



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 19, 2016 – 05:32 PM EST

PDB ID : 5MDZ
EMDB ID: : EMD-3493
Title : Structure of the 70S ribosome (empty A site)
Authors : James, N.R.; Brown, A.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on : 2016-11-13
Resolution : 3.10 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

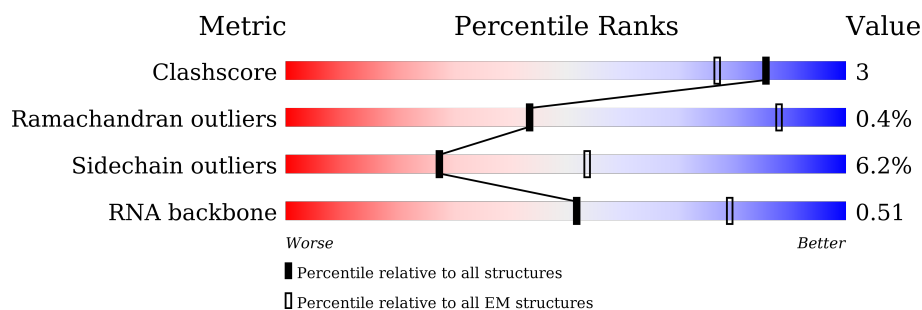
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.





















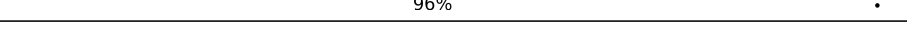






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1	2904	
2	2	1534	
3	3	120	
4	4	18	
5	5	78	
6	B	273	
7	C	209	
8	D	201	



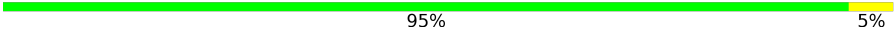


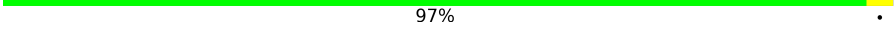



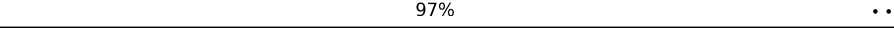
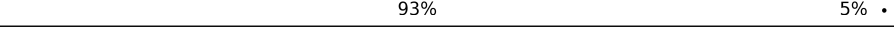
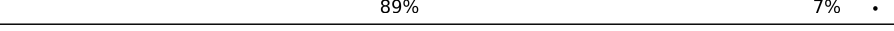

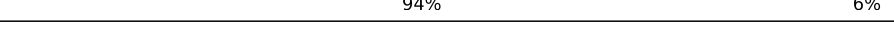

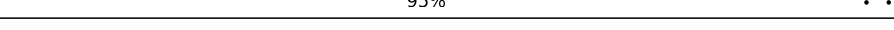

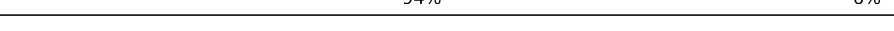
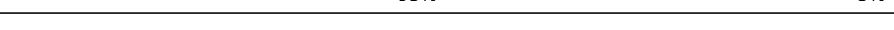


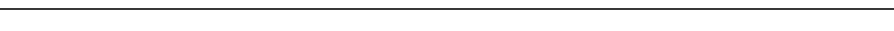

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Mol	Chain	Length	Quality of chain
9	E	179	 85% 13% ..
10	F	177	 92% 7% .
11	G	149	 89% 11% .
12	H	165	 61% 16% .. 21%
13	I	142	 78% 15% . 5%
14	J	142	 89% 11% .
15	K	123	 81% 19%
16	L	144	 92% 8%
17	M	136	 90% 9% .
18	N	127	 76% 18% 6%
19	O	117	 82% 16% ..
20	P	115	 92% 7% .
21	Q	118	 86% 13% .
22	R	103	 88% 11% .
23	S	110	 73% 27%
24	T	100	 84% 8% . 6%
25	U	104	 82% 16% ..
26	V	94	 96% .
27	W	85	 84% 6% 11%
28	X	78	 86% 10% ..
29	Y	63	 89% 10% .
30	Z	59	 85% 14% .
31	a	70	 86% 9% 6%
32	b	57	 88% 11% .
33	c	55	 89% 5% 5%

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Mol	Chain	Length	Quality of chain
34	d	46	 93% 7%
35	e	65	 91% 8% .
36	f	38	 95% 5%
37	g	241	 90% . 7%
38	h	233	 87% . 11%
39	i	206	 97% .
40	j	167	 89% 5% 7%
41	k	135	 72% . . 23%
42	l	179	 79% . . 16%
43	m	130	 97% . .
44	n	130	 93% 5% .
45	o	103	 89% 7% .
46	p	129	 87% . 9%
47	q	124	 94% 6% .
48	r	118	 91% 8% .
49	s	101	 95% . .
50	t	89	 85% 13% .
51	u	82	 94% 6%
52	v	84	 93% . 5%
53	w	75	 87% . 12%
54	x	92	 86% . 10%
55	y	87	 93% 6% .
56	z	71	 94% . .

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 146639 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	887	A	U	conflict	GB 802133627

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	5	Total	C	N	O	P	0	0
			109	49	22	33	5		

- Molecule 5 is a RNA chain called fMet-NH-tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	5	76	Total	C	N	O	P	S	0	0
			1622	725	292	528	76	1		

- Molecule 6 is a protein called 50S ribosomal protein L2.

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

- Molecule 7 is a protein called 50S ribosomal protein L3.

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

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L5.

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

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 11 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 12 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

- Molecule 13 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	135	Total	C	N	O	S	0	0
			984	622	171	185	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

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

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

- 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
			951	588	195	163	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	116	Total	C	N	O	0	0
			892	552	178	162		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 21 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	117	Total	C	N	O		0	0
			947	604	192	151			

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

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

- 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
			857	532	166	156	3		

- Molecule 24 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	103	Total	C	N	O		0	0
			788	498	148	142			

- Molecule 26 is a protein called 50S ribosomal protein L25.

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

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 28 is a protein called 50S ribosomal protein L28.

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

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 30 is a protein called 50S ribosomal protein L30.

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

- Molecule 31 is a protein called 50S ribosomal protein L31.

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

- Molecule 32 is a protein called 50S ribosomal protein L32.

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

- Molecule 33 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	c	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 34 is a protein called 50S ribosomal protein L34.

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

- Molecule 35 is a protein called 50S ribosomal protein L35.

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

- Molecule 36 is a protein called 50S ribosomal protein L36.

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

- Molecule 37 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 38 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 39 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 40 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 41 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 42 is a protein called 30S ribosomal protein S7.

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

- Molecule 43 is a protein called 30S ribosomal protein S8.

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

- Molecule 44 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 45 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 46 is a protein called 30S ribosomal protein S11.

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

- Molecule 47 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 48 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 49 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 50 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 51 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 52 is a protein called 30S ribosomal protein S17.

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

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 54 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 55 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

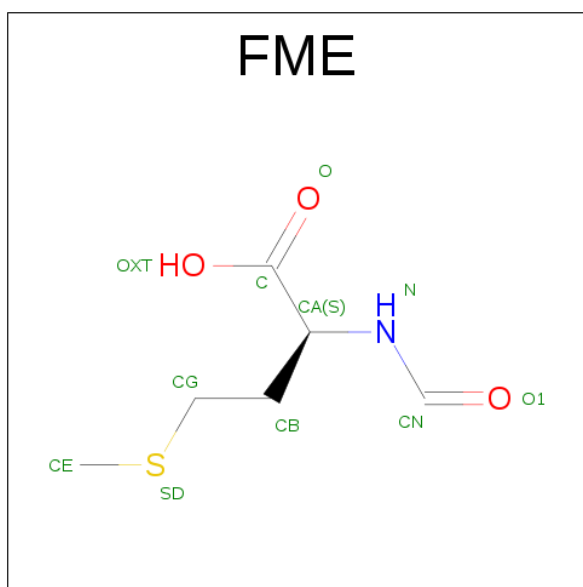
- Molecule 56 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	1	295	Total	Mg	0
			295	295	
57	b	1	Total	Mg	0
			1	1	
57	i	1	Total	Mg	0
			1	1	
57	n	1	Total	Mg	0
			1	1	
57	5	2	Total	Mg	0
			2	2	
57	2	128	Total	Mg	0
			128	128	
57	3	8	Total	Mg	0
			8	8	
57	f	1	Total	Mg	0
			1	1	

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					AltConf
58	5	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	a	1	Total	Zn	0
			1	1	
59	f	1	Total	Zn	0
			1	1	

