



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 02:23 pm GMT

PDB ID : 8QBT  
EMDB ID : EMD-18320  
Title : E. coli ApdP-stalled ribosomal complex  
Authors : Morici, M.; Wilson, D.N.  
Deposited on : 2023-08-25  
Resolution : 2.20 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

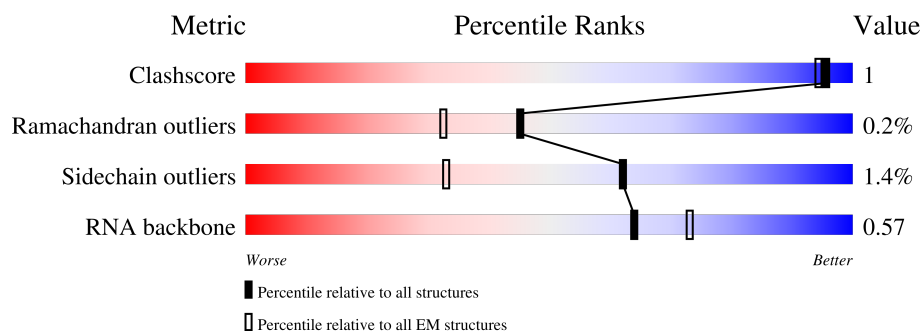
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.20 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	A	2903	77% 18% . .
2	B	120	82% 15% . .
3	C	273	95% . .
4	D	209	95% 5%
5	E	201	96% .
6	F	179	97% . .
7	G	177	93% . .



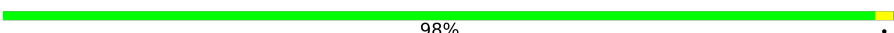









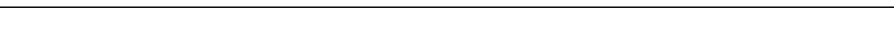



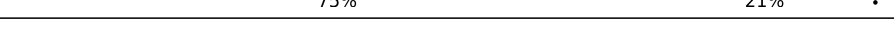


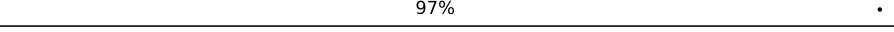
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Mol	Chain	Length	Quality of chain
8	H	149	
9	J	142	
10	K	123	
11	L	144	
12	M	136	
13	N	127	
14	O	117	
15	P	115	
16	Q	118	
17	R	103	
18	S	110	
19	T	100	
20	U	104	
21	V	94	
22	W	85	
23	X	78	
24	Y	63	
25	Z	59	
26	a	57	
27	b	55	
28	c	46	
29	d	65	
30	i	1540	
31	j	241	
32	m	167	

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Mol	Chain	Length	Quality of chain
33	n	135	 72% 26%
34	o	179	 83% 16%
35	p	130	 98% ..
36	q	130	 86% 10% .
37	s	129	 88% .. 9%
38	t	124	 89% 6% . .
39	u	118	 92% .. 5%
40	v	101	 89% 6% 5%
41	w	89	 97% .
42	y	84	 94% . 5%
43	z	75	 72% 27%
44	1	92	 78% 20%
45	2	87	 89% 10%
46	3	71	 51% 7% 41%
47	4	10	 90% 10%
48	5	77	 75% 21% .
48	6	77	 83% 10% 6%
49	7	76	 62% 37% .
50	e	38	 97% .
51	f	6	 100%

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 141132 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2841	Total	C	N	O	P	0	0
			60998	27210	11227	19720	2841		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2209	C	G	conflict	GB 991970073
A	2215	G	C	conflict	GB 991970073

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

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

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1285	811	235	237	2		

- Molecule 8 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 10 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 13 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 14 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	114	Total	C	N	O		0	0
			875	542	175	158			

- Molecule 15 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	112	Total	C	N	O	S	0	0
			900	564	176	159	1		

- Molecule 16 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	116	Total	C	N	O		0	0
			941	601	191	149			

- Molecule 17 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 18 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 19 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	92	Total	C	N	O	S	0	0
			730	461	138	130	1		

- Molecule 20 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	94	Total	C	N	O	S	
			753	479	137	134	3	0

- Molecule 22 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	84	Total	C	N	O	S	
			628	388	126	113	1	0

- Molecule 23 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	77	Total	C	N	O	S	
			625	388	129	106	2	0

- Molecule 24 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Y	63	Total	C	N	O	S	
			509	313	99	95	2	0

- Molecule 25 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Z	56	Total	C	N	O	S	
			435	272	84	77	2	0

- Molecule 26 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	a	56	Total	C	N	O	S	
			444	269	94	80	1	0

- Molecule 27 is a protein called Large ribosomal subunit protein bL33.



Mol	Chain	Residues	Atoms				AltConf	Trace
27	b	48	Total	C	N	O	0	0
			395	254	72	69		

- Molecule 28 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 29 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

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

- Molecule 31 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	215	Total	C	N	O	S	0	0
			1679	1067	299	307	6		

- Molecule 32 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 33 is a protein called 30S ribosomal protein S6, fully modified isoform.

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

- Molecule 34 is a protein called 30S ribosomal protein S7.

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

- Molecule 35 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 36 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	q	125	Total	C	N	O	S	0	0
			1001	622	200	176	3		

- Molecule 37 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	s	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 38 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	t	119	Total	C	N	O	S	0	0
			922	570	188	160	4		

- Molecule 39 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	112	Total	C	N	O	S	0	0
			867	535	175	154	3		

- Molecule 40 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	v	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 41 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	86	Total	C	N	O	S	0	0
			687	425	135	126	1		

- Molecule 42 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 43 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 44 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1	74	Total	C	N	O	S	0	0
			594	381	110	101	2		

- Molecule 45 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2	78	Total	C	N	O	S	0	0
			612	376	126	107	3		

- Molecule 46 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3	42	Total	C	N	O	S	0	0
			346	214	72	59	1		

- Molecule 47 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	4	10	Total	C	N	O	P	0	0
			214	95	40	69	10		

- Molecule 48 is a RNA chain called Pro-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	77	Total	C	N	O	P	0	0
			1644	733	295	540	76		
48	6	77	Total	C	N	O	P	0	0
			1648	733	295	543	77		

- Molecule 49 is a RNA chain called Ala-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	76	Total	C	N	O	P	0	0
			1618	722	289	532	75		

- Molecule 50 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	e	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 51 is a protein called ApdP nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	f	6	Total	C	N	O	S	0	0
			46	29	10	6	1		

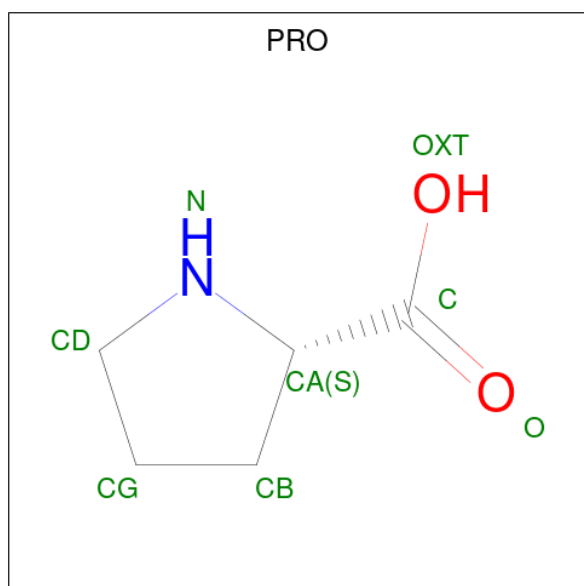
- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	A	178	Total	Mg	0
			178	178	
52	B	5	Total	Mg	0
			5	5	
52	C	1	Total	Mg	0
			1	1	
52	D	1	Total	Mg	0
			1	1	
52	a	1	Total	Mg	0
			1	1	
52	i	61	Total	Mg	0
			61	61	
52	6	1	Total	Mg	0
			1	1	

- Molecule 53 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
53	A	83	Total	K	0
			83	83	
53	C	3	Total	K	0
			3	3	
53	E	1	Total	K	0
			1	1	
53	U	1	Total	K	0
			1	1	
53	i	37	Total	K	0
			37	37	
53	n	1	Total	K	0
			1	1	
53	u	1	Total	K	0
			1	1	

- Molecule 54 is PROLINE (three-letter code: PRO) (formula:  $C_5H_9NO_2$ ).



Mol	Chain	Residues	Atoms				AltConf
54	5	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		AltConf
55	e	1	Total	Zn	0
			1	1	

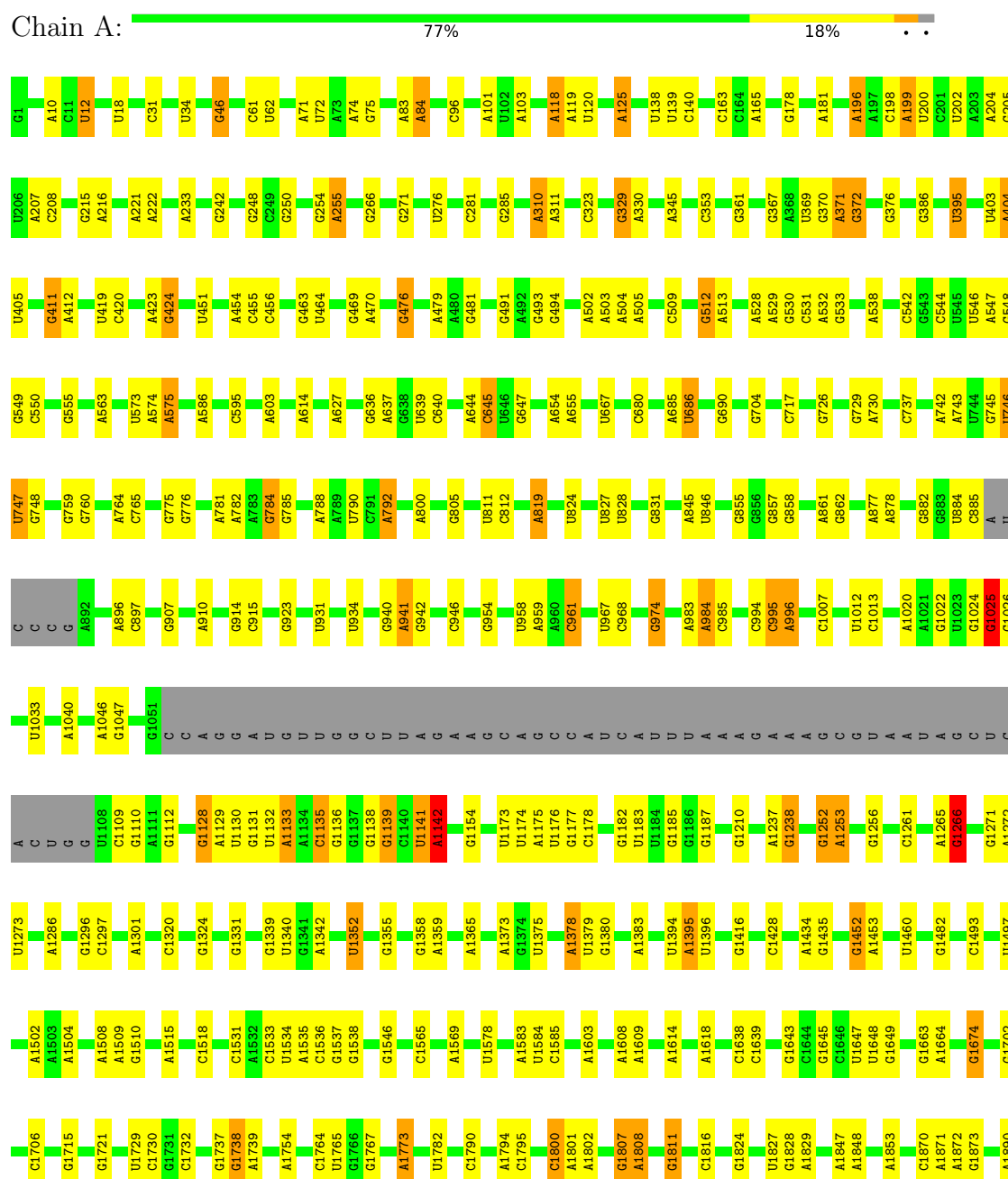
- Molecule 56 is water.

