	359	G
30	a	360	C
30	a	362	G
30	a	374	C
30	a	375	U
30	a	376	U
30	a	377	C
30	a	380	C
30	a	385	G
30	a	391	A
30	a	405	A
30	a	406	C
30	a	410	G
30	a	411	C
30	a	412	G
30	a	414	G
30	a	419	A
30	a	421	G
30	a	422	A
30	a	429	U
30	a	430	C
30	a	431	G
30	a	432	G
30	a	435	C
30	a	436	G
30	a	437	U
30	a	441	G
30	a	442	C
30	a	444	C
30	a	445	U
30	a	450	U
30	a	451	U

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Mol	Chain	Res	Type
30	a	456	A
30	a	461	C
30	a	463	A
30	a	465	U
30	a	467	C
30	a	470	U
30	a	471	U
30	a	474	A
30	a	475	A
30	a	477	A
30	a	479	G
30	a	483	G
30	a	485	A
30	a	493	G
30	a	494	G
30	a	497	C
30	a	503	C
30	a	504	A
30	a	505	G
30	a	507	A
30	a	508	A
30	a	509	G
30	a	510	C
30	a	514	G
30	a	519	A
30	a	520	C
30	a	521	U
30	a	525	U
30	a	526	G
30	a	527	C
30	a	530	G
30	a	536	G
30	a	539	G
30	a	540	U
30	a	541	A
30	a	542	A
30	a	544	A
30	a	546	G
30	a	551	U
30	a	552	G
30	a	553	G
30	a	556	A

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Mol	Chain	Res	Type
30	a	558	C
30	a	568	A
30	a	569	A
30	a	571	U
30	a	581	A
30	a	582	A
30	a	585	G
30	a	586	G
30	a	596	G
30	a	597	G
30	a	621	C
30	a	624	C
30	a	630	A
30	a	631	A
30	a	632	C
30	a	633	C
30	a	637	G
30	a	641	G
30	a	642	U
30	a	643	C
30	a	651	A
30	a	659	A
30	a	674	A
30	a	675	G
30	a	709	G
30	a	711	A
30	a	727	A
30	a	730	A
30	a	732	U
30	a	733	G
30	a	758	A
30	a	762	A
30	a	764	G
30	a	786	A
30	a	803	A
30	a	824	A
30	a	826	C
30	a	845	G
30	a	849	G
30	a	850	U
30	a	853	C
30	a	856	C

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Mol	Chain	Res	Type
30	a	869	C
30	a	880	U
30	a	924	A
30	a	925	A
30	a	936	G
30	a	941	C
30	a	944	C
30	a	945	A
30	a	970	U
30	a	971	U
30	a	976	G
30	a	978	A
30	a	979	A
30	a	981	G
30	a	985	A
30	a	986	G
30	a	987	A
30	a	994	C
30	a	1002	U
30	a	1003	G
30	a	1010	U
30	a	1014	A
30	a	1016	A
30	a	1030	G
30	a	1033	G
30	a	1035	C
30	a	1036	C
30	a	1039	U
30	a	1040	U
30	a	1041	C
30	a	1042	G
30	a	1044	G
30	a	1046	G
30	a	1049	G
30	a	1050	A
30	a	1051	G
30	a	1056	A
30	a	1058	G
30	a	1063	G
30	a	1065	A
30	a	1074	G
30	a	1075	U

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Mol	Chain	Res	Type
30	a	1096	U
30	a	1099	G
30	a	1104	G
30	a	1105	U
30	a	1111	A
30	a	1134	G
30	a	1136	U
30	a	1140	A
30	a	1148	G
30	a	1149	U
30	a	1155	A
30	a	1168	U
30	a	1176	A
30	a	1177	C
30	a	1178	A
30	a	1193	G
30	a	1205	A
30	a	1206	A
30	a	1221	U
30	a	1222	A
30	a	1223	U
30	a	1236	A
30	a	1237	C
30	a	1247	A
30	a	1257	A
30	a	1266	A
30	a	1267	G
30	a	1269	G
30	a	1289	A
30	a	1296	A
30	a	1307	C
30	a	1309	G
30	a	1311	U
30	a	1314	G
30	a	1328	A
30	a	1329	C
30	a	1331	C
30	a	1344	C
30	a	1345	U
30	a	1347	G
30	a	1355	A
30	a	1373	U