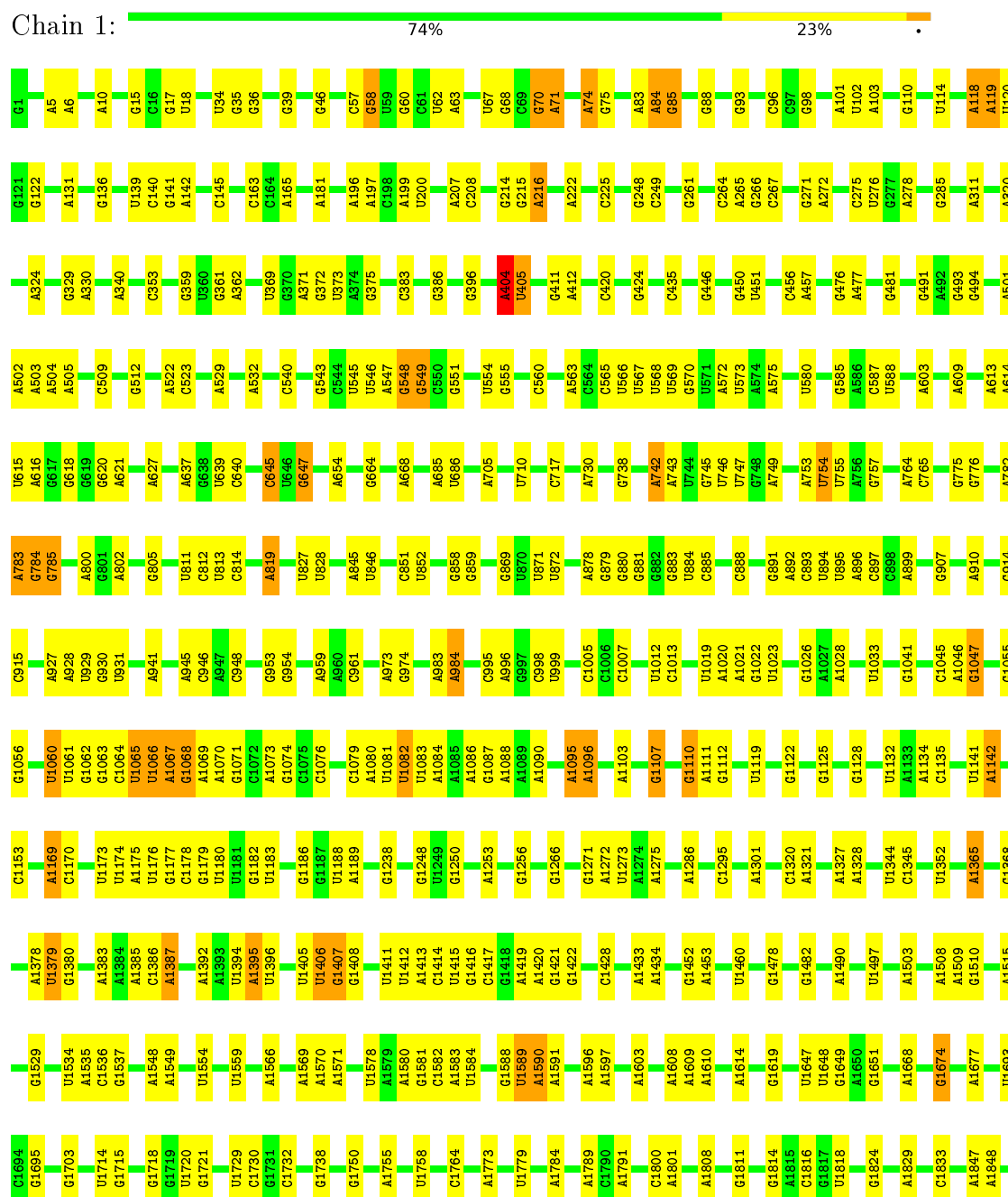
- Molecule 60 is water.

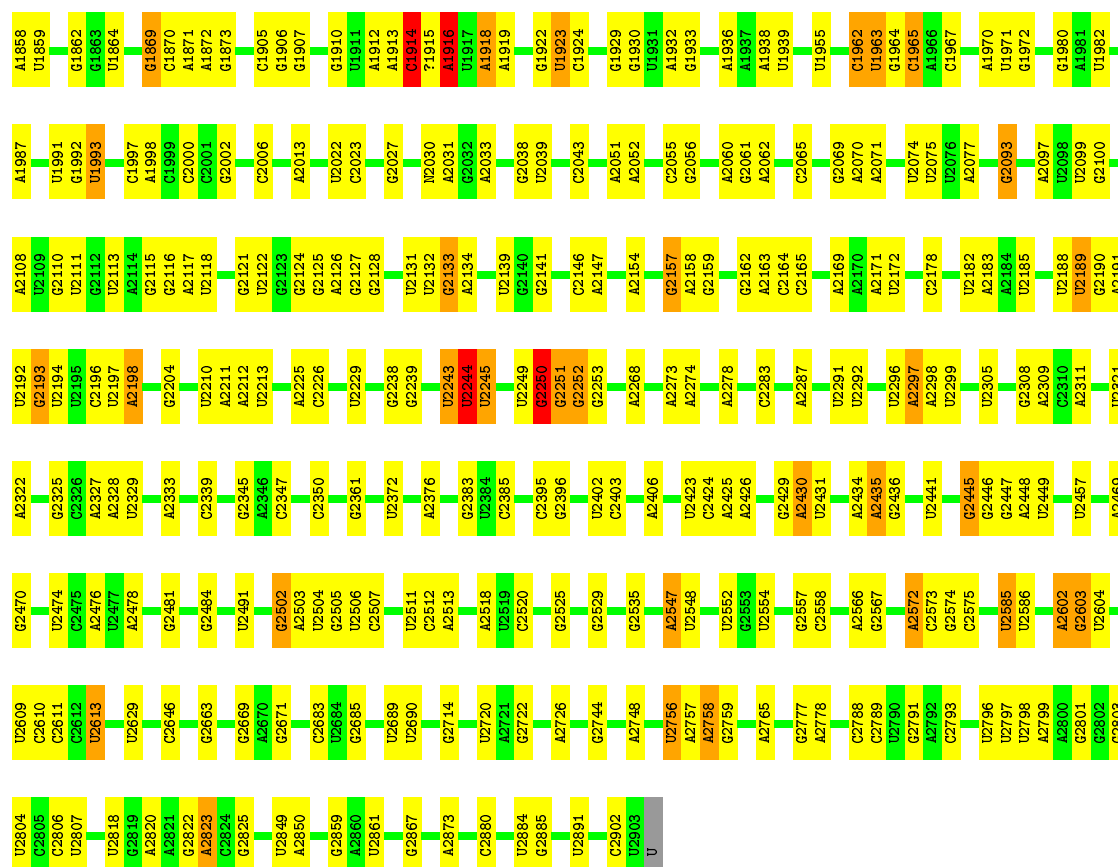
Mol	Chain	Residues	Atoms		AltConf
60	B	2	Total	O	0
			2	2	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

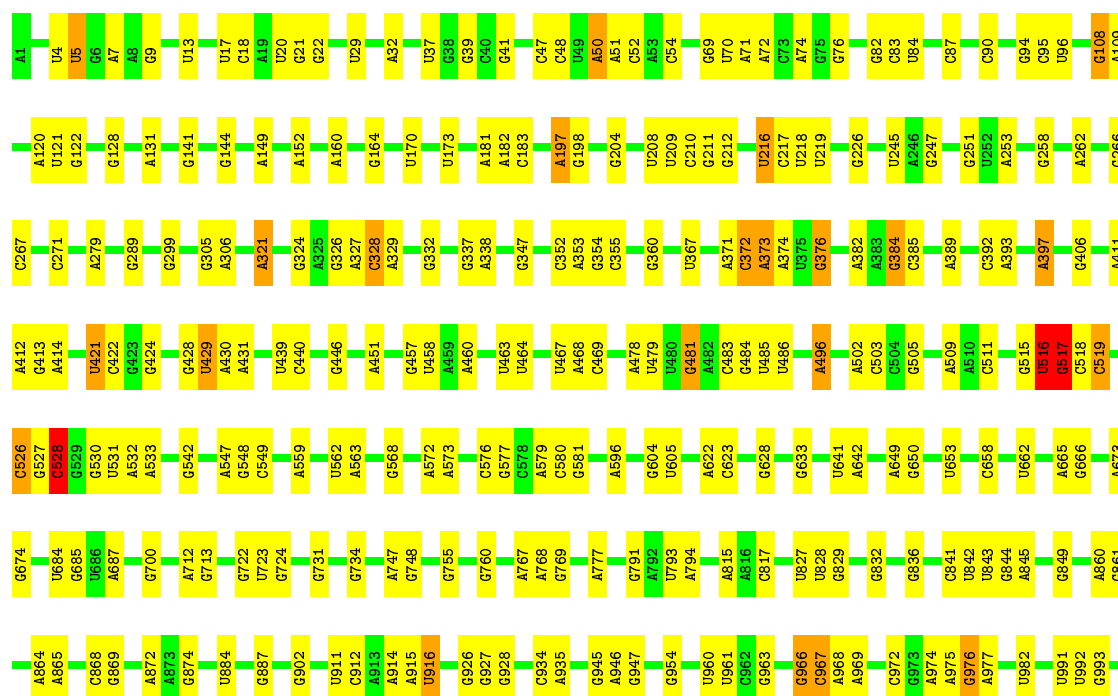
• Molecule 1: 23S ribosomal RNA

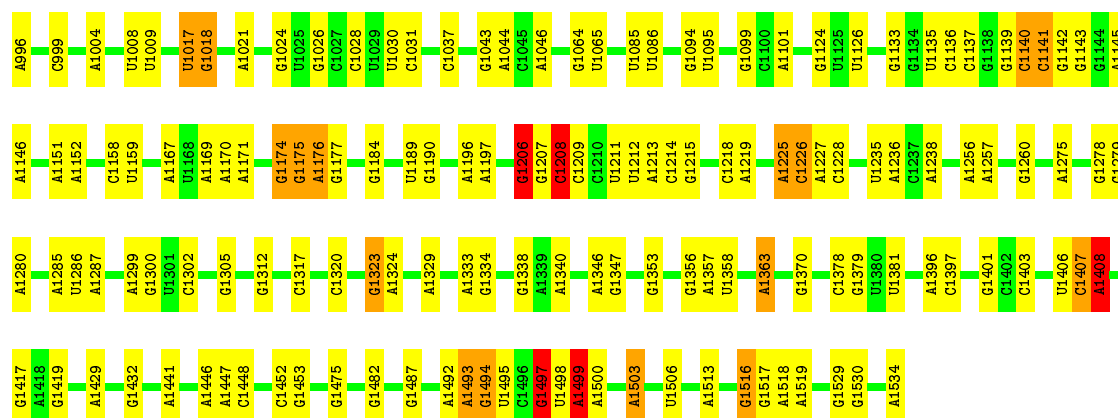




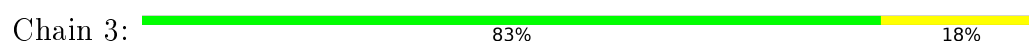
• Molecule 2: 16S ribosomal RNA

Chain 2: 73% 24% ..