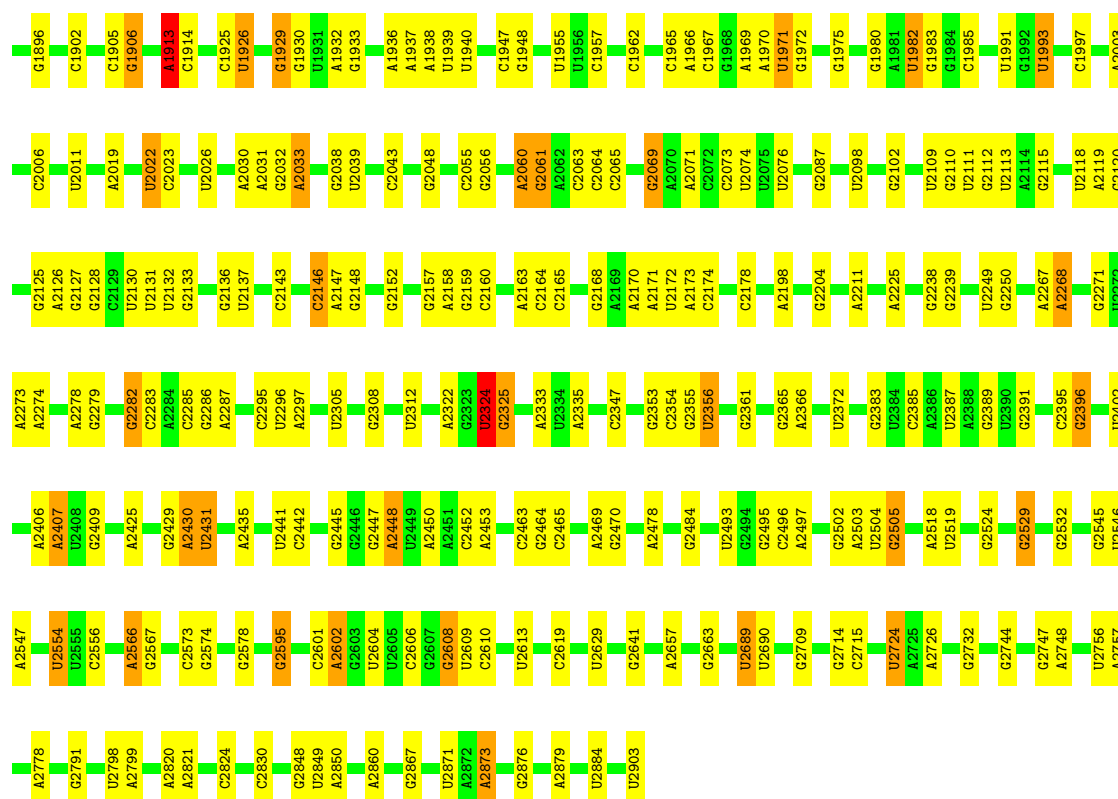
Mol	Chain	Residues	Atoms		AltConf
56	A	1006	Total 1006	O 1006	0
56	B	10	Total 10	O 10	0
56	C	14	Total 14	O 14	0
56	D	2	Total 2	O 2	0
56	E	3	Total 3	O 3	0
56	L	4	Total 4	O 4	0
56	N	3	Total 3	O 3	0
56	T	1	Total 1	O 1	0
56	a	4	Total 4	O 4	0
56	d	4	Total 4	O 4	0
56	i	176	Total 176	O 176	0
56	s	1	Total 1	O 1	0
56	4	3	Total 3	O 3	0
56	5	3	Total 3	O 3	0
56	6	2	Total 2	O 2	0
56	f	3	Total 3	O 3	0

### 3 Residue-property plots

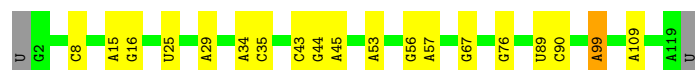
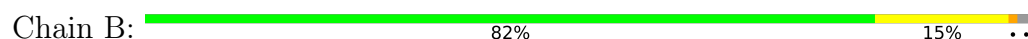
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: 23S rRNA





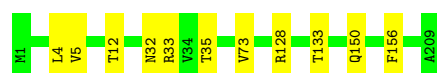
- Molecule 2: 5S rRNA



- Molecule 3: Large ribosomal subunit protein uL2



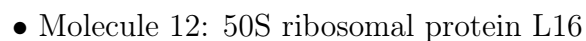
- Molecule 4: 50S ribosomal protein L3



- Molecule 5: Large ribosomal subunit protein uL4





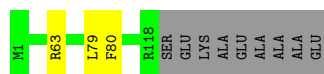


Chain M:  96% ..



- Molecule 13: Large ribosomal subunit protein bL17

Chain N:  91% • 7%




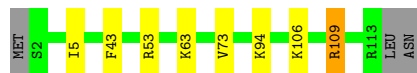
- Molecule 14: Large ribosomal subunit protein uL18

Chain O:  93% ...



- Molecule 15: Large ribosomal subunit protein bL19

Chain P:  90% 6% ..



- Molecule 16: Large ribosomal subunit protein bL20

Chain Q:  93% 5% •




- Molecule 17: Large ribosomal subunit protein bL21

Chain R:  89% 10% •




- Molecule 18: Large ribosomal subunit protein uL22

Chain S:  88% 12%



- Molecule 19: Large ribosomal subunit protein uL23

Chain T:  91% • 8%



- Molecule 20: Large ribosomal subunit protein uL24

Chain U:  94% • •



- Molecule 21: 50S ribosomal protein L25

Chain V:  95% 5%



- Molecule 22: Large ribosomal subunit protein bL27

Chain W:  92% 6% ••



- Molecule 23: Large ribosomal subunit protein bL28

Chain X:  92% 6% •



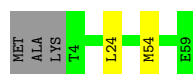
- Molecule 24: Large ribosomal subunit protein uL29

Chain Y:  95% 5%



- Molecule 25: Large ribosomal subunit protein uL30

Chain Z:  92% • 5%




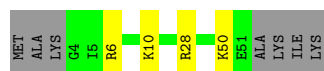
- Molecule 26: Large ribosomal subunit protein bL32

Chain a:  96% ..



- Molecule 27: Large ribosomal subunit protein bL33

Chain b:  80% 7% 13%



- Molecule 28: Large ribosomal subunit protein bL34

Chain c:  100%


There are no outlier residues recorded for this chain.

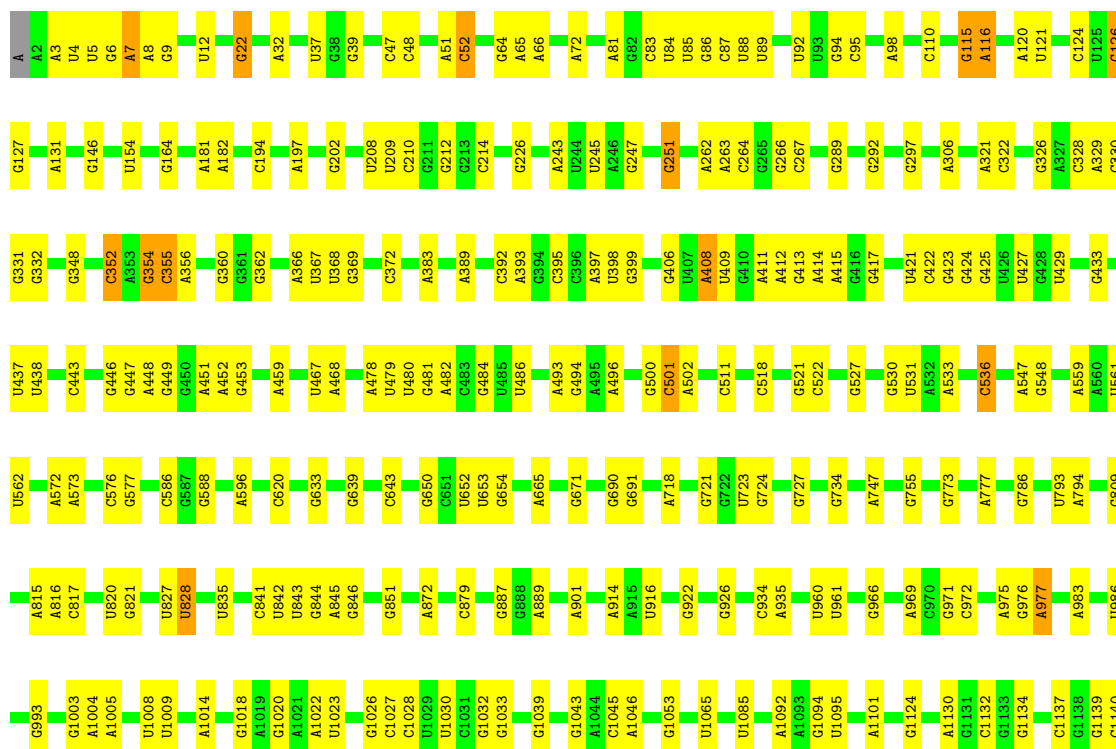
- Molecule 29: Large ribosomal subunit protein bL35

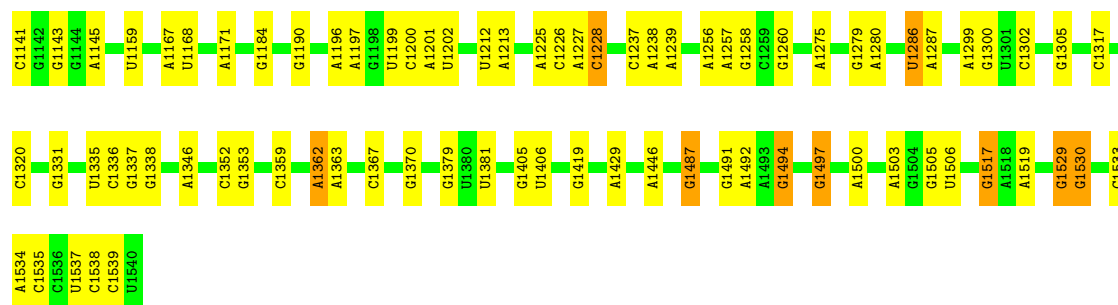
Chain d:  95% ..



- Molecule 30: 16S rRNA

Chain i:  78% 20% .





- Molecule 31: 30S ribosomal protein S2

Chain j: 87% 11%



- Molecule 32: Small ribosomal subunit protein uS5

Chain m: 88% 10%



- Molecule 33: 30S ribosomal protein S6, fully modified isoform

Chain n: 72% 26%



- Molecule 34: 30S ribosomal protein S7

Chain o: 83% 16%



- Molecule 35: Small ribosomal subunit protein uS8

Chain p: 98% 2%



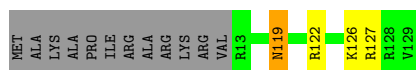
- Molecule 36: Small ribosomal subunit protein uS9

Chain q: 86% 10%



- Molecule 37: 30S ribosomal protein S11

Chain s: 88% .. 9%



- Molecule 38: 30S ribosomal protein S12

Chain t: 89% 6% ..



- Molecule 39: Small ribosomal subunit protein uS13

Chain u: 92% .. 5%



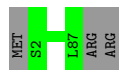
- Molecule 40: Small ribosomal subunit protein uS14

Chain v: 89% 6% 5%



- Molecule 41: Small ribosomal subunit protein uS15

Chain w: 97% .