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Mol	Chain	Res	Type
30	a	1389	U
30	a	1390	U
30	a	1406	C
30	a	1407	A
30	a	1415	U
30	a	1427	A
30	a	1449	U
30	a	1451	A
30	a	1455	A
30	a	1459	U
30	a	1462	U
30	a	1464	G
30	a	1497	G
30	a	1502	A
30	a	1504	G
30	a	1513	A
30	a	1515	G
30	a	1516	U
30	a	1527	G
30	a	1529	A
30	a	1530	G
30	a	1539	G
30	a	1540	G
37	y	9	A
37	y	14	A
37	y	18	U
37	y	19	G
37	y	20	G
37	y	21	U
37	y	22	A
37	y	47	G
37	y	48	U
37	y	49	C
37	y	59	A
37	y	75	C
37	w	9	A
37	w	14	A
37	w	18	U
37	w	19	G
37	w	20	G
37	w	21	U
37	w	22	A

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Mol	Chain	Res	Type
37	w	23	G
37	w	47	G
37	w	48	U
37	w	49	C
37	w	59	A
37	w	77	A
38	8	19	C

All (87) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	12	A
7	A	60	G
7	A	67	A
7	A	92	G
7	A	98	U
7	A	172	U
7	A	176	A
7	A	183	A
7	A	184	G
7	A	202	A
7	A	224	A
7	A	299	U
7	A	300	G
7	A	337	A
7	A	389	A
7	A	406	G
7	A	407	A
7	A	410	G
7	A	493	G
7	A	504	A
7	A	549	A
7	A	558	G
7	A	599	G
7	A	615	U
7	A	662	U
7	A	691	U
7	A	727	A
7	A	732	A
7	A	793	U
7	A	811	A
7	A	831	U

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Mol	Chain	Res	Type
7	A	852	G
7	A	855	G
7	A	874	U
7	A	990	C
7	A	1001	U
7	A	1004	U
7	A	1030	G
7	A	1041	C
7	A	1071	G
7	A	1092	A
7	A	1179	A
7	A	1180	C
7	A	1187	U
7	A	1188	A
7	A	1244	A
7	A	1246	G
7	A	1266	A
7	A	1278	G
7	A	1341	U
7	A	1344	C
7	A	1525	G
7	A	1530	G
7	A	1535	U
7	A	1543	U
7	A	1602	U
7	A	1653	A
7	A	1691	A
7	A	1751	U
7	A	1791	A
7	A	1876	A
7	A	1942	A
7	A	1947	A
7	A	2010	A
7	A	2026	A
7	A	2064	G
7	A	2127	U
7	A	2311	G
7	A	2315	A
7	A	2316	A
7	A	2348	C
7	A	2349	A
7	A	2435	C

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Mol	Chain	Res	Type
7	A	2459	A
7	A	2476	G
7	A	2533	U
7	A	2558	G
7	A	2610	G
7	A	2631	A
7	A	2785	U
7	A	2819	A
7	A	2892	G
8	B	37	A
8	B	48	G
8	B	49	G
8	B	85	U
8	B	106	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	2MA	A	2532	52,51,7	19,25,26	0.86	0	21,37,40	2.03	4 (19%)
7	PSU	A	2718	7	18,21,22	0.93	1 (5%)	22,30,33	0.82	0
7	OMG	A	2280	52,37,7	18,26,27	0.94	1 (5%)	19,38,41	0.97	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	2MA	A	2532	52,51,7	-	2/3/25/26	0/3/3/3
7	PSU	A	2718	7	-	1/7/25/26	0/2/2/2
7	OMG	A	2280	52,37,7	-	1/5/27/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2718	PSU	C6-C5	3.35	1.39	1.35
7	A	2280	OMG	C5-C6	-2.53	1.42	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2532	2MA	C5-C6-N1	-6.87	116.50	121.01
7	A	2532	2MA	C5-C6-N6	3.44	125.58	120.35
7	A	2532	2MA	CM2-C2-N1	3.36	122.40	117.15
7	A	2532	2MA	C2-N1-C6	2.62	122.16	118.08
7	A	2280	OMG	O2'-C2'-C1'	2.20	113.45	109.09
7	A	2280	OMG	O6-C6-C5	2.14	128.56	124.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2280	OMG	C1'-C2'-O2'-CM2
7	A	2718	PSU	O4'-C4'-C5'-O5'
7	A	2532	2MA	C4'-C5'-O5'-P
7	A	2532	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 248 ligands modelled in this entry, 247 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
53	PRO	y	101	37	5,7,8	0.67	0	7,8,10	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	PRO	y	101	37	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.