- Molecule 3: 5S ribosomal RNA



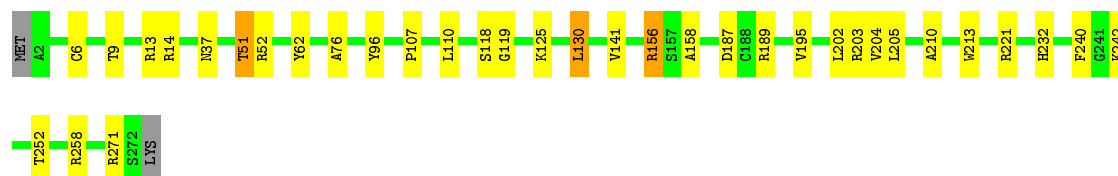
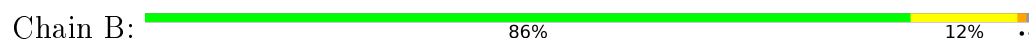
- Molecule 4: mRNA



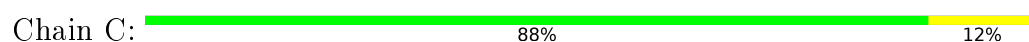
- Molecule 5: fMet-NH-tRNA(fMet)



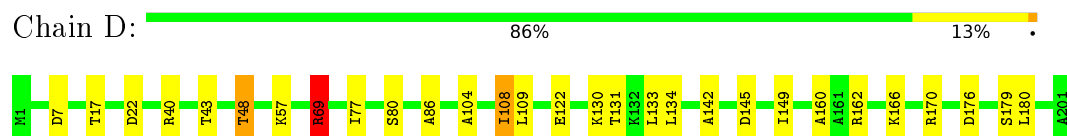
- Molecule 6: 50S ribosomal protein L2



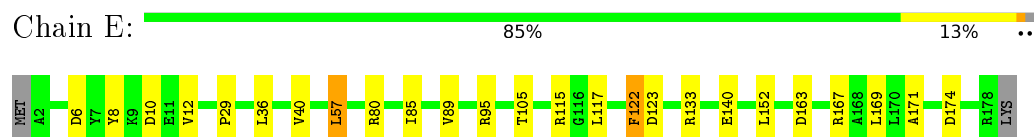
- Molecule 7: 50S ribosomal protein L3



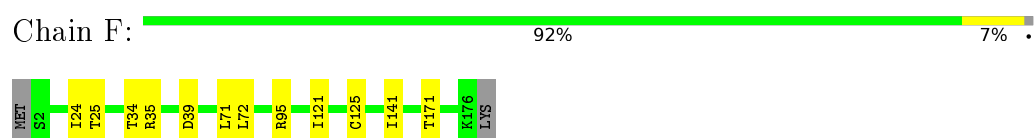
- Molecule 8: 50S ribosomal protein L4



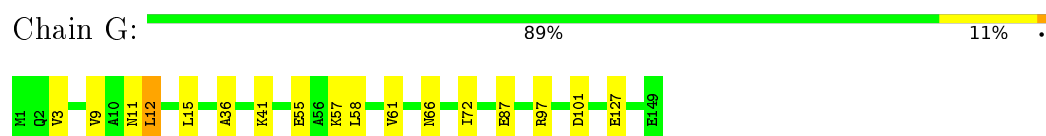
- Molecule 9: 50S ribosomal protein L5



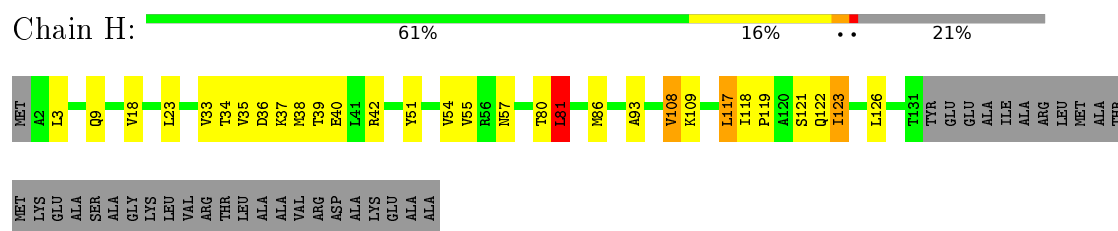
- Molecule 10: 50S ribosomal protein L6



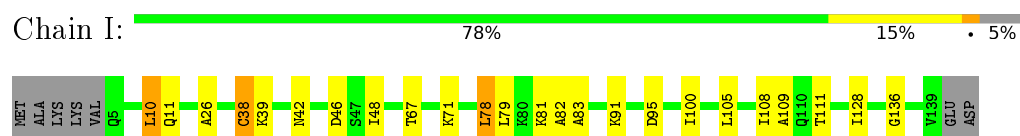
- Molecule 11: 50S ribosomal protein L9



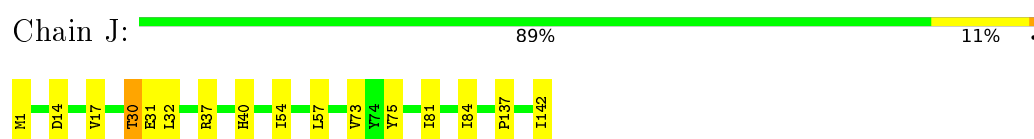
- Molecule 12: 50S ribosomal protein L10



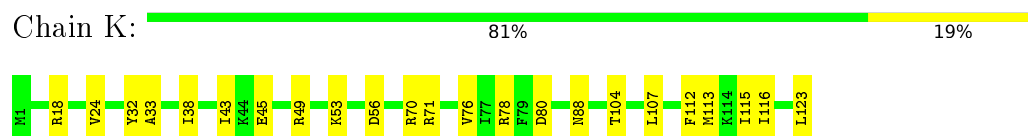
- Molecule 13: 50S ribosomal protein L11



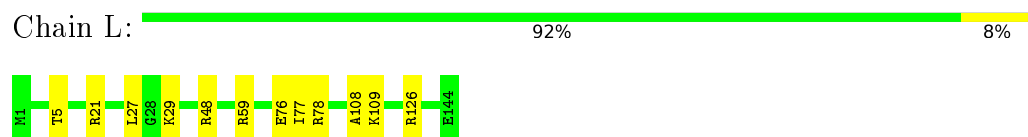
- Molecule 14: 50S ribosomal protein L13



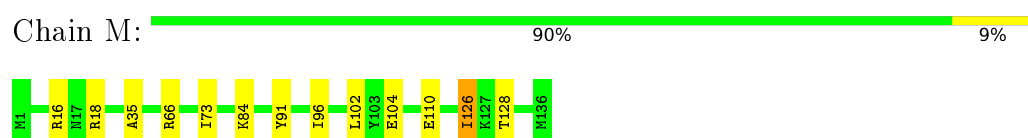
- Molecule 15: 50S ribosomal protein L14



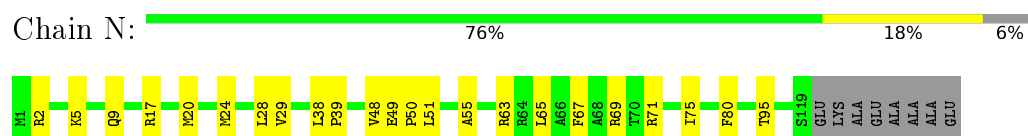
- Molecule 16: 50S ribosomal protein L15



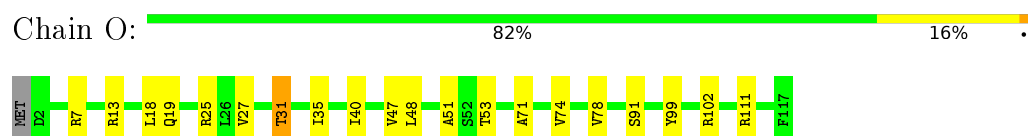
- Molecule 17: 50S ribosomal protein L16



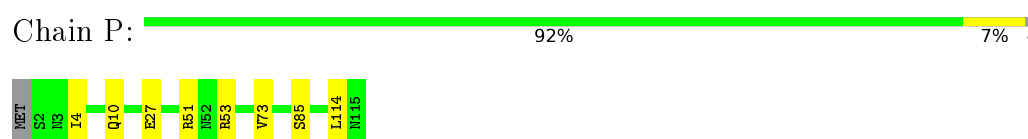
- Molecule 18: 50S ribosomal protein L17



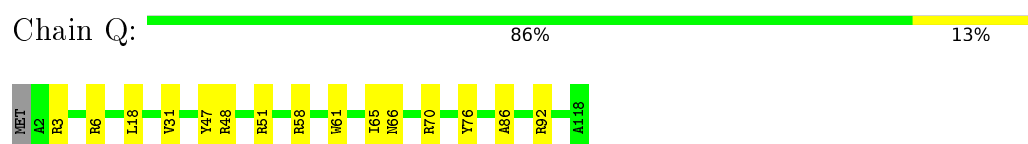
- Molecule 19: 50S ribosomal protein L18



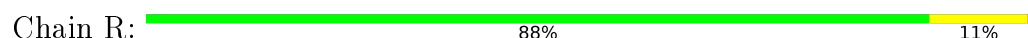
- Molecule 20: 50S ribosomal protein L19