- Molecule 42: Small ribosomal subunit protein uS17

Chain y: 94% . 5%



- Molecule 43: Small ribosomal subunit protein bS18

Chain z: 72% . 27%





- Molecule 50: Large ribosomal subunit protein bL36A

Chain e:  97%



- Molecule 51: ApdP nascent chain

Chain f:  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	205838	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: ZN, MG, PSU, K, 2MA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.61	1/68247 (0.0%)	1.29	302/106469 (0.3%)
2	B	0.51	0/2828	1.17	7/4410 (0.2%)
3	C	0.42	0/2121	0.87	4/2852 (0.1%)
4	D	0.41	0/1586	0.72	0/2134
5	E	0.38	0/1571	0.68	0/2113
6	F	0.29	0/1434	0.64	0/1926
7	G	0.31	0/1303	0.65	0/1759
8	H	0.31	0/364	0.66	0/490
9	J	0.35	0/1152	0.67	0/1551
10	K	0.36	0/947	0.81	0/1268
11	L	0.40	0/1054	0.76	0/1403
12	M	0.37	0/1093	0.76	1/1460 (0.1%)
13	N	0.38	0/958	0.77	0/1281
14	O	0.32	0/885	0.70	1/1187 (0.1%)
15	P	0.37	0/912	0.77	0/1220
16	Q	0.41	0/954	0.75	1/1271 (0.1%)
17	R	0.40	0/829	0.80	1/1107 (0.1%)
18	S	0.38	0/864	0.71	0/1156
19	T	0.32	0/736	0.67	0/984
20	U	0.30	0/787	0.71	0/1051
21	V	0.31	0/766	0.67	0/1025
22	W	0.41	0/636	0.76	0/841
23	X	0.38	0/635	0.79	1/848 (0.1%)
24	Y	0.29	0/510	0.63	0/677
25	Z	0.33	0/439	0.68	0/587
26	a	0.41	0/450	0.81	0/599
27	b	0.37	0/402	0.73	0/536
28	c	0.44	0/380	0.90	0/498
29	d	0.41	0/513	0.77	0/676
30	i	0.55	0/36966	1.20	85/57666 (0.1%)
31	j	0.30	0/1710	0.69	0/2306
32	m	0.33	0/1118	0.69	0/1504

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	n	0.29	0/835	0.67	0/1128
34	o	0.30	0/1195	0.70	1/1602 (0.1%)
35	p	0.29	0/989	0.65	0/1326
36	q	0.38	0/1013	0.76	0/1350
37	s	0.34	0/893	0.79	2/1205 (0.2%)
38	t	0.32	0/935	0.80	0/1256
39	u	0.31	0/875	0.74	0/1170
40	v	0.33	0/785	0.68	0/1043
41	w	0.31	0/695	0.58	0/931
42	y	0.28	0/657	0.71	0/881
43	z	0.30	0/462	0.65	0/621
44	1	0.32	0/609	0.67	0/822
45	2	0.30	0/616	0.69	0/814
46	3	0.40	0/349	0.86	0/461
47	4	0.61	0/238	1.16	0/369
48	5	0.56	0/1837	1.20	3/2864 (0.1%)
48	6	0.60	1/1841 (0.1%)	1.20	4/2868 (0.1%)
49	7	0.61	0/1807	1.10	1/2816 (0.0%)
50	e	0.36	0/303	0.91	0/397
51	f	0.39	0/46	0.81	0/60
All	All	0.54	2/152130 (0.0%)	1.15	414/228839 (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	A	0	6
3	C	0	6
4	D	0	2
5	E	0	1
9	J	0	1
11	L	0	1
12	M	0	2
13	N	0	1
14	O	0	1
15	P	0	1
16	Q	0	1
17	R	0	2
22	W	0	4
23	X	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	a	0	1
27	b	0	2
29	d	0	1
32	m	0	2
33	n	0	2
36	q	0	5
38	t	0	4
39	u	0	3
All	All	0	51

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	6	1	C	OP3-P	-7.30	1.52	1.61
1	A	2069	G	C8-N7	5.36	1.34	1.30

All (414) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2061	G	O5'-P-OP2	-28.61	76.37	110.70
1	A	575	A	O5'-P-OP1	-20.21	86.45	110.70
1	A	1139	G	O5'-P-OP2	-18.09	88.99	110.70
1	A	1395	A	O5'-P-OP1	-17.95	89.16	110.70
1	A	2250	G	O5'-P-OP2	-17.42	89.80	110.70
1	A	2430	A	O5'-P-OP2	-17.30	89.93	110.70
1	A	2554	U	O5'-P-OP1	-17.17	90.10	110.70
1	A	819	A	O5'-P-OP1	-15.46	91.79	105.70
1	A	1253	A	O5'-P-OP1	-15.29	91.94	105.70
1	A	255	A	O5'-P-OP1	-14.51	92.64	105.70
1	A	2296	U	O3'-P-O5'	-14.45	76.55	104.00
1	A	685	A	O3'-P-O5'	-13.42	78.50	104.00
30	i	1519	A	O5'-P-OP2	-13.05	93.96	105.70
30	i	1494	G	O5'-P-OP2	-12.39	94.55	105.70
1	A	2602	A	O5'-P-OP2	-11.67	95.20	105.70
1	A	2061	G	O5'-P-OP1	11.60	124.62	110.70
1	A	961	C	O5'-P-OP2	-10.99	95.81	105.70
1	A	995	C	O5'-P-OP1	10.97	123.87	110.70
1	A	512	G	O4'-C1'-N9	10.75	116.80	108.20
1	A	1266	G	O5'-P-OP1	-10.73	96.04	105.70
1	A	686	U	O5'-P-OP1	10.68	123.52	110.70
1	A	574	A	O5'-P-OP1	-10.65	96.12	105.70
30	i	110	C	O5'-P-OP2	10.48	123.27	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	i	115	G	P-O3'-C3'	10.37	132.15	119.70
1	A	2022	U	O5'-P-OP1	-10.31	96.42	105.70
1	A	994	C	O3'-P-O5'	-10.12	84.77	104.00
1	A	2505	G	O5'-P-OP2	-10.03	96.67	105.70
3	C	221	ARG	NE-CZ-NH2	-9.99	115.30	120.30
1	A	2361	G	O5'-P-OP2	-9.98	96.72	105.70
30	i	500	G	O3'-P-O5'	-9.97	85.05	104.00
1	A	1352	U	O5'-P-OP2	-9.97	96.73	105.70
30	i	501	C	O3'-P-O5'	-9.97	85.06	104.00
2	B	99	A	O5'-P-OP1	-9.89	96.80	105.70
1	A	1811	G	O5'-P-OP2	-9.78	96.90	105.70
1	A	574	A	O5'-P-OP2	9.77	122.42	110.70
1	A	2430	A	O5'-P-OP1	9.58	122.19	110.70
30	i	889	A	O3'-P-O5'	-9.56	85.84	104.00
1	A	2033	A	O5'-P-OP2	-9.52	97.13	105.70
1	A	83	A	O3'-P-O5'	-9.43	86.08	104.00
1	A	2022	U	O5'-P-OP2	9.29	121.85	110.70
1	A	2065	C	O5'-P-OP2	-9.29	97.34	105.70
1	A	1939	U	P-O3'-C3'	-9.24	108.61	119.70
1	A	470	A	O5'-P-OP1	9.22	121.77	110.70
1	A	941	A	O5'-P-OP1	-9.07	97.54	105.70
1	A	2431	U	O5'-P-OP1	-9.06	97.55	105.70
1	A	1395	A	O5'-P-OP2	9.01	121.51	110.70
1	A	743	A	O5'-P-OP2	-8.97	97.63	105.70
1	A	996	A	O5'-P-OP1	-8.96	97.64	105.70
1	A	1790	C	O5'-P-OP2	-8.87	97.71	105.70
1	A	1940	U	O5'-P-OP2	-8.83	97.75	105.70
1	A	2848	G	O4'-C1'-N9	8.66	115.13	108.20
1	A	1394	U	OP1-P-O3'	8.59	124.09	105.20
1	A	1375	U	C5-C4-O4	8.58	131.05	125.90
1	A	1905	C	O5'-P-OP2	-8.56	98.00	105.70
1	A	2546	U	O3'-P-O5'	-8.52	87.81	104.00
30	i	1487	G	O5'-P-OP2	-8.48	98.07	105.70
1	A	1565	C	O3'-P-O5'	-8.44	87.96	104.00
1	A	1807	G	O5'-P-OP2	-8.43	98.11	105.70
1	A	746	PSU	P-O3'-C3'	8.41	129.80	119.70
1	A	329	G	O5'-P-OP2	-8.28	98.25	105.70
30	i	972	C	O5'-P-OP2	-8.25	98.28	105.70
17	R	80	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	1373	A	O3'-P-O5'	-8.17	88.47	104.00
30	i	22	G	O5'-P-OP2	-8.17	98.35	105.70
30	i	1529	G	O3'-P-O5'	-8.12	88.57	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	A	O3'-P-O5'	-8.12	88.58	104.00
1	A	1237	A	O3'-P-O5'	-8.09	88.64	104.00
1	A	940	G	O3'-P-O5'	8.05	119.29	104.00
1	A	575	A	O5'-P-OP2	8.04	120.35	110.70
1	A	2465	C	O5'-P-OP2	-7.98	98.51	105.70
30	i	1491	G	O3'-P-O5'	-7.98	88.83	104.00
1	A	329	G	O3'-P-O5'	-7.97	88.86	104.00
1	A	2268	A	O5'-P-OP2	-7.95	98.55	105.70
1	A	1238	G	O5'-P-OP1	7.86	120.13	110.70
1	A	2071	A	O5'-P-OP2	-7.77	98.71	105.70
1	A	1985	C	O5'-P-OP2	-7.75	98.73	105.70
1	A	2724	U	O5'-P-OP2	-7.72	98.75	105.70
1	A	1639	C	O5'-P-OP1	-7.68	98.79	105.70
30	i	773	G	O5'-P-OP2	-7.65	98.81	105.70
1	A	2452	C	O5'-P-OP2	-7.65	98.81	105.70
3	C	258	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	A	1025	G	O3'-P-O5'	7.61	118.45	104.00
1	A	1643	G	O3'-P-O5'	-7.57	89.61	104.00
1	A	2463	C	O5'-P-OP2	-7.48	98.97	105.70
1	A	2445	G	C2-N3-C4	7.48	115.64	111.90
1	A	959	A	O5'-P-OP1	-7.47	98.98	105.70
1	A	395	U	O4'-C1'-N1	7.42	114.14	108.20
1	A	1518	C	O3'-P-O5'	-7.42	89.90	104.00
1	A	370	G	O3'-P-O5'	-7.39	89.95	104.00
1	A	205	G	O5'-P-OP1	7.38	119.56	110.70
1	A	2608	G	O5'-P-OP2	-7.37	99.07	105.70
1	A	424	G	O5'-P-OP1	7.32	119.48	110.70
1	A	1905	C	O3'-P-O5'	-7.30	90.12	104.00
1	A	476	G	O5'-P-OP2	-7.30	99.13	105.70
30	i	1517	G	O5'-P-OP2	-7.30	99.13	105.70
30	i	1406	U	O5'-P-OP2	-7.29	99.14	105.70
1	A	2442	C	O5'-P-OP2	-7.25	99.17	105.70
1	A	1847	A	O3'-P-O5'	-7.24	90.25	104.00
1	A	2602	A	O5'-P-OP1	7.23	119.37	110.70
1	A	196	A	O5'-P-OP1	-7.21	99.21	105.70
1	A	2048	G	O5'-P-OP2	-7.17	99.24	105.70
1	A	1702	G	O3'-P-O5'	-7.09	90.53	104.00
1	A	1936	A	O4'-C1'-N9	7.03	113.83	108.20
30	i	561	U	O3'-P-O5'	-7.02	90.65	104.00
1	A	204	A	O3'-P-O5'	-6.99	90.72	104.00
1	A	747	U	O3'-P-O5'	-6.99	90.73	104.00
1	A	2353	G	O3'-P-O5'	-6.96	90.77	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	958	U	OP1-P-O3'	6.93	120.44	105.20
1	A	2278	A	O3'-P-O5'	-6.90	90.90	104.00
48	5	57	C	C2'-C3'-O3'	6.89	124.72	113.70
2	B	29	A	O5'-P-OP2	-6.89	99.50	105.70
1	A	198	C	O5'-P-OP1	-6.88	99.51	105.70
1	A	704	G	O4'-C1'-N9	6.85	113.68	108.20
1	A	1828	G	C5-C6-O6	-6.83	124.50	128.60
1	A	2006	C	O5'-P-OP2	-6.81	99.57	105.70
30	i	1201	A	P-O3'-C3'	6.79	127.85	119.70
30	i	251	G	O4'-C1'-N9	-6.73	102.82	108.20
1	A	2249	U	OP2-P-O3'	6.72	119.98	105.20
1	A	2578	G	O5'-P-OP1	-6.70	99.67	105.70
2	B	15	A	O4'-C1'-N9	6.70	113.56	108.20
1	A	2824	C	O5'-P-OP2	-6.70	99.67	105.70
1	A	1355	G	C4-C5-N7	-6.68	108.13	110.80
30	i	326	G	C5-C6-O6	-6.67	124.60	128.60
1	A	2524	G	O3'-P-O5'	-6.66	91.36	104.00
1	A	2545	G	O5'-P-OP2	-6.65	99.71	105.70
1	A	745	G	C5-C6-O6	-6.64	124.61	128.60
30	i	292	G	O5'-P-OP2	-6.61	99.75	105.70
1	A	2076	U	O4'-C1'-N1	6.61	113.48	108.20
1	A	1355	G	C5-C6-O6	6.55	132.53	128.60
30	i	352	C	O3'-P-O5'	-6.53	91.60	104.00
30	i	1279	G	O3'-P-O5'	-6.49	91.66	104.00
1	A	974	G	C5-C6-O6	-6.49	124.71	128.60
30	i	586	C	O5'-P-OP2	-6.46	99.88	105.70
1	A	2556	C	O5'-P-OP2	-6.46	99.89	105.70
1	A	1971	U	O3'-P-O5'	-6.45	91.75	104.00
48	6	47	U	P-O3'-C3'	6.44	127.43	119.70
48	6	56	C	C2'-C3'-O3'	6.44	124.00	113.70
1	A	372	G	O5'-P-OP1	-6.43	99.91	105.70
1	A	781	A	O3'-P-O5'	-6.43	91.78	104.00
1	A	831	G	O5'-P-OP1	-6.40	99.94	105.70
1	A	760	G	O5'-P-OP2	-6.38	99.96	105.70
1	A	1252	G	O3'-P-O5'	6.37	116.11	104.00
1	A	2354	C	O3'-P-O5'	-6.36	91.91	104.00
1	A	2391	G	O4'-C1'-N9	6.36	113.29	108.20
1	A	974	G	N1-C6-O6	6.36	123.72	119.90
1	A	2850	A	O5'-P-OP1	6.36	118.33	110.70
1	A	984	A	O4'-C1'-N9	6.35	113.28	108.20
1	A	1913	A	C2'-C3'-O3'	6.32	123.82	113.70
30	i	1494	G	O5'-P-OP1	6.31	118.27	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	48	U	O3'-P-O5'	-6.28	92.07	104.00
1	A	1355	G	N9-C4-C5	6.28	107.91	105.40
30	i	828	U	O5'-P-OP2	-6.28	100.05	105.70
1	A	2606	C	O5'-P-OP2	-6.27	100.05	105.70
30	i	1497	G	O5'-P-OP2	-6.27	100.06	105.70
30	i	1199	U	O3'-P-O5'	-6.26	92.10	104.00
30	i	1500	A	O5'-P-OP2	-6.25	100.08	105.70
1	A	46	G	O5'-P-OP2	-6.23	100.09	105.70
1	A	2064	C	OP2-P-O3'	6.22	118.89	105.20
1	A	528	A	O5'-P-OP1	6.21	118.16	110.70
1	A	1185	G	O5'-P-OP2	-6.21	100.11	105.70
1	A	667	U	O3'-P-O5'	-6.21	92.20	104.00
1	A	455	C	O5'-P-OP2	-6.20	100.12	105.70
1	A	2715	C	O5'-P-OP2	-6.19	100.13	105.70
1	A	464	U	O5'-P-OP2	-6.18	100.14	105.70
1	A	742	A	OP2-P-O3'	6.18	118.80	105.20
1	A	1969	A	O3'-P-O5'	-6.17	92.28	104.00
1	A	2074	U	O5'-P-OP2	-6.15	100.16	105.70
30	i	1190	G	O3'-P-O5'	-6.14	92.33	104.00
1	A	1913	A	P-O3'-C3'	6.13	127.06	119.70
30	i	986	U	O3'-P-O5'	-6.13	92.36	104.00
1	A	759	G	O5'-P-OP2	-6.13	100.19	105.70
1	A	1355	G	C5-C6-N1	-6.12	108.44	111.50
30	i	297	G	O3'-P-O5'	-6.08	92.45	104.00
1	A	404	A	P-O3'-C3'	6.07	126.99	119.70
1	A	1802	A	O5'-P-OP1	-6.07	100.23	105.70
30	i	124	C	O5'-P-OP2	-6.07	100.23	105.70
1	A	1663	G	O5'-P-OP2	-6.07	100.24	105.70
30	i	809	G	O5'-P-OP2	-6.07	100.24	105.70
1	A	2267	A	O4'-C1'-N9	-6.07	103.35	108.20
1	A	1378	A	O4'-C1'-N9	6.05	113.04	108.20
1	A	2496	C	P-O5'-C5'	-6.05	111.22	120.90
1	A	1975	G	O5'-P-OP2	-6.04	100.26	105.70
1	A	1131	G	O3'-P-O5'	-6.04	92.52	104.00
1	A	1906	G	O3'-P-O5'	-6.03	92.54	104.00
30	i	1530	G	O4'-C1'-N9	6.02	113.01	108.20
1	A	2747	G	O3'-P-O5'	-6.01	92.58	104.00
1	A	310	A	O3'-P-O5'	-6.01	92.58	104.00
1	A	748	G	C1'-O4'-C4'	-6.01	105.09	109.90
1	A	1452	G	O3'-P-O5'	-6.00	92.60	104.00
30	i	115	G	C4'-C3'-O3'	6.00	125.00	113.00
1	A	995	C	O5'-P-OP2	-5.98	100.32	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1324	G	O4'-C1'-N9	5.98	112.98	108.20
1	A	857	G	OP2-P-O3'	5.97	118.33	105.20
30	i	115	G	O3'-P-O5'	5.96	115.33	104.00
1	A	1925	C	O3'-P-O5'	-5.93	92.74	104.00
1	A	2389	G	O5'-P-OP2	-5.92	100.37	105.70
1	A	1210	G	C5-N7-C8	-5.91	101.35	104.30
1	A	31	C	O5'-P-OP2	-5.91	100.38	105.70
1	A	1800	C	O5'-P-OP2	-5.90	100.39	105.70
30	i	1405	G	OP2-P-O3'	5.90	118.17	105.20
1	A	370	G	O4'-C1'-N9	-5.89	103.49	108.20
1	A	479	A	C3'-C2'-C1'	-5.88	96.79	101.50
1	A	1358	G	O3'-P-O5'	-5.88	92.83	104.00
2	B	8	C	O3'-P-O5'	-5.88	92.83	104.00
1	A	2033	A	O5'-P-OP1	5.86	117.73	110.70
1	A	1936	A	C1'-O4'-C4'	-5.85	105.22	109.90
1	A	923	G	O5'-P-OP2	-5.84	100.44	105.70
1	A	1948	G	O5'-P-OP2	-5.80	100.48	105.70