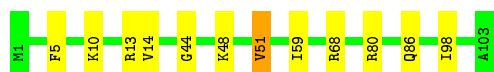


- Molecule 21: 50S ribosomal protein L20



- Molecule 22: 50S ribosomal protein L21

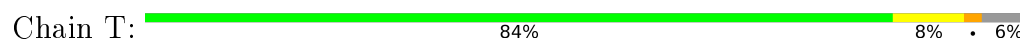




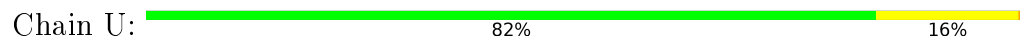
- Molecule 23: 50S ribosomal protein L22



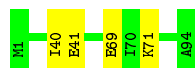
- Molecule 24: 50S ribosomal protein L23



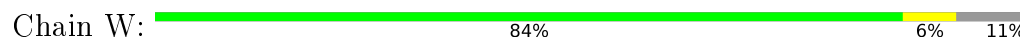
- Molecule 25: 50S ribosomal protein L24



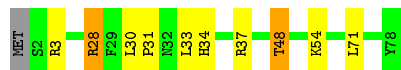
- Molecule 26: 50S ribosomal protein L25



- Molecule 27: 50S ribosomal protein L27




- Molecule 28: 50S ribosomal protein L28



- Molecule 29: 50S ribosomal protein L29




- Molecule 30: 50S ribosomal protein L30

Chain Z:  85% 14%




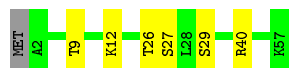
- Molecule 31: 50S ribosomal protein L31

Chain a:  86% 9% 6%




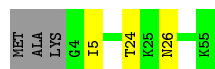
- Molecule 32: 50S ribosomal protein L32

Chain b:  88% 11%



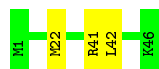
- Molecule 33: 50S ribosomal protein L33

Chain c:  89% 5% 5%




- Molecule 34: 50S ribosomal protein L34

Chain d:  93% 7%



- Molecule 35: 50S ribosomal protein L35

Chain e:  91% 8%




- Molecule 36: 50S ribosomal protein L36

Chain f:  95% 5%



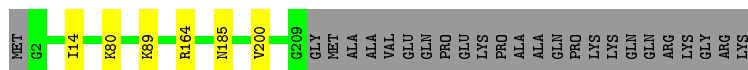
- Molecule 37: 30S ribosomal protein S2

Chain g:  90% 7%



- Molecule 38: 30S ribosomal protein S3

Chain h: 87% 11%



- Molecule 39: 30S ribosomal protein S4

Chain i: 97%



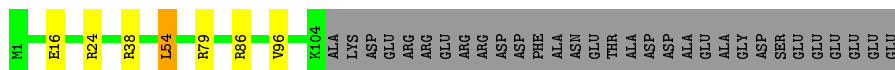
- Molecule 40: 30S ribosomal protein S5

Chain j: 89% 5% 7%



- Molecule 41: 30S ribosomal protein S6

Chain k: 72% 23%



- Molecule 42: 30S ribosomal protein S7

Chain l: 79% 16%



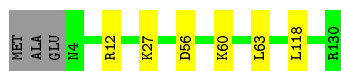
- Molecule 43: 30S ribosomal protein S8

Chain m: 97%




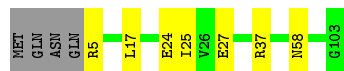
- Molecule 44: 30S ribosomal protein S9

Chain n: 93% 5%




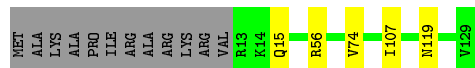
- Molecule 45: 30S ribosomal protein S10

Chain o:  89% 7%



- Molecule 46: 30S ribosomal protein S11

Chain p:  87% 9%




- Molecule 47: 30S ribosomal protein S12

Chain q:  94% 6%



- Molecule 48: 30S ribosomal protein S13

Chain r:  91% 8%




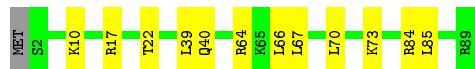
- Molecule 49: 30S ribosomal protein S14

Chain s:  95%



- Molecule 50: 30S ribosomal protein S15

Chain t:  85% 13%



- Molecule 51: 30S ribosomal protein S16

Chain u:  94% 6%




- Molecule 52: 30S ribosomal protein S17

Chain v:  93% • 5%



- Molecule 53: 30S ribosomal protein S18

Chain w:  87% • 12%



- Molecule 54: 30S ribosomal protein S19

Chain x:  86% • 10%



- Molecule 55: 30S ribosomal protein S20

Chain y:  93% • 6%



- Molecule 56: 30S ribosomal protein S21

Chain z:  94% • •



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	140027	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	134615	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 0TD, 2MA, 2MG, 1MG, 3TD, G7M, 8AN, UR3, 7MG, 5MU, ZN, OMU, 6MZ, FME, OMC, MG, OMG, H2U, 5MC, 4OC, 4SU, PSU

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 >2	RMSZ	# Z >2
1	1	0.36	0/69284	0.72	18/108079 (0.0%)
10	F	0.39	0/1333	0.67	0/1805
11	G	0.43	0/1122	0.69	0/1515
12	H	0.49	0/993	0.80	1/1340 (0.1%)
13	I	0.45	0/998	0.69	0/1348
14	J	0.49	0/1152	0.75	0/1551
15	K	0.41	0/955	0.77	0/1279
16	L	0.40	0/1062	0.76	0/1413
17	M	0.46	0/1093	0.81	0/1460
18	N	0.51	0/964	0.87	0/1289
19	O	0.46	0/902	0.81	0/1209
2	2	0.28	0/36583	0.71	15/57046 (0.0%)
20	P	0.41	0/929	0.72	0/1242
21	Q	0.59	0/960	0.91	0/1278
22	R	0.37	0/829	0.66	0/1107
23	S	0.48	0/864	0.82	0/1156
24	T	0.41	0/752	0.71	0/1005
25	U	0.34	0/796	0.67	2/1062 (0.2%)
26	V	0.40	0/766	0.67	0/1025
27	W	0.38	0/589	0.71	0/779
28	X	0.48	0/635	0.81	1/848 (0.1%)
29	Y	0.53	0/502	0.82	0/667
3	3	0.26	0/2872	0.69	0/4478
30	Z	0.44	0/452	0.77	0/605
31	a	0.42	0/531	0.68	0/709
32	b	0.40	0/450	0.79	0/599
33	c	0.34	0/433	0.64	0/576
34	d	0.52	0/380	0.98	0/498
35	e	0.45	0/513	0.82	0/676
36	f	0.37	0/303	0.78	0/397
37	g	0.47	0/1791	0.71	0/2413

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	h	0.43	0/1663	0.71	0/2241
39	i	0.46	0/1665	0.73	0/2227
4	4	0.35	0/122	0.59	0/188
40	j	0.45	0/1165	0.75	0/1568
41	k	0.43	0/867	0.75	1/1171 (0.1%)
42	l	0.50	0/1195	0.81	0/1602
43	m	0.41	0/989	0.69	0/1326
44	n	0.42	0/1034	0.75	0/1375
45	o	0.39	0/800	0.75	0/1082
46	p	0.40	0/893	0.69	0/1205
47	q	0.35	0/960	0.74	0/1286
48	r	0.47	0/909	0.82	0/1215
49	s	0.49	0/817	0.78	0/1088
5	5	0.27	0/1672	0.77	2/2603 (0.1%)
50	t	0.53	0/722	0.85	0/964
51	u	0.44	0/659	0.77	0/884
52	v	0.33	0/657	0.62	0/881
53	w	0.45	0/553	0.77	0/743
54	x	0.38	0/680	0.62	0/915
55	y	0.57	0/675	0.85	0/895
56	z	0.55	0/597	0.88	0/792
6	B	0.39	0/2121	0.77	0/2852
7	C	0.43	0/1586	0.70	0/2134
8	D	0.45	0/1571	0.77	2/2113 (0.1%)
9	E	0.44	0/1434	0.77	0/1926
All	All	0.37	0/157794	0.73	42/235730 (0.0%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	516	PSU	P-O3'-C3'	14.64	137.27	119.70
1	1	2252	G	N9-C1'-C2'	-10.99	99.72	114.00
2	2	1401	G	N9-C1'-C2'	-10.73	100.05	114.00
5	5	20	H2U	P-O3'-C3'	10.49	132.29	119.70
2	2	528	C	N1-C1'-C2'	-10.28	100.64	114.00
2	2	1499	A	N9-C1'-C2'	-10.26	100.66	114.00
2	2	526	C	N1-C1'-C2'	-8.77	102.35	112.00
2	2	1208	C	N1-C1'-C2'	-8.58	102.56	112.00
2	2	1206	G	N9-C1'-C2'	-8.43	102.73	112.00
2	2	1406	U	N1-C1'-C2'	-7.83	103.38	112.00
5	5	20	H2U	O3'-P-O5'	7.39	118.03	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1206	G	C4'-C3'-O3'	7.17	127.35	113.00
1	1	2245	U	N1-C1'-C2'	-7.11	104.17	112.00
1	1	1910	G	N9-C1'-C2'	-6.73	104.59	112.00
2	2	1403	C	N1-C1'-C2'	-6.67	104.66	112.00
2	2	1401	G	C4'-C3'-O3'	6.61	126.22	113.00
1	1	1914	C	C4'-C3'-O3'	6.60	126.21	113.00
1	1	2250	G	C4'-C3'-O3'	-6.60	95.54	109.40
1	1	1379	U	C2'-C3'-O3'	6.57	124.21	113.70
1	1	2243	U	N1-C1'-C2'	-6.57	104.78	112.00
2	2	1408	A	N9-C1'-C2'	-6.49	104.86	112.00
2	2	515	G	N9-C1'-C2'	-6.44	104.92	112.00
2	2	1497	G	N9-C1'-C2'	-6.31	105.06	112.00
12	H	81	LEU	CA-CB-CG	6.10	129.33	115.30
1	1	754	U	N1-C1'-C2'	5.88	121.65	114.00
2	2	517	G	C5'-C4'-C3'	5.67	125.07	116.00
1	1	2244	U	C1'-C2'-O2'	-5.60	93.81	110.60
41	k	54	LEU	CA-CB-CG	5.58	128.14	115.30
25	U	22	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	1	783	A	C4'-C3'-O3'	5.50	123.99	113.00
25	U	22	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	1	1914	C	C3'-C2'-C1'	5.30	105.74	101.50
28	X	28	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	1	742	A	C8-N9-C1'	-5.19	118.36	127.70
1	1	404	A	C2'-C3'-O3'	5.18	121.98	113.70
8	D	69	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	1	2244	U	C4'-C3'-O3'	5.17	123.34	113.00
1	1	2252	G	C4'-C3'-O3'	5.12	123.23	113.00
1	1	1916	A	N9-C1'-C2'	-5.09	106.40	112.00
8	D	69	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	1	742	A	C4-N9-C1'	5.08	135.45	126.30
1	1	2243	U	C4'-C3'-O3'	5.08	123.15	113.00

There are no chirality outliers.

There are no planarity outliers.

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	1	62336	0	31368	223	0
2	2	32929	0	16594	124	0
3	3	2569	0	1301	2	0
4	4	109	0	55	0	0
5	5	1622	0	830	5	0
6	B	2082	0	2154	17	0
7	C	1565	0	1616	15	0
8	D	1552	0	1619	12	0
9	E	1410	0	1444	7	0
10	F	1313	0	1358	6	0
11	G	1111	0	1148	5	0
12	H	980	0	1013	16	0
13	I	984	0	1035	11	0
14	J	1129	0	1162	9	0
15	K	946	0	1023	10	0
16	L	1053	0	1129	6	0
17	M	1074	0	1157	5	0
18	N	951	0	994	9	0
19	O	892	0	923	9	0
20	P	917	0	962	4	0
21	Q	947	0	1019	11	0
22	R	816	0	839	6	0
23	S	857	0	922	15	0
24	T	746	0	811	7	0
25	U	788	0	843	10	0
26	V	753	0	780	0	0
27	W	582	0	599	3	0
28	X	625	0	652	5	0
29	Y	501	0	531	4	0
30	Z	448	0	488	5	0
31	a	522	0	520	0	0
32	b	444	0	458	0	0
33	c	426	0	464	0	0
34	d	377	0	418	0	0
35	e	504	0	572	0	0
36	f	302	0	342	0	0
37	g	1760	0	1787	0	0
38	h	1636	0	1710	0	0
39	i	1643	0	1707	0	0
40	j	1152	0	1196	0	0
41	k	848	0	846	0	0
42	l	1181	0	1238	0	0
43	m	979	0	1031	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	n	1022	0	1070	0	0
45	o	790	0	831	0	0
46	p	877	0	887	0	0
47	q	957	0	1017	0	0
48	r	900	0	965	0	0
49	s	805	0	844	0	0
50	t	714	0	734	0	0
51	u	649	0	666	0	0
52	v	648	0	691	0	0
53	w	544	0	560	0	0
54	x	663	0	688	0	0
55	y	669	0	719	0	0
56	z	589	0	629	0	0
57	1	295	0	0	0	0
57	2	128	0	0	0	0
57	3	8	0	0	0	0
57	5	2	0	0	0	0
57	b	1	0	0	0	0
57	f	1	0	0	0	0
57	i	1	0	0	0	0
57	n	1	0	0	0	0
58	5	10	0	10	0	0
59	a	1	0	0	0	0
59	f	1	0	0	0	0
60	B	2	0	0	0	0
All	All	146639	0	98969	506	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 3.