1	A	2689	U	C5-C6-N1	-5.80	119.80	122.70
1	A	2026	U	O3'-P-O5'	-5.80	92.98	104.00
1	A	1706	C	O4'-C1'-N1	5.80	112.84	108.20
1	A	2069	G	C5-N7-C8	-5.79	101.41	104.30
1	A	2060	A	O3'-P-O5'	5.78	114.99	104.00
1	A	2445	G	N1-C2-N2	5.78	121.40	116.20
1	A	2873	A	C1'-O4'-C4'	-5.77	105.28	109.90
1	A	784	G	P-O3'-C3'	5.76	126.61	119.70
1	A	1261	C	O5'-P-OP2	-5.76	100.52	105.70
1	A	1265	A	O3'-P-O5'	5.76	114.94	104.00
1	A	2011	U	O5'-P-OP2	-5.75	100.52	105.70
1	A	2409	G	O3'-P-O5'	-5.75	93.07	104.00
1	A	792	A	O5'-P-OP2	-5.74	100.54	105.70
30	i	52	C	OP2-P-O3'	5.73	117.81	105.20
1	A	1138	G	O3'-P-O5'	5.73	114.88	104.00
12	M	16	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	745	G	N3-C2-N2	-5.72	115.89	119.90
1	A	967	U	O3'-P-O5'	-5.72	93.12	104.00
30	i	1228	C	O5'-P-OP2	-5.72	100.55	105.70
1	A	242	G	C3'-C2'-C1'	-5.70	96.94	101.50
37	s	122	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	1971	U	O4'-C1'-N1	5.68	112.75	108.20
30	i	816	A	O3'-P-O5'	-5.68	93.22	104.00
1	A	2641	G	C4'-C3'-C2'	-5.67	96.92	102.60
30	i	1362	A	OP2-P-O3'	5.67	117.67	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	15	A	C3'-C2'-C1'	-5.67	96.97	101.50
30	i	1367	C	O3'-P-O5'	-5.66	93.24	104.00
1	A	1896	G	O3'-P-O5'	-5.66	93.25	104.00
1	A	1929	G	O5'-P-OP1	5.65	117.48	110.70
1	A	1025	G	O4'-C1'-N9	-5.65	103.68	108.20
1	A	1983	G	OP2-P-O3'	5.64	117.61	105.20
1	A	2448	A	O5'-P-OP1	-5.64	100.62	105.70
3	C	221	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	2249	U	O5'-P-OP2	-5.59	100.67	105.70
1	A	1133	A	C1'-O4'-C4'	-5.59	105.43	109.90
30	i	727	G	O5'-P-OP2	-5.58	100.67	105.70
1	A	72	U	C3'-C2'-C1'	-5.58	97.04	101.50
23	X	28	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	A	62	U	O3'-P-O5'	-5.56	93.43	104.00
14	O	102	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	A	371	A	O5'-P-OP2	5.56	117.37	110.70
1	A	595	C	O5'-P-OP2	-5.55	100.70	105.70
1	A	2529	G	O4'-C1'-N9	-5.55	103.76	108.20
30	i	835	U	O3'-P-O5'	-5.55	93.45	104.00
37	s	127	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	376	G	O3'-P-O5'	-5.54	93.47	104.00
1	A	2595	G	O5'-P-OP2	-5.54	100.71	105.70
1	A	1939	U	O4'-C1'-N1	5.54	112.63	108.20
1	A	538	A	O5'-P-OP2	-5.53	100.72	105.70
30	i	827	U	O3'-P-O5'	5.53	114.50	104.00
1	A	729	G	C1'-O4'-C4'	-5.52	105.48	109.90
16	Q	58	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	2830	C	O5'-P-OP2	-5.51	100.75	105.70
1	A	2296	U	OP1-P-O3'	5.49	117.29	105.20
1	A	1890	A	O5'-P-OP2	-5.49	100.76	105.70
1	A	1142	A	O4'-C1'-N9	5.49	112.59	108.20
1	A	1154	G	O3'-P-O5'	-5.48	93.58	104.00
1	A	1638	C	OP2-P-O3'	5.48	117.25	105.20
30	i	356	A	OP1-P-O3'	5.48	117.25	105.20
1	A	1737	G	O3'-P-O5'	-5.48	93.59	104.00
30	i	536	C	O5'-P-OP2	-5.47	100.78	105.70
30	i	116	A	C5-N7-C8	-5.46	101.17	103.90
1	A	529	A	O3'-P-O5'	-5.45	93.64	104.00
1	A	1339	G	O5'-P-OP2	-5.45	100.79	105.70
1	A	2073	C	O4'-C1'-N1	5.45	112.56	108.20
1	A	1808	A	O4'-C1'-N9	-5.45	103.84	108.20
30	i	652	U	O3'-P-O5'	-5.44	93.67	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	G	O3'-P-O5'	-5.43	93.67	104.00
30	i	879	C	OP2-P-O3'	5.43	117.16	105.20
30	i	1092	A	O3'-P-O5'	-5.43	93.67	104.00
1	A	1767	G	OP2-P-O3'	5.43	117.15	105.20
30	i	820	U	O5'-P-OP2	-5.43	100.82	105.70
1	A	2447	G	O5'-P-OP1	-5.42	100.82	105.70
1	A	2030	A	C5-C6-N6	5.41	128.03	123.70
1	A	2879	A	O3'-P-O5'	-5.41	93.72	104.00
1	A	18	U	O5'-P-OP2	-5.40	100.84	105.70
1	A	2356	U	O3'-P-O5'	-5.40	93.73	104.00
1	A	2484	G	C4'-C3'-C2'	-5.40	97.20	102.60
30	i	126	G	O3'-P-O5'	-5.40	93.74	104.00
1	A	513	A	O5'-P-OP2	-5.40	100.84	105.70
1	A	1546	G	OP1-P-O3'	5.39	117.06	105.20
30	i	7	A	C1'-O4'-C4'	-5.39	105.59	109.90
1	A	1024	G	C5-C6-O6	-5.37	125.38	128.60
30	i	263	A	O3'-P-O5'	-5.37	93.81	104.00
1	A	2493	U	O3'-P-O5'	-5.36	93.81	104.00
1	A	2279	G	O3'-P-O5'	-5.36	93.82	104.00
1	A	745	G	C6-N1-C2	-5.36	121.89	125.10
1	A	1502	A	O3'-P-O5'	-5.36	93.83	104.00
1	A	2003	A	O3'-P-O5'	-5.35	93.83	104.00
30	i	1239	A	O3'-P-O5'	-5.35	93.83	104.00
30	i	1237	C	OP1-P-O3'	5.35	116.97	105.20
30	i	354	G	OP2-P-O3'	5.35	116.96	105.20
1	A	2282	G	O4'-C1'-N9	5.33	112.47	108.20
1	A	1135	C	OP1-P-O3'	5.32	116.91	105.20
30	i	352	C	OP2-P-O3'	5.32	116.90	105.20
34	o	2	PRO	CA-N-CD	-5.32	104.05	111.50
1	A	242	G	O3'-P-O5'	-5.32	93.90	104.00
30	i	1331	G	O4'-C1'-N9	5.32	112.45	108.20
1	A	2876	G	O5'-P-OP2	-5.32	100.92	105.70
30	i	691	G	O5'-P-OP2	-5.31	100.92	105.70
30	i	671	G	O5'-P-OP2	-5.31	100.92	105.70
1	A	2519	U	O3'-P-O5'	-5.30	93.93	104.00
2	B	16	G	O3'-P-O5'	-5.30	93.94	104.00
1	A	1130	U	O4'-C1'-N1	5.29	112.43	108.20
30	i	916	U	O5'-P-OP2	-5.28	100.94	105.70
1	A	2285	C	O4'-C1'-N1	5.28	112.43	108.20
30	i	872	A	C1'-O4'-C4'	-5.28	105.68	109.90
1	A	512	G	C1'-O4'-C4'	-5.28	105.68	109.90
1	A	1957	C	OP2-P-O3'	5.27	116.80	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	i	355	C	O3'-P-O5'	-5.27	93.98	104.00
30	i	901	A	O3'-P-O5'	-5.27	93.98	104.00
1	A	542	C	O3'-P-O5'	-5.27	93.99	104.00
1	A	2464	G	C2-N3-C4	-5.26	109.27	111.90
1	A	1765	U	OP2-P-O3'	5.26	116.78	105.20
1	A	2871	U	O3'-P-O5'	-5.25	94.02	104.00
1	A	1962	C	N3-C4-N4	-5.25	114.33	118.00
1	A	737	C	O3'-P-O5'	-5.25	94.03	104.00
1	A	2604	U	O4'-C1'-N1	5.24	112.39	108.20
30	i	243	A	OP1-P-O3'	5.24	116.74	105.20
1	A	2286	G	C5-N7-C8	-5.24	101.68	104.30
1	A	1253	A	O4'-C1'-N9	-5.24	104.01	108.20
30	i	362	G	O3'-P-O5'	-5.24	94.05	104.00
1	A	2601	C	O3'-P-O5'	-5.23	94.06	104.00
1	A	690	G	O5'-P-OP2	-5.23	100.99	105.70
1	A	994	C	OP2-P-O3'	5.22	116.70	105.20
1	A	2619	C	OP2-P-O3'	5.22	116.69	105.20
1	A	2453	A	O4'-C1'-N9	5.22	112.38	108.20
48	6	43	U	O4'-C1'-N1	5.21	112.37	108.20
1	A	2146	C	P-O3'-C3'	5.21	125.95	119.70
30	i	522	C	O5'-P-OP1	-5.21	101.01	105.70
3	C	11	PRO	N-CA-C	-5.21	98.56	112.10
1	A	1359	A	O3'-P-O5'	-5.21	94.11	104.00
1	A	1926	U	P-O5'-C5'	-5.21	112.57	120.90
1	A	1962	C	C2-N1-C1'	-5.20	113.08	118.80
1	A	2860	A	O3'-P-O5'	-5.20	94.12	104.00
1	A	942	G	O5'-P-OP2	-5.20	101.02	105.70
1	A	1674	G	C3'-C2'-C1'	5.19	105.65	101.50
1	A	2365	G	O5'-P-OP2	-5.18	101.03	105.70
30	i	690	G	O5'-P-OP2	-5.18	101.03	105.70
49	7	15	G	P-O3'-C3'	5.18	125.92	119.70
1	A	2267	A	OP1-P-O3'	5.18	116.59	105.20
1	A	2732	G	O4'-C1'-N9	5.17	112.34	108.20
1	A	784	G	OP1-P-O3'	5.17	116.58	105.20
1	A	2464	G	N9-C4-C5	-5.17	103.33	105.40
1	A	2495	G	OP2-P-O3'	5.17	116.58	105.20
1	A	199	A	C1'-O4'-C4'	-5.16	105.77	109.90
1	A	1939	U	C1'-O4'-C4'	-5.16	105.77	109.90
1	A	1394	U	O4'-C1'-N1	-5.16	104.07	108.20
1	A	323	C	O4'-C1'-N1	5.16	112.32	108.20
1	A	1827	U	O5'-P-OP2	-5.15	101.06	105.70
1	A	205	G	C3'-C2'-C1'	-5.15	97.38	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	i	977	A	O3'-P-O5'	-5.15	94.22	104.00
1	A	2430	A	C1'-O4'-C4'	-5.15	105.78	109.90
30	i	264	C	OP1-P-O3'	5.14	116.52	105.20
1	A	419	U	O3'-P-O5'	-5.14	94.23	104.00
1	A	1966	A	P-O3'-C3'	-5.14	113.53	119.70
1	A	2610	C	OP1-P-O3'	5.13	116.50	105.20
1	A	2566	A	O4'-C1'-N9	5.13	112.31	108.20
1	A	454	A	O4'-C1'-N9	-5.13	104.10	108.20
1	A	1808	A	O5'-P-OP2	-5.13	101.08	105.70
1	A	329	G	O5'-P-OP1	5.12	116.85	110.70
1	A	800	A	O4'-C1'-N9	-5.12	104.11	108.20
1	A	1947	C	OP2-P-O3'	5.11	116.44	105.20
48	5	3	G	C2'-C3'-O3'	5.11	121.87	113.70
30	i	786	G	O3'-P-O5'	-5.11	94.30	104.00
1	A	824	U	O5'-P-OP2	-5.10	101.11	105.70
1	A	2387	U	O5'-P-OP2	-5.10	101.11	105.70
1	A	84	A	C3'-C2'-C1'	-5.10	97.42	101.50
1	A	1962	C	C5-C4-N4	5.10	123.77	120.20
30	i	110	C	P-O5'-C5'	-5.10	112.74	120.90
30	i	408	A	C3'-C2'-C1'	5.09	105.58	101.50
1	A	202	U	O4'-C1'-N1	5.09	112.27	108.20
1	A	1645	G	OP1-P-O3'	5.09	116.39	105.20
30	i	1359	C	OP2-P-O3'	5.09	116.39	105.20
1	A	555	G	O3'-P-O5'	-5.08	94.34	104.00
30	i	12	U	O3'-P-O5'	-5.08	94.34	104.00
30	i	262	A	O3'-P-O5'	-5.08	94.34	104.00
1	A	84	A	O5'-P-OP2	5.07	116.79	110.70
1	A	1128	G	C1'-O4'-C4'	-5.07	105.84	109.90
1	A	1773	A	O4'-C1'-N9	5.06	112.25	108.20
1	A	2324	U	O3'-P-O5'	5.05	113.60	104.00
1	A	2286	G	C3'-C2'-C1'	5.05	105.54	101.50
1	A	1396	U	OP1-P-O3'	5.05	116.31	105.20
1	A	680	C	C6-N1-C2	-5.04	118.28	120.30
30	i	1429	A	O3'-P-O5'	-5.04	94.42	104.00
1	A	1902	C	O5'-P-OP2	-5.04	101.16	105.70
30	i	1352	C	O3'-P-O5'	-5.04	94.42	104.00
30	i	194	C	O3'-P-O5'	-5.04	94.42	104.00
48	6	46	G	C3'-C2'-C1'	5.04	105.53	101.50
1	A	2497	A	OP1-P-O3'	5.03	116.27	105.20
1	A	198	C	N3-C4-C5	-5.02	119.89	121.90
2	B	43	C	O3'-P-O5'	5.02	113.54	104.00
1	A	726	G	O3'-P-O5'	-5.02	94.47	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	i	331	G	OP1-P-O3'	5.02	116.24	105.20
1	A	907	G	O3'-P-O5'	-5.02	94.47	104.00
1	A	125	A	O5'-P-OP2	-5.01	101.19	105.70
30	i	1286	U	O3'-P-O5'	-5.01	94.47	104.00
30	i	322	C	O3'-P-O5'	-5.01	94.47	104.00
30	i	643	C	O3'-P-O5'	-5.01	94.48	104.00
1	A	855	G	O3'-P-O5'	-5.01	94.48	104.00
1	A	1342	A	O5'-P-OP2	-5.01	101.19	105.70
1	A	2366	A	O5'-P-OP2	-5.01	101.19	105.70
1	A	255	A	O4'-C1'-N9	5.01	112.21	108.20
1	A	1297	C	OP2-P-O3'	5.01	116.21	105.20
1	A	254	G	O3'-P-O5'	5.00	113.51	104.00
1	A	2447	G	C3'-C2'-C1'	-5.00	97.50	101.50