All (506) 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)
1:1:1021:A:N1	1:1:1141:U:O4	1.63	1.31
1:1:2074:U:O4	1:1:2435:A:N6	1.60	1.31
2:2:1358:U:O4	2:2:1363:A:N1	1.60	1.29
1:1:2074:U:N3	1:1:2435:A:N1	1.83	1.25
2:2:563:A:N1	2:2:884:U:O4	1.73	1.21
1:1:2297:A:N1	1:1:2321:U:C4	2.29	1.00
2:2:13:U:N3	2:2:915:A:C6	2.29	1.00
2:2:13:U:O4	2:2:20:U:O4	1.79	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:67:U:N3	1:1:74:A:C6	2.36	0.94
2:2:13:U:N3	2:2:915:A:N6	2.16	0.94
2:2:13:U:C4	2:2:915:A:N6	2.36	0.93
1:1:2013:A:N6	1:1:2613:U:H3	1.68	0.92
2:2:13:U:C4	2:2:20:U:O4	2.24	0.91
1:1:1406:U:O2'	1:1:1407:G:C5'	2.19	0.91
1:1:783:A:N3	1:1:783:A:H2'	1.89	0.86
1:1:67:U:N3	1:1:74:A:N6	2.25	0.85
25:U:34:VAL:HG13	25:U:67:VAL:HG22	1.58	0.83
1:1:1406:U:O2'	1:1:1407:G:H5''	1.79	0.82
1:1:1021:A:N6	1:1:1141:U:H3	1.77	0.81
1:1:1019:U:H3	1:1:1142:A:N6	1.77	0.81
1:1:1914:C:H2'	1:1:1915:3TD:O4	1.81	0.81
2:2:37:U:N3	2:2:397:A:N6	2.28	0.80
1:1:2297:A:N1	1:1:2321:U:O4	2.14	0.80
1:1:1019:U:H3	1:1:1142:A:H61	1.28	0.80
1:1:2298:A:C4	1:1:2321:U:C5	2.70	0.80
1:1:585:G:N7	21:Q:6:ARG:NH1	2.29	0.79
1:1:2189:U:O4'	1:1:2189:U:OP1	2.00	0.79
1:1:1406:U:O2'	1:1:1407:G:O5'	2.01	0.79
1:1:1021:A:H61	1:1:1141:U:H3	1.29	0.78
1:1:2756:U:N3	1:1:2758:A:C6	2.52	0.77
1:1:2756:U:N3	1:1:2758:A:N6	2.32	0.77
7:C:4:LEU:HD23	7:C:29:VAL:HG11	1.65	0.77
1:1:1406:U:O2'	1:1:1407:G:P	2.41	0.77
2:2:1358:U:C4	2:2:1363:A:N1	2.52	0.77
13:I:82:ALA:HB2	13:I:108:ILE:HD11	1.67	0.76
1:1:2074:U:C4	1:1:2435:A:N6	2.53	0.76
1:1:1021:A:N1	1:1:1141:U:C4	2.55	0.75
25:U:36:VAL:HG11	25:U:39:ILE:HD12	1.68	0.74
12:H:36:ASP:O	12:H:39:THR:OG1	2.05	0.74
19:O:31:THR:O	19:O:102:ARG:NH1	2.19	0.74
2:2:517:G:O2'	2:2:530:G:H4'	1.88	0.73
2:2:827:U:H3	2:2:872:A:N6	1.87	0.72
1:1:2298:A:C4	1:1:2321:U:H5	2.04	0.72
1:1:67:U:C4	1:1:74:A:N6	2.57	0.72
1:1:742:A:H2'	1:1:743:A:C8	2.26	0.71
5:5:19:G:H5'	5:5:20:H2U:O2	1.91	0.71
1:1:1021:A:H3'	1:1:1021:A:N3	2.07	0.69
1:1:1596:A:H2'	1:1:1597:A:C8	2.27	0.69
1:1:572:A:OP2	22:R:80:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:516:PSU:H3'	2:2:517:G:C8	2.27	0.69
2:2:915:A:N6	2:2:916:U:C4	2.60	0.69
1:1:927:A:H2'	1:1:928:A:C8	2.28	0.69
2:2:13:U:O4	2:2:21:G:C2	2.46	0.69
1:1:2756:U:C4	1:1:2758:A:N6	2.62	0.68
2:2:37:U:H3	2:2:397:A:N6	1.90	0.68
1:1:2435:A:O2'	1:1:2436:G:O5'	2.10	0.67
2:2:563:A:N1	2:2:884:U:C4	2.60	0.67
1:1:1153:C:OP1	21:Q:92:ARG:NH1	2.27	0.67
1:1:1779:U:H5	1:1:1784:A:N7	1.93	0.66
1:1:2445:2MG:HM23	1:1:2446:G:H1'	1.75	0.66
2:2:1407:5MC:C2'	2:2:1408:A:H5'	2.24	0.66
10:F:24:ILE:HD13	10:F:72:LEU:HD21	1.77	0.66
1:1:2013:A:N6	1:1:2613:U:N3	2.33	0.66
2:2:827:U:N3	2:2:872:A:N6	2.45	0.64
23:S:36:LEU:HD13	23:S:48:LYS:HA	1.80	0.64
1:1:1082:U:N3	1:1:1086:A:N6	2.45	0.64
2:2:1358:U:O4	2:2:1363:A:C2	2.47	0.64
5:5:19:G:H3'	5:5:20:H2U:H5''	1.80	0.64
2:2:1358:U:H3	2:2:1363:A:N6	1.96	0.63
2:2:516:PSU:O2'	2:2:519:C:N3	2.31	0.63
1:1:1107:G:H4'	12:H:81:LEU:HB3	1.81	0.63
2:2:37:U:O2	2:2:548:G:C2	2.52	0.63
2:2:13:U:O4	2:2:20:U:C4	2.51	0.63
10:F:121:ILE:HD12	10:F:141:ILE:HG22	1.79	0.62
1:1:2297:A:C2	1:1:2321:U:C4	2.86	0.62
1:1:1789:A:OP2	6:B:221:ARG:NH1	2.31	0.62
1:1:2683:C:OP1	20:P:51:ARG:NH2	2.32	0.62
1:1:754:U:H2'	1:1:755:U:C6	2.35	0.62
1:1:1998:A:OP2	7:C:141:ARG:NH2	2.32	0.62
1:1:2189:U:O4'	1:1:2189:U:P	2.57	0.62
2:2:1358:U:N3	2:2:1363:A:N6	2.46	0.62
1:1:568:U:H1'	1:1:2030:6MZ:H9C1	1.79	0.62
24:T:50:LEU:HD23	29:Y:26:PHE:CE1	2.35	0.61
1:1:84:A:N1	1:1:98:G:O2'	2.32	0.61
1:1:2720:U:OP1	20:P:53:ARG:NH2	2.34	0.61
2:2:13:U:C5	2:2:20:U:O4	2.53	0.60
1:1:70:G:H4'	1:1:71:A:OP1	2.02	0.60
1:1:2297:A:C2	1:1:2321:U:C5	2.89	0.60
2:2:658:C:H1'	24:T:22:THR:HG21	118.55	0.60
12:H:23:LEU:HD12	12:H:118:ILE:HG12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1218:C:H2'	2:2:1219:A:C8	2.36	0.59
2:2:13:U:C2	2:2:915:A:N6	2.70	0.59
1:1:1590:A:H2'	1:1:1591:A:C8	2.38	0.59
1:1:1021:A:C2	1:1:1141:U:O4	2.50	0.59
2:2:439:U:O2	2:2:440:C:C6	2.56	0.59
1:1:2572:A:C8	7:C:149:ASN:OD1	2.56	0.59
25:U:36:VAL:CG1	25:U:39:ILE:HD12	2.32	0.58
5:5:18:G:N2	5:5:57:A:H2'	2.19	0.58
13:I:109:ALA:HB2	13:I:128:ILE:HD12	1.85	0.58
13:I:78:LEU:HD22	13:I:108:ILE:HG23	1.86	0.58
2:2:927:G:O3'	2:2:928:G:P	2.61	0.58
2:2:563:A:N6	2:2:884:U:N3	2.51	0.58
23:S:20:VAL:HG11	23:S:44:ALA:HA	1.86	0.57
1:1:2245:U:O2'	1:1:2436:G:OP2	2.22	0.57
2:2:321:A:N7	2:2:328:C:O2'	2.34	0.57
7:C:33:ARG:NH1	7:C:53:GLY:O	2.36	0.57
1:1:1406:U:HO2'	1:1:1407:G:C5'	2.09	0.57
2:2:966:2MG:HM22	5:5:34:C:H5''	1.86	0.56
1:1:1818:U:OP2	6:B:156:ARG:NH1	2.38	0.56
2:2:528:C:H6	2:2:528:C:H5''	1.71	0.56
8:D:104:ALA:O	8:D:108:ILE:HG23	2.05	0.56
1:1:1614:A:C2	23:S:93:ALA:HB2	2.40	0.56
13:I:105:LEU:HD22	13:I:128:ILE:HG22	1.86	0.56
16:L:77:ILE:HD11	16:L:108:ALA:HB1	1.87	0.56
1:1:580:U:O3'	21:Q:31:VAL:HG13	2.05	0.56
17:M:66:ARG:NH1	17:M:104:GLU:OE1	2.39	0.56
28:X:31:PRO:HG2	28:X:33:LEU:HD13	1.87	0.56
2:2:496:A:N3	2:2:496:A:H2'	2.19	0.56
21:Q:86:ALA:O	22:R:51:VAL:HG23	2.05	0.56
1:1:2502:G:H5''	1:1:2503:2MA:H5''	1.87	0.56
1:1:2445:2MG:OP1	8:D:69:ARG:NH2	2.34	0.56
2:2:1206:G:H2'	2:2:1207:2MG:C8	2.40	0.55
1:1:2249:U:H3'	1:1:2250:G:C5'	2.36	0.55
1:1:1962:5MC:O2'	1:1:1964:G:OP2	2.25	0.55
1:1:404:A:O2'	1:1:405:U:OP2	2.22	0.55
8:D:108:ILE:HD11	8:D:180:LEU:HD13	1.89	0.55
1:1:2552:OMU:H6	1:1:2552:OMU:O5'	2.07	0.55
24:T:50:LEU:HD23	29:Y:26:PHE:CZ	2.42	0.55
1:1:523:C:O2	1:1:554:U:O2'	2.25	0.55
2:2:1207:2MG:O5'	2:2:1207:2MG:H8	1.89	0.54
2:2:563:A:N6	2:2:884:U:H3	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:58:LEU:O	11:G:61:VAL:HG22	2.08	0.54
1:1:811:U:H2'	16:L:21:ARG:HA	1.89	0.54
2:2:966:2MG:H5''	2:2:967:5MC:OP2	2.08	0.54
2:2:961:U:O4	2:2:974:A:N1	2.40	0.54
27:W:37:ILE:HD11	27:W:82:ILE:HD11	1.90	0.54
8:D:130:LYS:HB2	8:D:133:LEU:HD12	1.89	0.54
2:2:13:U:C2	2:2:915:A:C6	2.95	0.54
1:1:1056:G:O2'	1:1:1103:A:N6	2.41	0.54
2:2:945:G:C2	2:2:946:A:C8	2.96	0.54
8:D:131:THR:HG22	8:D:160:ALA:O	2.08	0.54
19:O:35:ILE:HG21	19:O:71:ALA:HA	1.89	0.54
23:S:59:GLU:CG	23:S:66:ILE:HD11	2.38	0.53
1:1:2192:U:H2'	1:1:2193:G:C8	2.43	0.53
2:2:767:A:H2'	2:2:768:A:O4'	2.08	0.53
19:O:27:VAL:HG21	19:O:40:ILE:HD12	1.89	0.53
2:2:769:G:H4'	2:2:1513:A:H4'	1.88	0.53
2:2:13:U:C4	2:2:21:G:C2	2.96	0.53
2:2:439:U:O2	2:2:440:C:C5	2.61	0.53
2:2:1518:MA6:N6	2:2:1519:MA6:H93	2.22	0.53
12:H:80:THR:C	12:H:81:LEU:HD13	2.29	0.53
2:2:673:A:H2'	2:2:674:G:C8	2.44	0.53
9:E:8:TYR:HA	9:E:12:VAL:HB	1.91	0.53
1:1:1047:G:HO2'	1:1:1110:G:H1	1.57	0.52
1:1:2074:U:C4	1:1:2435:A:N1	2.71	0.52
2:2:197:A:O3'	2:2:198:G:P	2.67	0.52
1:1:2298:A:C5	1:1:2321:U:O4	2.62	0.52
12:H:38:MET:O	12:H:42:ARG:N	2.35	0.52
12:H:108:VAL:O	12:H:108:VAL:HG12	2.10	0.52
18:N:38:LEU:N	18:N:39:PRO:CD	2.73	0.52
1:1:2196:C:O3'	1:1:2197:U:P	2.67	0.52
2:2:13:U:C4	2:2:915:A:C6	2.92	0.52
21:Q:58:ARG:HA	21:Q:61:TRP:CE3	2.45	0.52
25:U:94:ARG:HB3	25:U:103:ILE:HD12	1.91	0.52
25:U:13:VAL:CG2	25:U:39:ILE:HD13	2.39	0.52
1:1:929:U:H1'	30:Z:26:GLY:O	2.10	0.52
1:1:1980:G:O2'	1:1:1982:U:OP2	2.28	0.52
1:1:2328:A:H2'	1:1:2329:U:C6	2.44	0.52
1:1:639:U:H2'	1:1:640:C:C6	2.45	0.52
2:2:966:2MG:H2'	2:2:966:2MG:N3	2.25	0.52
2:2:864:A:C2	2:2:865:A:C2	2.98	0.52
2:2:1499:A:O2'	2:2:1500:A:H5'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1614:A:N1	23:S:93:ALA:HB2	2.25	0.51
1:1:1918:A:O2'	1:1:1919:A:N7	2.38	0.51
1:1:587:C:OP2	16:L:21:ARG:NH1	2.43	0.51
1:1:783:A:N3	1:1:783:A:C2'	2.70	0.51
1:1:1693:U:O2'	6:B:14:ARG:NH2	2.43	0.51
1:1:1814:G:H4'	6:B:51:THR:HG21	1.93	0.51
23:S:59:GLU:HG3	23:S:66:ILE:HD11	1.92	0.51
1:1:2000:C:OP1	18:N:5:LYS:NZ	2.36	0.51
1:1:2074:U:H2'	1:1:2075:U:C6	2.46	0.51
1:1:523:C:H4'	1:1:540:C:O2	2.10	0.51
1:1:118:A:C8	1:1:119:A:C8	2.99	0.51
12:H:118:ILE:HB	12:H:119:PRO:HD3	1.93	0.51
10:F:121:ILE:HD12	10:F:141:ILE:CG2	2.40	0.51
15:K:43:ILE:HD12	15:K:56:ASP:HB2	1.93	0.51
3:3:106:G:H2'	3:3:107:G:O4'	2.10	0.51
1:1:1869:G:N2	1:1:1871:A:O2'	2.44	0.51
25:U:12:ILE:HG21	25:U:80:ALA:HB2	1.92	0.51
1:1:1141:U:O2	1:1:1142:A:N6	2.44	0.50
1:1:1964:G:H4'	1:1:1965:C:OP2	2.11	0.50
2:2:1407:5MC:C3'	2:2:1408:A:H5'	2.40	0.50
14:J:17:VAL:HG23	14:J:137:PRO:HB2	1.92	0.50
18:N:55:ALA:HA	18:N:80:PHE:CE1	2.47	0.50
1:1:2074:U:O4	1:1:2435:A:C6	2.55	0.50
1:1:2243:U:H2'	1:1:2244:U:C6	2.46	0.50
2:2:5:U:O4'	2:2:5:U:O2	2.29	0.50
1:1:1824:G:O2'	6:B:252:THR:HG21	2.11	0.50
2:2:108:G:N3	2:2:108:G:H5''	2.27	0.50
15:K:71:ARG:NH2	15:K:123:LEU:O	2.42	0.50
14:J:30:THR:HG22	14:J:31:GLU:N	2.27	0.50
23:S:24:ILE:HD13	23:S:36:LEU:HD11	1.93	0.50
23:S:55:ILE:HG23	23:S:66:ILE:HD12	1.93	0.50
2:2:1499:A:OP2	2:2:1499:A:H3'	2.12	0.50
15:K:113:MET:O	15:K:116:ILE:HG13	2.11	0.50
2:2:1356:G:H2'	2:2:1357:A:C8	2.47	0.50
14:J:32:LEU:CD2	14:J:54:ILE:HG21	2.42	0.50
2:2:1140:C:HO2'	2:2:1141:C:P	2.35	0.50
1:1:2298:A:N3	1:1:2321:U:C5	2.80	0.50
1:1:742:A:C2	1:1:743:A:C6	3.00	0.50
1:1:1433:A:H2'	1:1:1434:A:O4'	2.13	0.49
2:2:1208:C:H2'	2:2:1209:C:C6	2.47	0.49
6:B:107:PRO:HD2	6:B:110:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2646:C:O5'	1:1:2646:C:H6	1.95	0.49
2:2:872:A:N3	2:2:872:A:H2'	2.27	0.49
7:C:25:THR:HG21	7:C:193:VAL:HG22	1.94	0.49
22:R:14:VAL:HG21	22:R:98:ILE:HG13	1.94	0.49
1:1:2557:G:H2'	1:1:2558:C:C6	2.47	0.49
2:2:50:A:O2'	2:2:360:G:N2	2.45	0.49
2:2:1169:A:H2'	2:2:1170:A:C8	2.48	0.49
11:G:3:VAL:HG22	11:G:36:ALA:HB1	1.95	0.49
29:Y:18:LEU:HB2	29:Y:53:VAL:HG11	1.94	0.49
30:Z:24:LEU:HD11	30:Z:54:MET:CE	2.42	0.49
2:2:1174:G:H2'	2:2:1175:G:H5'	1.95	0.49
7:C:156:PHE:CE1	14:J:81:ILE:HD13	2.48	0.49
2:2:516:PSU:H3'	2:2:517:G:H8	1.75	0.49
6:B:210:ALA:HA	6:B:213:TRP:CE3	2.48	0.49
18:N:67:PHE:O	18:N:71:ARG:N	2.45	0.49
1:1:85:G:OP2	25:U:7:ARG:HB2	2.13	0.49
1:1:2297:A:C6	1:1:2321:U:O4	2.65	0.49
1:1:2074:U:C2	1:1:2435:A:N1	2.76	0.49
1:1:560:C:O2	21:Q:48:ARG:NH1	2.41	0.49
2:2:13:U:O4	2:2:21:G:N3	2.46	0.49
7:C:4:LEU:HD23	7:C:29:VAL:CG1	2.39	0.49
2:2:1493:A:O2'	2:2:1494:G:P	2.71	0.48
23:S:29:VAL:HB	23:S:55:ILE:HD11	1.95	0.48
23:S:25:ARG:NH1	23:S:74:ILE:O	2.46	0.48
27:W:37:ILE:HG21	27:W:80:ILE:HG21	1.95	0.48
1:1:2038:G:H2'	1:1:2039:U:O4'	2.13	0.48
10:F:35:ARG:HD3	10:F:71:LEU:HD13	1.93	0.48
1:1:1412:U:C4	1:1:1413:A:N7	2.81	0.48
13:I:38:CYS:SG	13:I:39:LYS:N	2.86	0.48
22:R:14:VAL:CG2	22:R:98:ILE:HG13	2.43	0.48
1:1:1922:G:C2'	1:1:1923:U:H5'	2.44	0.48
12:H:23:LEU:HA	12:H:118:ILE:HG12	1.96	0.48
1:1:1588:G:C6	1:1:1589:U:O4	2.67	0.48
1:1:2585:U:O2	1:1:2585:U:O4'	2.31	0.48
13:I:82:ALA:CB	13:I:108:ILE:HD11	2.39	0.48
23:S:4:ILE:HG12	23:S:106:VAL:HG22	1.95	0.48
1:1:570:G:H2'	1:1:2030:6MZ:N7	2.28	0.48
13:I:10:LEU:HD22	13:I:26:ALA:HB1	1.96	0.48
19:O:51:ALA:HB3	19:O:78:VAL:HB	1.95	0.48
1:1:565:C:H2'	1:1:566:U:O4'	2.13	0.48
7:C:121:THR:HB	7:C:127:PHE:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1067:A:O2'	1:1:1068:G:O4'	2.31	0.48
1:1:2685:G:OP1	15:K:78:ARG:NH2	2.47	0.48
2:2:1017:U:O2'	2:2:1018:G:O4'	2.31	0.48
2:2:927:G:O2'	2:2:1503:A:N7	2.36	0.48
28:X:3:ARG:HD2	28:X:30:LEU:HD22	1.94	0.48
2:2:13:U:O2	2:2:915:A:N7	2.47	0.48
2:2:604:G:H2'	2:2:605:U:O4'	2.14	0.48
1:1:1814:G:C4'	6:B:51:THR:HG21	2.44	0.48
19:O:27:VAL:CG2	19:O:40:ILE:HD12	2.44	0.48
2:2:1516:2MG:N2	2:2:1519:MA6:OP2	2.45	0.47
10:F:24:ILE:CD1	10:F:72:LEU:HD21	2.43	0.47
22:R:5:PHE:HB3	22:R:59:ILE:HD12	1.96	0.47
2:2:371:A:H2'	2:2:372:C:O4'	2.14	0.47
5:5:21:A:N6	5:5:46:A:O2'	2.47	0.47
1:1:1406:U:H3	1:1:1596:A:H2	1.59	0.47
1:1:1993:U:H4'	7:C:133:THR:HG22	1.96	0.47
2:2:1064:G:O2'	2:2:1190:G:N2	2.47	0.47
2:2:373:A:C2	2:2:374:A:C8	3.03	0.47
2:2:911:U:H2'	2:2:912:C:C6	2.49	0.47
14:J:84:ILE:HG23	14:J:84:ILE:O	2.14	0.47
1:1:2065:C:H4'	1:1:2251:OMG:HM22	1.97	0.47
1:1:2093:G:O2'	1:1:2198:A:N1	2.41	0.47
22:R:51:VAL:HG22	22:R:51:VAL:O	2.15	0.46
1:1:1695:G:N7	6:B:14:ARG:NH2	2.64	0.46
1:1:2074:U:C4	1:1:2435:A:C6	3.04	0.46
7:C:152:PRO:HG3	7:C:156:PHE:CZ	2.50	0.46
1:1:1720:U:H2'	1:1:1721:G:O4'	2.16	0.46
1:1:1020:A:C6	1:1:1141:U:O2	2.68	0.46
1:1:2065:C:H4'	1:1:2251:OMG:CM2	2.45	0.46
1:1:2445:2MG:HM23	1:1:2446:G:C1'	2.45	0.46
1:1:2756:U:C4	1:1:2759:G:C6	3.03	0.46
2:2:1175:G:N3	2:2:1176:A:C8	2.83	0.46
2:2:868:C:H2'	2:2:869:G:O4'	2.16	0.46