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1025	G	Sidechain
1	A	250	G	Sidechain
1	A	2595	G	Sidechain
1	A	395	U	Sidechain
1	A	463	G	Sidechain
1	A	512	G	Sidechain
3	C	109	GLY	Peptide
3	C	156	ARG	Sidechain
3	C	177	ARG	Sidechain
3	C	221	ARG	Sidechain
3	C	258	ARG	Sidechain
3	C	271	ARG	Sidechain
4	D	128	ARG	Sidechain
4	D	33	ARG	Sidechain
5	E	88	ARG	Sidechain
9	J	120	ARG	Sidechain
11	L	59	ARG	Sidechain
12	M	16	ARG	Sidechain
12	M	55	ARG	Sidechain
13	N	63	ARG	Sidechain
14	O	9	ARG	Sidechain
15	P	109	ARG	Sidechain
16	Q	51	ARG	Sidechain
17	R	79	ARG	Sidechain

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Mol	Chain	Res	Type	Group
17	R	80	ARG	Sidechain
22	W	20	ARG	Sidechain
22	W	39	ARG	Sidechain
22	W	55	ARG	Sidechain
22	W	77	ARG	Sidechain
23	X	16	ASN	Peptide
23	X	3	ARG	Sidechain
26	a	40	ARG	Sidechain
27	b	50	LYS	Peptide
27	b	6	ARG	Sidechain
29	d	13	ARG	Sidechain
32	m	138	ARG	Sidechain
32	m	93	ARG	Sidechain
33	n	38	ARG	Sidechain
33	n	79	ARG	Sidechain
36	q	123	ARG	Sidechain
36	q	124	ARG	Sidechain
36	q	33	ARG	Sidechain
36	q	45	ARG	Sidechain
36	q	99	ARG	Sidechain
38	t	114	ARG	Sidechain
38	t	36	ARG	Sidechain
38	t	83	ARG	Sidechain
38	t	99	ARG	Sidechain
39	u	101	ARG	Sidechain
39	u	107	ARG	Sidechain
39	u	90	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60998	0	30646	50	0
2	B	2529	0	1281	1	0
3	C	2082	0	2153	3	0
4	D	1565	0	1616	9	0
5	E	1552	0	1619	4	0
6	F	1410	0	1444	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1285	0	1341	3	0
8	H	359	0	381	1	0
9	J	1129	0	1162	4	0
10	K	938	0	1012	5	0
11	L	1045	0	1117	13	0
12	M	1074	0	1157	2	0
13	N	945	0	989	1	0
14	O	875	0	906	2	0
15	P	900	0	945	5	0
16	Q	941	0	1014	3	0
17	R	816	0	839	5	0
18	S	857	0	922	8	0
19	T	730	0	795	1	0
20	U	779	0	830	2	0
21	V	753	0	780	3	0
22	W	628	0	642	3	0
23	X	625	0	652	1	0
24	Y	509	0	543	2	0
25	Z	435	0	470	1	0
26	a	444	0	458	0	0
27	b	395	0	422	0	0
28	c	377	0	418	0	0
29	d	504	0	572	0	0
30	i	33015	0	16604	0	0
31	j	1679	0	1705	0	0
32	m	1105	0	1148	0	0
33	n	817	0	808	0	0
34	o	1181	0	1238	0	0
35	p	979	0	1031	0	0
36	q	1001	0	1044	0	0
37	s	877	0	887	0	0
38	t	922	0	978	0	0
39	u	867	0	921	0	0
40	v	774	0	824	0	0
41	w	687	0	702	0	0
42	y	648	0	691	0	0
43	z	455	0	478	0	0
44	1	594	0	610	1	0
45	2	612	0	650	0	0
46	3	346	0	369	3	0
47	4	214	0	111	1	0
48	5	1644	0	832	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	6	1648	0	831	2	0
49	7	1618	0	823	0	0
50	e	302	0	340	0	0
51	f	46	0	53	0	0
52	6	1	0	0	0	0
52	A	178	0	0	0	0
52	B	5	0	0	0	0
52	C	1	0	0	0	0
52	D	1	0	0	0	0
52	a	1	0	0	0	0
52	i	61	0	0	0	0
53	A	83	0	0	0	0
53	C	3	0	0	0	0
53	E	1	0	0	0	0
53	U	1	0	0	0	0
53	i	37	0	0	0	0
53	n	1	0	0	0	0
53	u	1	0	0	0	0
54	5	7	0	7	1	0
55	e	1	0	0	0	0
56	4	3	0	0	0	0
56	5	3	0	0	0	0
56	6	2	0	0	0	0
56	A	1006	0	0	0	0
56	B	10	0	0	0	0
56	C	14	0	0	0	0
56	D	2	0	0	0	0
56	E	3	0	0	0	0
56	L	4	0	0	0	0
56	N	3	0	0	0	0
56	T	1	0	0	0	0
56	a	4	0	0	0	0
56	d	4	0	0	0	0
56	f	3	0	0	0	0
56	i	176	0	0	0	0
56	s	1	0	0	0	0
All	All	141132	0	90811	119	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 (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3:37:PHE:O	46:3:41:PRO:HD2	1.76	0.84
48:5:8:U:H5	48:5:14:A:N7	1.86	0.73
18:S:59:GLU:HB3	18:S:66:ILE:HD11	1.78	0.65
1:A:1824:G:O2'	3:C:252:THR:HG21	1.97	0.64
54:5:101:PRO:N	48:6:76:A:HO2'	1.97	0.62
20:U:72:ILE:HD12	20:U:96:PHE:CE1	2.37	0.60
48:5:8:U:O5'	48:5:8:U:O2	2.20	0.59
11:L:77:ILE:HD13	11:L:108:ALA:HB1	1.85	0.58
5:E:4:VAL:HA	5:E:11:ALA:HA	1.86	0.58
16:Q:88:VAL:HG13	17:R:48:LYS:HE2	1.86	0.57
1:A:636:G:C6	11:L:111:ILE:HD11	2.40	0.56
1:A:2324:U:H3'	1:A:2325:G:H5''	1.86	0.56
1:A:1266:G:H5''	18:S:15:GLN:HE22	1.71	0.56
1:A:1993:U:H4'	4:D:133:THR:HG22	1.88	0.55
1:A:2032:G:O2'	4:D:150:GLN:NE2	2.39	0.55
21:V:6:ALA:HB1	21:V:40:ILE:HG23	1.88	0.54
18:S:72:THR:HG21	18:S:108:SER:HB3	1.89	0.54
3:C:29:PRO:HG2	3:C:34:LEU:HD11	1.89	0.54
20:U:7:ARG:O	20:U:25:VAL:O	2.26	0.54
44:1:31:LEU:HB2	44:1:49:ILE:HG22	1.89	0.53
8:H:5:LEU:HD11	8:H:12:LEU:HD23	1.90	0.53
1:A:811:U:H2'	11:L:21:ARG:HA	1.92	0.51
3:C:107:PRO:HD2	3:C:110:LEU:HD22	1.92	0.51
4:D:156:PHE:CE1	9:J:81:ILE:HD13	2.45	0.51
46:3:37:PHE:O	46:3:41:PRO:CD	2.52	0.51
1:A:1932:A:H2'	1:A:1933:G:O4'	2.11	0.51
17:R:51:VAL:HB	17:R:52:PRO:HD2	1.92	0.50
6:F:25:VAL:O	6:F:28:VAL:HG12	2.12	0.50
11:L:85:VAL:HB	11:L:94:THR:HG22	1.93	0.50
18:S:59:GLU:HA	18:S:64:ALA:HA	1.94	0.50
9:J:110:PRO:O	9:J:115:GLY:HA3	2.12	0.49
5:E:149:ILE:HG22	5:E:192:ALA:HB1	1.94	0.48
15:P:43:PHE:CE1	15:P:63:LYS:HE2	2.47	0.48
1:A:2273:A:H2'	1:A:2274:A:C8	2.46	0.48
11:L:77:ILE:CD1	11:L:108:ALA:HB1	2.42	0.48
11:L:95:LEU:HD11	11:L:125:LEU:HD21	1.95	0.48
1:A:954:G:OP2	12:M:16:ARG:NH2	2.38	0.48
17:R:48:LYS:HE3	17:R:49:ILE:O	2.14	0.47
18:S:55:ILE:HG23	18:S:66:ILE:HD12	1.96	0.47
5:E:5:LEU:HD23	5:E:120:VAL:HG12	1.96	0.47
4:D:4:LEU:HD22	4:D:32:ASN:HB2	1.97	0.47
11:L:110:VAL:O	11:L:111:ILE:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:125:TYR:OH	9:J:132:HIS:NE2	2.44	0.47
1:A:1296:G:OP1	1:A:2709:G:O2'	2.26	0.47
11:L:77:ILE:HD11	11:L:101:ILE:HG21	1.97	0.47
4:D:35:THR:HG22	4:D:73:VAL:HG21	1.96	0.46
7:G:164:TYR:HB2	7:G:167:GLU:HG3	1.97	0.46
48:5:8:U:C5	48:5:14:A:N7	2.75	0.46
11:L:70:LYS:O	11:L:74:THR:HG23	2.15	0.46
1:A:1853:A:N1	1:A:2087:G:H1'	2.30	0.46
1:A:2395:C:H2'	1:A:2396:G:O4'	2.16	0.46
11:L:77:ILE:N	11:L:77:ILE:HD12	2.30	0.46
1:A:494:G:H4'	18:S:6:LYS:HB2	1.98	0.46
1:A:1980:G:O2'	1:A:1982:U:OP2	2.33	0.46
13:N:79:LEU:O	13:N:80:PHE:HB2	2.16	0.46
1:A:493:G:H2'	1:A:494:G:O4'	2.16	0.46
21:V:4:ILE:CG2	21:V:42:LEU:HD22	2.46	0.46
1:A:1434:A:H2'	1:A:1435:G:C8	2.50	0.45
1:A:2532:G:O2'	1:A:2657:A:N1	2.49	0.45
7:G:24:ILE:HD11	7:G:43:VAL:HG11	1.97	0.45
10:K:91:SER:O	10:K:93:GLN:N	2.49	0.45
1:A:1378:A:O2'	1:A:1380:G:N7	2.50	0.45
5:E:189:THR:O	5:E:192:ALA:HB3	2.16	0.44
1:A:1434:A:H2'	1:A:1435:G:H8	1.81	0.44
1:A:118:A:N3	1:A:178:G:H1'	2.33	0.44
1:A:788:A:OP1	1:A:790:U:H5	2.01	0.44
1:A:1007:C:OP1	9:J:39:LYS:HD2	2.18	0.44
19:T:8:LEU:HD11	24:Y:22:LEU:HB2	2.00	0.44
1:A:476:G:H4'	1:A:502:A:N1	2.33	0.44
11:L:74:THR:HG22	11:L:107:PHE:HB2	1.99	0.44
1:A:636:G:C5	11:L:111:ILE:HD11	2.53	0.43
14:O:34:HIS:HA	14:O:53:THR:OG1	2.17	0.43
10:K:76:VAL:HG12	15:P:73:VAL:HB	2.00	0.43
1:A:1182:G:H2'	1:A:1183:U:O4'	2.19	0.43
1:A:2356:U:H4'	22:W:20:ARG:HG3	2.01	0.43
1:A:1721:G:N2	1:A:1738:G:O2'	2.52	0.43
25:Z:24:LEU:HD11	25:Z:54:MET:CE	2.49	0.43
16:Q:76:TYR:CZ	16:Q:80:ILE:HG13	2.54	0.43
1:A:411:G:P	1:A:2407:A:OP2	2.77	0.42
1:A:207:A:H2'	1:A:208:C:O4'	2.19	0.42
24:Y:7:ARG:O	24:Y:8:GLU:C	2.58	0.42
4:D:12:THR:CG2	15:P:5:ILE:HG23	2.49	0.42
1:A:644:A:H2'	1:A:645:C:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1664:A:N3	10:K:67:LYS:NZ	2.68	0.42
1:A:1340:U:C5	1:A:1603:A:C8	3.07	0.42
18:S:20:VAL:HG11	18:S:44:ALA:HA	2.01	0.42
1:A:639:U:H2'	1:A:640:C:C6	2.55	0.42
1:A:2019:A:H4'	16:Q:34:VAL:HG21	2.02	0.42
1:A:2038:G:H2'	1:A:2039:U:O4'	2.20	0.42
1:A:1141:U:H4'	1:A:1142:A:O4'	2.20	0.41
6:F:57:LEU:HD23	6:F:57:LEU:HA	1.94	0.41
10:K:63:VAL:HG12	10:K:107:LEU:HD11	2.01	0.41
46:3:16:LEU:H	46:3:16:LEU:HG	1.51	0.41
1:A:2063:C:O2	1:A:2450:A:N1	2.53	0.41
1:A:1020:A:N1	1:A:1141:U:O2'	2.43	0.41
1:A:1614:A:C2	18:S:93:ALA:HB2	2.55	0.41
7:G:121:ILE:HD12	7:G:141:ILE:CG2	2.50	0.41
10:K:41:ILE:HD11	10:K:86:LEU:HD22	2.02	0.41
1:A:861:A:H2'	1:A:862:G:O4'	2.20	0.41
17:R:5:PHE:HB3	17:R:59:ILE:HD12	2.01	0.41
1:A:1320:C:N3	1:A:1331:G:O6	2.54	0.41
1:A:1993:U:H4'	4:D:133:THR:CG2	2.50	0.41
15:P:106:LYS:O	15:P:109:ARG:HG2	2.21	0.41
23:X:7:VAL:HG23	23:X:51:VAL:HG12	2.02	0.41
1:A:1913:A:C6	48:5:39:A:H5'	2.56	0.41
4:D:5:VAL:HB	4:D:32:ASN:HD21	1.85	0.41
22:W:37:ILE:HG21	22:W:80:ILE:HG21	2.02	0.41
1:A:12:U:O2	1:A:12:U:H2'	2.21	0.41
4:D:5:VAL:H	4:D:32:ASN:ND2	2.18	0.41
17:R:14:VAL:HG21	17:R:20:VAL:HG21	2.03	0.41
47:4:18:G:H1	48:6:34:U:H3	1.69	0.41
1:A:2295:C:OP2	14:O:9:ARG:NH2	2.55	0.40
11:L:59:ARG:HG2	11:L:59:ARG:HH11	1.87	0.40
1:A:1794:A:H2'	1:A:1795:C:C6	2.57	0.40
1:A:1754:A:C8	15:P:94:LYS:CE	3.04	0.40
2:B:76:G:OP1	21:V:9:ARG:NH1	2.47	0.40
12:M:66:ARG:NH1	12:M:104:GLU:OE2	2.52	0.40
1:A:2271:G:H5'	22:W:20:ARG:HD2	2.03	0.40
1:A:2469:A:H2'	1:A:2470:G:O4'	2.21	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	
3	C	269/273 (98%)	256 (95%)	13 (5%)	0	100	100
4	D	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
5	E	199/201 (99%)	188 (94%)	10 (5%)	1 (0%)	25	28
6	F	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
7	G	167/177 (94%)	158 (95%)	9 (5%)	0	100	100
8	H	45/149 (30%)	42 (93%)	2 (4%)	1 (2%)	5	3
9	J	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
10	K	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
11	L	141/144 (98%)	133 (94%)	7 (5%)	1 (1%)	19	19
12	M	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
13	N	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
14	O	112/117 (96%)	107 (96%)	5 (4%)	0	100	100
15	P	110/115 (96%)	107 (97%)	3 (3%)	0	100	100
16	Q	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	R	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
18	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
19	T	90/100 (90%)	88 (98%)	2 (2%)	0	100	100
20	U	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
21	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
22	W	82/85 (96%)	80 (98%)	2 (2%)	0	100	100
23	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
24	Y	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
25	Z	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
26	a	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
27	b	46/55 (84%)	46 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	c	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
29	d	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	j	213/241 (88%)	187 (88%)	25 (12%)	1 (0%)	25	28
32	m	148/167 (89%)	139 (94%)	9 (6%)	0	100	100
33	n	98/135 (73%)	88 (90%)	10 (10%)	0	100	100
34	o	149/179 (83%)	136 (91%)	13 (9%)	0	100	100
35	p	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
36	q	123/130 (95%)	105 (85%)	16 (13%)	2 (2%)	8	6
37	s	115/129 (89%)	106 (92%)	8 (7%)	1 (1%)	14	14
38	t	117/124 (94%)	103 (88%)	13 (11%)	1 (1%)	14	14
39	u	110/118 (93%)	100 (91%)	10 (9%)	0	100	100
40	v	92/101 (91%)	87 (95%)	3 (3%)	2 (2%)	5	3
41	w	84/89 (94%)	82 (98%)	2 (2%)	0	100	100
42	y	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
43	z	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
44	1	72/92 (78%)	71 (99%)	1 (1%)	0	100	100
45	2	74/87 (85%)	71 (96%)	3 (4%)	0	100	100
46	3	40/71 (56%)	39 (98%)	1 (2%)	0	100	100
50	e	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4	2
51	f	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	4751/5225 (91%)	4480 (94%)	260 (6%)	11 (0%)	45	52

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	190	ALA
11	L	111	ILE
37	s	119	ASN
40	v	23	LYS
36	q	51	PRO
36	q	91	ASP
50	e	37	GLN
8	H	15	LEU
31	j	123	ASP
38	t	17	ALA

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Mol	Chain	Res	Type
40	v	32	SER

### 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	
3	C	216/218 (99%)	215 (100%)	1 (0%)	86	93
4	D	164/164 (100%)	164 (100%)	0	100	100
5	E	165/165 (100%)	164 (99%)	1 (1%)	84	91
6	F	148/150 (99%)	147 (99%)	1 (1%)	81	90
7	G	133/138 (96%)	132 (99%)	1 (1%)	79	88
8	H	38/114 (33%)	37 (97%)	1 (3%)	41	54
9	J	116/116 (100%)	115 (99%)	1 (1%)	75	86
10	K	103/104 (99%)	102 (99%)	1 (1%)	73	84
11	L	102/103 (99%)	102 (100%)	0	100	100
12	M	109/109 (100%)	107 (98%)	2 (2%)	54	69
13	N	98/103 (95%)	98 (100%)	0	100	100
14	O	84/87 (97%)	83 (99%)	1 (1%)	67	80
15	P	97/100 (97%)	96 (99%)	1 (1%)	73	84
16	Q	89/90 (99%)	89 (100%)	0	100	100
17	R	84/84 (100%)	83 (99%)	1 (1%)	67	80
18	S	93/93 (100%)	91 (98%)	2 (2%)	47	61
19	T	79/84 (94%)	79 (100%)	0	100	100
20	U	83/85 (98%)	83 (100%)	0	100	100
21	V	78/78 (100%)	78 (100%)	0	100	100
22	W	61/63 (97%)	61 (100%)	0	100	100
23	X	67/68 (98%)	67 (100%)	0	100	100
24	Y	55/55 (100%)	55 (100%)	0	100	100
25	Z	47/49 (96%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	a	47/48 (98%)	47 (100%)	0	100	100
27	b	44/49 (90%)	42 (96%)	2 (4%)	23	30
28	c	38/38 (100%)	38 (100%)	0	100	100
29	d	51/52 (98%)	50 (98%)	1 (2%)	50	65
31	j	177/199 (89%)	172 (97%)	5 (3%)	38	51
32	m	113/126 (90%)	112 (99%)	1 (1%)	75	86
33	n	87/116 (75%)	86 (99%)	1 (1%)	70	82
34	o	124/147 (84%)	122 (98%)	2 (2%)	58	73
35	p	104/105 (99%)	102 (98%)	2 (2%)	52	67
36	q	103/107 (96%)	97 (94%)	6 (6%)	17	20
37	s	90/99 (91%)	88 (98%)	2 (2%)	47	61
38	t	100/104 (96%)	95 (95%)	5 (5%)	20	26
39	u	90/96 (94%)	88 (98%)	2 (2%)	47	61
40	v	79/84 (94%)	75 (95%)	4 (5%)	20	25
41	w	73/77 (95%)	73 (100%)	0	100	100
42	y	74/78 (95%)	73 (99%)	1 (1%)	62	77
43	z	48/65 (74%)	47 (98%)	1 (2%)	48	63
44	1	65/79 (82%)	65 (100%)	0	100	100
45	2	60/66 (91%)	59 (98%)	1 (2%)	56	71
46	3	35/61 (57%)	31 (89%)	4 (11%)	4	4
50	e	34/34 (100%)	34 (100%)	0	100	100
51	f	5/5 (100%)	5 (100%)	0	100	100
All	All	3950/4255 (93%)	3896 (99%)	54 (1%)	62	77

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	43	ARG
5	E	5	LEU
6	F	83	TYR
7	G	168	VAL
8	H	5	LEU
9	J	96	ARG
10	K	98	ARG

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Mol	Chain	Res	Type
12	M	59	ARG
12	M	84	LYS
14	O	25	ARG
15	P	53	ARG
17	R	71	LYS
18	S	29	VAL
18	S	69	LEU
27	b	10	LYS
27	b	28	ARG
29	d	31	HIS
31	j	23	TRP
31	j	40	ILE
31	j	43	LEU
31	j	50	PHE
31	j	151	ILE
32	m	52	LYS
33	n	1	MET
34	o	5	ARG
34	o	131	LYS
35	p	51	VAL
35	p	67	GLN
36	q	30	ILE
36	q	46	MET
36	q	48	VAL
36	q	52	LEU
36	q	98	LEU
36	q	106	ARG
37	s	119	ASN
37	s	126	LYS
38	t	16	VAL
38	t	18	LYS
38	t	36	ARG
38	t	75	GLN
38	t	80	ILE
39	u	63	PHE
39	u	107	ARG
40	v	10	GLU
40	v	24	ARG
40	v	33	ASP
40	v	42	TRP
42	y	4	LYS
43	z	66	SER

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Mol	Chain	Res	Type
45	2	54	MET
46	3	16	LEU
46	3	17	ARG
46	3	25	LYS
46	3	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	226	ASN
4	D	32	ASN
4	D	150	GLN
5	E	94	GLN
5	E	163	ASN
7	G	143	GLN
10	K	3	GLN
13	N	62	ASN
14	O	38	GLN
18	S	15	GLN
19	T	15	HIS
20	U	66	GLN
21	V	49	ASN
23	X	16	ASN
23	X	17	ASN
24	Y	15	ASN
26	a	5	GLN
28	c	13	ASN
31	j	19	GLN
31	j	89	GLN
31	j	103	ASN
31	j	146	ASN
32	m	12	GLN
32	m	89	HIS
34	o	28	ASN
34	o	148	ASN
38	t	5	ASN
38	t	75	GLN
40	v	43	ASN
41	w	37	ASN
45	2	48	GLN
45	2	52	ASN
50	e	35	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2837/2903 (97%)	345 (12%)	55 (1%)
2	B	117/120 (97%)	13 (11%)	1 (0%)
30	i	1538/1540 (99%)	280 (18%)	0
47	4	9/10 (90%)	0	0
48	5	76/77 (98%)	15 (19%)	4 (5%)
48	6	76/77 (98%)	11 (14%)	4 (5%)
49	7	75/76 (98%)	28 (37%)	3 (4%)
All	All	4728/4803 (98%)	692 (14%)	67 (1%)

All (692) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	34	U
1	A	46	G
1	A	61	C
1	A	71	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	96	C
1	A	101	A
1	A	103	A
1	A	118	A
1	A	119	A
1	A	120	U
1	A	138	U
1	A	139	U
1	A	163	C
1	A	165	A
1	A	181	A
1	A	196	A
1	A	199	A
1	A	200	U
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	233	A
1	A	248	G

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Mol	Chain	Res	Type
1	A	255	A
1	A	266	G
1	A	271	G
1	A	276	U
1	A	281	C
1	A	285	G
1	A	311	A
1	A	329	G
1	A	330	A
1	A	353	C
1	A	361	G
1	A	367	G
1	A	371	A
1	A	372	G
1	A	386	G
1	A	403	U
1	A	405	U
1	A	411	G
1	A	412	A
1	A	420	C
1	A	424	G
1	A	451	U
1	A	456	C
1	A	481	G
1	A	491	G
1	A	503	A
1	A	504	A
1	A	505	A
1	A	509	C
1	A	530	G
1	A	531	C
1	A	532	A
1	A	533	G
1	A	544	C
1	A	546	U
1	A	547	A
1	A	548	G
1	A	549	G
1	A	550	C
1	A	563	A
1	A	573	U
1	A	575	A

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Mol	Chain	Res	Type
1	A	586	A
1	A	603	A
1	A	614	A
1	A	627	A
1	A	637	A
1	A	645	C
1	A	647	G
1	A	654	A
1	A	655	A
1	A	686	U
1	A	717	C
1	A	730	A
1	A	747	U
1	A	764	A
1	A	765	C
1	A	775	G
1	A	776	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	792	A
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	845	A
1	A	846	U
1	A	858	G
1	A	877	A
1	A	878	A
1	A	882	G
1	A	884	U
1	A	885	C
1	A	896	A
1	A	897	C
1	A	910	A
1	A	914	G
1	A	915	C
1	A	931	U
1	A	934	U
1	A	941	A

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Mol	Chain	Res	Type
1	A	946	C
1	A	961	C
1	A	968	C
1	A	974	G
1	A	983	A
1	A	984	A
1	A	985	C
1	A	995	C
1	A	996	A
1	A	1012	U
1	A	1013	C
1	A	1022	G
1	A	1026	G
1	A	1033	U
1	A	1040	A
1	A	1046	A
1	A	1047	G
1	A	1109	C
1	A	1110	G
1	A	1112	G
1	A	1128	G
1	A	1129	A
1	A	1132	U
1	A	1133	A
1	A	1135	C
1	A	1136	G
1	A	1139	G
1	A	1142	A
1	A	1173	U
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1178	C
1	A	1187	G
1	A	1238	G
1	A	1253	A
1	A	1256	G
1	A	1266	G
1	A	1271	G
1	A	1272	A
1	A	1273	U

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Mol	Chain	Res	Type
1	A	1301	A
1	A	1352	U
1	A	1365	A
1	A	1379	U
1	A	1383	A
1	A	1395	A
1	A	1416	G
1	A	1428	C
1	A	1452	G
1	A	1453	A
1	A	1460	U
1	A	1482	G
1	A	1493	C
1	A	1504	A
1	A	1508	A
1	A	1509	A
1	A	1510	G
1	A	1515	A
1	A	1531	C
1	A	1533	C
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1538	G
1	A	1569	A
1	A	1578	U
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1608	A
1	A	1609	A
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1674	G
1	A	1715	G
1	A	1729	U
1	A	1730	C
1	A	1732	C
1	A	1738	G
1	A	1739	A

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Mol	Chain	Res	Type
1	A	1764	C
1	A	1773	A
1	A	1782	U
1	A	1800	C
1	A	1801	A
1	A	1807	G
1	A	1808	A
1	A	1811	G
1	A	1816	C
1	A	1829	A
1	A	1848	A
1	A	1870	C
1	A	1871	A
1	A	1873	G
1	A	1906	G
1	A	1914	C
1	A	1926	U
1	A	1929	G
1	A	1930	G
1	A	1937	A
1	A	1938	A
1	A	1955	U
1	A	1965	C
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1982	U
1	A	1991	U
1	A	1993	U
1	A	1997	C
1	A	2022	U
1	A	2023	C
1	A	2031	A
1	A	2033	A
1	A	2043	C
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2069	G
1	A	2098	U

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Mol	Chain	Res	Type
1	A	2102	G
1	A	2109	U
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2115	G
1	A	2118	U
1	A	2119	A
1	A	2120	G
1	A	2125	G
1	A	2126	A
1	A	2127	G
1	A	2128	G
1	A	2130	U
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2136	G
1	A	2137	U
1	A	2143	C
1	A	2146	C
1	A	2147	A
1	A	2148	G
1	A	2152	G
1	A	2157	G
1	A	2158	A
1	A	2159	G
1	A	2160	C
1	A	2163	A
1	A	2164	C
1	A	2165	C
1	A	2168	G
1	A	2170	A
1	A	2171	A
1	A	2172	U
1	A	2173	A
1	A	2174	C
1	A	2178	C
1	A	2198	A
1	A	2204	G
1	A	2211	A

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Mol	Chain	Res	Type
1	A	2225	A
1	A	2238	G
1	A	2239	G
1	A	2268	A
1	A	2283	C
1	A	2287	A
1	A	2297	A
1	A	2305	U
1	A	2308	G
1	A	2312	U
1	A	2322	A
1	A	2325	G
1	A	2333	A
1	A	2335	A
1	A	2347	C
1	A	2355	G
1	A	2372	U
1	A	2383	G
1	A	2385	C
1	A	2396	G
1	A	2402	U
1	A	2406	A
1	A	2407	A
1	A	2425	A
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2435	A
1	A	2441	U
1	A	2448	A
1	A	2478	A
1	A	2502	G
1	A	2505	G
1	A	2518	A
1	A	2529	G
1	A	2547	A
1	A	2554	U
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2574	G
1	A	2602	A

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Mol	Chain	Res	Type
1	A	2608	G
1	A	2609	U
1	A	2613	U
1	A	2629	U
1	A	2663	G
1	A	2689	U
1	A	2690	U
1	A	2714	G
1	A	2724	U
1	A	2726	A
1	A	2744	G
1	A	2748	A
1	A	2757	A
1	A	2778	A
1	A	2791	G
1	A	2798	U
1	A	2799	A
1	A	2820	A
1	A	2821	A
1	A	2867	G
1	A	2884	U
1	A	2903	U
2	B	25	U
2	B	34	A
2	B	35	C
2	B	44	G
2	B	45	A
2	B	53	A
2	B	56	G
2	B	57	A
2	B	67	G
2	B	89	U
2	B	90	C
2	B	99	A
2	B	109	A
30	i	3	A
30	i	4	U
30	i	5	U
30	i	6	G
30	i	7	A
30	i	8	A
30	i	9	G

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Mol	Chain	Res	Type
30	i	22	G
30	i	32	A
30	i	37	U
30	i	39	G
30	i	47	C
30	i	48	C
30	i	51	A
30	i	52	C
30	i	64	G
30	i	65	A
30	i	66	A
30	i	72	A
30	i	81	A
30	i	83	C
30	i	84	U
30	i	85	U
30	i	86	G
30	i	87	C
30	i	88	U
30	i	89	U
30	i	92	U
30	i	94	G
30	i	95	C
30	i	98	A
30	i	115	G
30	i	116	A
30	i	120	A
30	i	121	U
30	i	126	G
30	i	127	G
30	i	131	A
30	i	146	G
30	i	154	U
30	i	164	G
30	i	181	A
30	i	182	A
30	i	197	A
30	i	202	G
30	i	208	U
30	i	209	U
30	i	210	C
30	i	212	G

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Mol	Chain	Res	Type
30	i	214	C
30	i	226	G
30	i	245	U
30	i	247	G
30	i	251	G
30	i	266	G
30	i	267	C
30	i	289	G
30	i	306	A
30	i	321	A
30	i	328	C
30	i	329	A
30	i	330	C
30	i	332	G
30	i	348	G
30	i	352	C
30	i	354	G
30	i	355	C
30	i	360	G
30	i	366	A
30	i	367	U
30	i	368	U
30	i	369	G
30	i	372	C
30	i	383	A
30	i	389	A
30	i	392	C
30	i	393	A
30	i	395	C
30	i	397	A
30	i	398	U
30	i	399	G
30	i	406	G
30	i	408	A
30	i	409	U
30	i	411	A
30	i	412	A
30	i	413	G
30	i	414	A
30	i	415	A
30	i	417	G
30	i	421	U

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Mol	Chain	Res	Type
30	i	422	C
30	i	423	G
30	i	424	G
30	i	425	G
30	i	427	U
30	i	429	U
30	i	433	G
30	i	437	U
30	i	438	U
30	i	443	C
30	i	446	G
30	i	447	G
30	i	448	A
30	i	449	G
30	i	451	A
30	i	452	A
30	i	453	G
30	i	459	A
30	i	467	U
30	i	468	A
30	i	478	A
30	i	479	U
30	i	480	U
30	i	481	G
30	i	482	A
30	i	484	G
30	i	486	U
30	i	493	A
30	i	494	G
30	i	496	A
30	i	501	C
30	i	502	A
30	i	511	C
30	i	518	C
30	i	521	G
30	i	527	G
30	i	530	G
30	i	531	U
30	i	533	A
30	i	536	C
30	i	547	A
30	i	548	G

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Mol	Chain	Res	Type
30	i	559	A
30	i	562	U
30	i	572	A
30	i	573	A
30	i	576	C
30	i	577	G
30	i	588	G
30	i	596	A
30	i	620	C
30	i	633	G
30	i	639	G
30	i	650	G
30	i	653	U
30	i	654	G
30	i	665	A
30	i	718	A
30	i	721	G
30	i	723	U
30	i	724	G
30	i	734	G
30	i	747	A
30	i	755	G
30	i	777	A
30	i	793	U
30	i	794	A
30	i	815	A
30	i	817	C
30	i	821	G
30	i	828	U
30	i	841	C
30	i	842	U
30	i	843	U
30	i	844	G
30	i	845	A
30	i	846	G
30	i	851	G
30	i	887	G
30	i	914	A
30	i	922	G
30	i	926	G
30	i	934	C
30	i	935	A

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Mol	Chain	Res	Type
30	i	960	U
30	i	961	U
30	i	966	G
30	i	969	A
30	i	971	G
30	i	975	A
30	i	976	G
30	i	977	A
30	i	983	A
30	i	993	G
30	i	1003	G
30	i	1004	A
30	i	1005	A
30	i	1008	U
30	i	1009	U
30	i	1014	A
30	i	1018	G
30	i	1020	G
30	i	1022	A
30	i	1023	U
30	i	1026	G
30	i	1027	C
30	i	1028	C
30	i	1030	U
30	i	1032	G
30	i	1033	G
30	i	1039	G
30	i	1043	G
30	i	1045	C
30	i	1046	A
30	i	1053	G
30	i	1065	U
30	i	1085	U
30	i	1094	G
30	i	1095	U
30	i	1101	A
30	i	1124	G
30	i	1130	A
30	i	1132	C
30	i	1134	G
30	i	1137	C
30	i	1139	G

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Mol	Chain	Res	Type
30	i	1140	C
30	i	1141	C
30	i	1143	G
30	i	1145	A
30	i	1159	U
30	i	1167	A
30	i	1168	U
30	i	1171	A
30	i	1184	G
30	i	1196	A
30	i	1197	A
30	i	1200	C
30	i	1202	U
30	i	1212	U
30	i	1213	A
30	i	1225	A
30	i	1226	C
30	i	1227	A
30	i	1228	C
30	i	1238	A
30	i	1256	A
30	i	1257	A
30	i	1258	G
30	i	1260	G
30	i	1275	A
30	i	1280	A
30	i	1286	U
30	i	1287	A
30	i	1299	A
30	i	1300	G
30	i	1302	C
30	i	1305	G
30	i	1317	C
30	i	1320	C
30	i	1335	U
30	i	1336	C
30	i	1337	G
30	i	1338	G
30	i	1346	A
30	i	1353	G
30	i	1362	A
30	i	1363	A

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Mol	Chain	Res	Type
30	i	1370	G
30	i	1379	G
30	i	1381	U
30	i	1419	G
30	i	1446	A
30	i	1487	G
30	i	1492	A
30	i	1494	G
30	i	1497	G
30	i	1503	A
30	i	1505	G
30	i	1506	U
30	i	1517	G
30	i	1529	G
30	i	1530	G
30	i	1533	C
30	i	1534	A
30	i	1535	C
30	i	1537	U
30	i	1538	C
30	i	1539	C
48	5	4	C
48	5	9	A
48	5	20	G
48	5	21	U
48	5	22	A
48	5	44	U
48	5	47	G
48	5	48	U
48	5	49	C
48	5	50	G
48	5	57	C
48	5	58	G
48	5	73	G
48	5	74	A
48	5	75	C
48	6	19	G
48	6	20	U
48	6	21	A
48	6	43	U
48	6	46	G
48	6	47	U

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Mol	Chain	Res	Type
48	6	48	C
48	6	49	G
48	6	56	C
48	6	57	G
48	6	76	A
49	7	6	U
49	7	8	U
49	7	11	C
49	7	12	U
49	7	13	C
49	7	14	A
49	7	16	C
49	7	17	U
49	7	18	G
49	7	19	G
49	7	20	G
49	7	21	A
49	7	34	U
49	7	35	G
49	7	37	A
49	7	46	G
49	7	47	U
49	7	48	C
49	7	51	C
49	7	55	U
49	7	56	C
49	7	58	A
49	7	59	U
49	7	67	A
49	7	72	C
49	7	74	C
49	7	75	C
49	7	76	A

All (67) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	125	A
1	A	140	C
1	A	199	A
1	A	221	A
1	A	271	G

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Mol	Chain	Res	Type
1	A	310	A
1	A	345	A
1	A	369	U
1	A	404	A
1	A	503	A
1	A	548	G
1	A	549	G
1	A	614	A
1	A	746	PSU
1	A	764	A
1	A	776	G
1	A	784	G
1	A	805	G
1	A	827	U
1	A	984	A
1	A	995	C
1	A	1025	G
1	A	1128	G
1	A	1133	A
1	A	1135	C
1	A	1141	U
1	A	1175	A
1	A	1252	G
1	A	1266	G
1	A	1286	A
1	A	1497	U
1	A	1583	A
1	A	1608	A
1	A	1618	A
1	A	1647	U
1	A	1738	G
1	A	1808	A
1	A	1872	A
1	A	1913	A
1	A	2022	U
1	A	2109	U
1	A	2146	C
1	A	2158	A
1	A	2170	A
1	A	2225	A
1	A	2282	G
1	A	2287	A

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Mol	Chain	Res	Type
1	A	2324	U
1	A	2335	A
1	A	2518	A
1	A	2602	A
1	A	2756	U
1	A	2798	U
1	A	2849	U
1	A	2873	A
2	B	34	A
48	5	3	G
48	5	20	G
48	5	47	G
48	5	57	C
48	6	19	G
48	6	46	G
48	6	47	U
48	6	56	C
49	7	15	G
49	7	74	C
49	7	75	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	$\# Z  > 2$
1	PSU	A	2504	53,1	18,21,22	1.04	1 (5%)	22,30,33	1.00	1 (4%)
1	2MA	A	2503	53,1,52	19,25,26	0.91	0	21,37,40	2.14	4 (19%)
1	PSU	A	746	1,52	18,21,22	0.96	1 (5%)	22,30,33	1.59	4 (18%)

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
1	PSU	A	2504	53,1	-	0/7/25/26	0/2/2/2
1	2MA	A	2503	53,1,52	-	1/3/25/26	0/3/3/3
1	PSU	A	746	1,52	-	1/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2504	PSU	C6-C5	3.55	1.39	1.35
1	A	746	PSU	C6-C5	3.35	1.39	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2503	2MA	C5-C6-N1	-7.57	116.04	121.01
1	A	746	PSU	O3'-C3'-C4'	4.47	123.98	111.05
1	A	2503	2MA	C5-C6-N6	3.93	126.33	120.35
1	A	746	PSU	C3'-C2'-C1'	3.42	105.62	101.64
1	A	2503	2MA	CM2-C2-N1	3.08	121.97	117.15
1	A	746	PSU	C6-C5-C4	-2.42	116.50	118.20
1	A	2503	2MA	C2-N1-C6	2.35	121.75	118.08
1	A	2504	PSU	C5-C6-N1	-2.06	119.02	122.11
1	A	746	PSU	O2'-C2'-C3'	2.02	118.35	111.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	746	PSU	O4'-C1'-C5-C6
1	A	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 377 ligands modelled in this entry, 376 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	$\# Z  > 2$
54	PRO	5	101	48	5,7,8	0.54	0	7,8,10	0.99	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
54	PRO	5	101	48	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	5	101	PRO	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.