9:E:36:LEU:HB3	9:E:57:LEU:HD21	1.97	0.46
14:J:30:THR:CG2	14:J:31:GLU:N	2.79	0.46
15:K:18:ARG:HB2	15:K:45:GLU:HB3	1.97	0.46
1:1:2291:U:H2'	1:1:2292:U:C6	2.51	0.46
2:2:946:A:H2'	2:2:947:G:C8	2.50	0.46
12:H:117:LEU:O	12:H:117:LEU:HD12	2.15	0.46
1:1:1275:A:N1	1:1:1295:C:O2'	2.46	0.46
1:1:1394:U:H4'	1:1:1603:A:H4'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:998:C:OP2	21:Q:58:ARG:NH2	2.49	0.46
2:2:429:U:N3	2:2:431:A:N6	2.64	0.46
2:2:915:A:C8	2:2:915:A:H3'	2.50	0.46
25:U:94:ARG:CB	25:U:103:ILE:HD12	2.45	0.46
2:2:563:A:C2	2:2:884:U:O4	2.62	0.46
24:T:30:ILE:HD13	24:T:93:LEU:HD12	1.97	0.46
1:1:2070:A:H2'	1:1:2071:A:O4'	2.16	0.46
1:1:2298:A:C6	1:1:2299:U:C2	3.04	0.46
1:1:784:G:H5'	1:1:785:G:OP1	2.15	0.46
1:1:1095:A:O2'	1:1:1096:A:O4'	2.33	0.45
1:1:1385:A:O2'	1:1:1396:U:O2	2.34	0.45
1:1:1914:C:H2'	1:1:1915:3TD:C4	2.43	0.45
23:S:17:VAL:HG12	23:S:76:VAL:HG21	1.98	0.45
9:E:57:LEU:HD22	9:E:89:VAL:CG2	2.46	0.45
1:1:1047:G:N2	1:1:1110:G:O2'	2.50	0.45
1:1:2547:A:H2'	1:1:2548:U:C6	2.52	0.45
19:O:18:LEU:HD23	19:O:25:ARG:HD2	1.99	0.45
1:1:1915:3TD:H2'	1:1:1916:A:C8	2.51	0.45
1:1:68:G:N2	1:1:74:A:OP2	2.49	0.45
8:D:170:ARG:NH2	8:D:176:ASP:OD1	2.49	0.45
17:M:96:ILE:HG21	17:M:126:ILE:HD12	1.98	0.45
21:Q:47:TYR:CD1	21:Q:47:TYR:C	2.90	0.45
1:1:1327:A:H2'	1:1:1328:A:O4'	2.17	0.45
11:G:55:GLU:HA	11:G:58:LEU:HD12	1.99	0.45
3:3:48:U:H2'	3:3:49:C:C6	2.52	0.45
9:E:29:PRO:HB2	9:E:169:LEU:HD22	1.99	0.45
1:1:645:C:H2'	1:1:647:G:C8	2.52	0.45
2:2:1498:UR3:C4'	2:2:1519:MA6:H2	2.47	0.45
1:1:340:A:O2'	8:D:162:ARG:NH1	2.50	0.45
1:1:742:A:C2	1:1:755:U:N3	2.80	0.45
2:2:17:U:H2'	2:2:18:C:C6	2.52	0.45
6:B:76:ALA:HB2	6:B:96:TYR:CD1	2.51	0.45
18:N:28:LEU:HD23	18:N:48:VAL:HG21	1.98	0.45
1:1:2822:G:OP1	7:C:164:GLN:NE2	2.47	0.44
1:1:930:G:H1'	30:Z:25:LEU:HD11	1.98	0.44
1:1:1007:C:OP1	14:J:37:ARG:NH2	2.50	0.44
2:2:337:G:H2'	2:2:338:A:C8	2.52	0.44
7:C:186:LEU:HD21	20:P:4:ILE:HG21	1.98	0.44
1:1:2445:2MG:HM21	1:1:2449:U:O4	2.18	0.44
6:B:6:CYS:SG	6:B:13:ARG:NH1	2.90	0.44
1:1:1386:C:H2'	1:1:1387:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1939:5MU:OP1	1:1:2604:U:O2'	2.36	0.44
1:1:2074:U:N3	1:1:2435:A:C6	2.73	0.44
1:1:2133:G:O2'	1:1:2157:G:N2	2.51	0.44
2:2:397:A:H3'	2:2:397:A:N3	2.33	0.44
2:2:684:U:H2'	2:2:685:G:O4'	2.18	0.44
1:1:2395:C:H2'	1:1:2396:G:O4'	2.18	0.44
1:1:39:G:H1'	8:D:43:THR:HG21	1.99	0.44
21:Q:76:TYR:OH	21:Q:92:ARG:NH1	2.50	0.44
29:Y:59:GLU:O	29:Y:63:ALA:HB3	2.18	0.44
1:1:1962:5MC:H4'	1:1:1963:U:OP1	2.18	0.44
1:1:2245:U:O2	1:1:2435:A:H2'	2.18	0.44
2:2:13:U:C2	2:2:915:A:C5	3.06	0.44
2:2:976:G:C8	2:2:1358:U:O2	2.71	0.44
1:1:1021:A:N6	1:1:1141:U:N3	2.47	0.44
2:2:1176:A:H2'	2:2:1177:G:O4'	2.16	0.44
2:2:376:G:C2	2:2:389:A:C2	3.06	0.44
1:1:1060:U:OP2	13:I:71:LYS:NZ	2.46	0.44
1:1:954:G:OP2	17:M:16:ARG:NH2	2.50	0.44
2:2:915:A:H8	2:2:915:A:O5'	2.00	0.44
17:M:35:ALA:HB2	17:M:102:LEU:HD11	2.00	0.44
1:1:959:A:N3	1:1:2457:PSU:O2'	2.49	0.43
1:1:1095:A:H2'	1:1:1096:A:C8	2.53	0.43
1:1:214:G:N2	1:1:216:A:N3	2.66	0.43
2:2:109:A:C6	2:2:326:G:C6	3.05	0.43
2:2:1417:G:C6	2:2:1482:G:C6	3.06	0.43
1:1:1589:U:C2	1:1:1590:A:C8	3.06	0.43
2:2:324:G:N2	2:2:327:A:C8	2.86	0.43
2:2:421:U:O2	2:2:421:U:O4'	2.37	0.43
7:C:172:VAL:HG11	7:C:175:LEU:HD21	2.01	0.43
12:H:121:SER:OG	12:H:126:LEU:HD11	2.18	0.43
1:1:1055:G:H4'	12:H:33:VAL:HA	2.00	0.43
15:K:24:VAL:HG13	15:K:33:ALA:HB2	2.00	0.43
1:1:1932:A:H2'	1:1:1933:G:O4'	2.19	0.43
2:2:1499:A:O2'	2:2:1500:A:C5'	2.66	0.43
15:K:107:LEU:HD21	15:K:115:ILE:HG21	2.01	0.43
1:1:1142:A:N3	1:1:1142:A:H2'	2.34	0.43
1:1:2252:G:H2'	1:1:2253:G:H8	1.84	0.43
1:1:1020:A:C2	1:1:1141:U:C2	3.07	0.43
1:1:1365:A:O5'	28:X:28:ARG:NH2	2.52	0.43
1:1:74:A:N7	1:1:88:G:C5	2.86	0.43
1:1:57:C:H2'	1:1:58:G:O4'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:973:A:O4'	1:1:1188:U:C6	2.72	0.42
1:1:2252:G:O2'	1:1:2253:G:H5'	2.18	0.42
14:J:73:VAL:HG11	14:J:75:TYR:CZ	2.53	0.42
15:K:76:VAL:HG12	20:P:73:VAL:HB	2.01	0.42
18:N:49:GLU:HB2	18:N:50:PRO:HD3	2.00	0.42
1:1:1394:U:C4	1:1:1395:A:C6	3.07	0.42
1:1:2469:A:N6	1:1:2481:G:O2'	2.52	0.42
1:1:745:1MG:HN21	1:1:745:1MG:HM11	1.66	0.42
2:2:1126:U:OP1	19:O:7:ARG:NH2	128.14	0.42
2:2:1323:G:H2'	2:2:1324:A:C8	2.54	0.42
2:2:622:A:C8	2:2:623:C:C6	3.08	0.42
6:B:37:ASN:HB2	6:B:62:TYR:HB2	2.01	0.42
21:Q:65:ILE:CD1	21:Q:92:ARG:HB2	2.50	0.42
1:1:2756:U:C4	1:1:2759:G:O6	2.72	0.42
1:1:2788:C:H2'	1:1:2789:C:C6	2.55	0.42
1:1:819:A:C4	1:1:1189:A:C2	3.07	0.42
2:2:384:G:H2'	2:2:385:C:C6	2.54	0.42
1:1:320:A:H2'	8:D:131:THR:HG21	2.01	0.42
25:U:12:ILE:CG2	25:U:80:ALA:HB2	2.49	0.42
1:1:2803:G:H2'	1:1:2804:U:C5	2.55	0.42
1:1:705:A:O4'	6:B:9:THR:HG21	2.19	0.42
1:1:813:U:H2'	1:1:814:C:C6	2.53	0.42
2:2:842:U:H3'	2:2:843:U:C5'	2.48	0.42
24:T:61:LEU:C	24:T:61:LEU:HD12	2.39	0.42
1:1:142:A:O2'	24:T:1:MET:N	2.47	0.42
1:1:567:U:OP2	16:L:29:LYS:NZ	2.53	0.42
15:K:38:ILE:HD11	15:K:112:PHE:CZ	2.55	0.42
1:1:1028:A:N6	1:1:1125:G:H2'	2.34	0.42
2:2:1498:UR3:O4'	2:2:1519:MA6:H2	2.20	0.42
2:2:37:U:O2	2:2:548:G:N2	2.52	0.42
19:O:99:TYR:OH	19:O:111:ARG:NH1	2.53	0.42
1:1:2511:U:O4	1:1:2575:C:N3	2.53	0.42
1:1:2602:A:H5''	1:1:2603:G:C5'	2.49	0.42
2:2:481:G:O2'	2:2:483:C:N4	2.52	0.42
30:Z:27:LEU:O	30:Z:38:ARG:NE	2.46	0.42
1:1:1065:U:O2'	1:1:1066:U:O5'	2.34	0.42
1:1:879:G:H2'	1:1:880:G:O4'	2.19	0.42
8:D:134:LEU:HB2	8:D:160:ALA:HB1	2.02	0.42
12:H:123:ILE:HD13	12:H:123:ILE:O	2.20	0.42
1:1:1082:U:C4	1:1:1086:A:N6	2.88	0.42
1:1:36:G:N3	1:1:450:G:O2'	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:429:U:O2	2:2:430:A:N7	2.53	0.42
6:B:240:PHE:O	6:B:240:PHE:CD2	2.73	0.42
13:I:109:ALA:HB2	13:I:128:ILE:CD1	2.49	0.42
14:J:32:LEU:HD23	14:J:54:ILE:HD13	2.01	0.42
1:1:1570:A:H2'	1:1:1571:A:C8	2.55	0.42
8:D:48:THR:HG23	8:D:86:ALA:HB3	2.02	0.42
12:H:18:VAL:HG22	12:H:86:MET:HE2	2.02	0.42
1:1:1021:A:C3'	1:1:1021:A:N3	2.78	0.41
1:1:1082:U:N3	1:1:1086:A:C6	2.87	0.41
1:1:1250:G:OP2	16:L:21:ARG:NH2	2.52	0.41
1:1:749:A:N1	1:1:753:A:O2'	2.48	0.41
1:1:948:C:H1'	1:1:984:A:C8	2.55	0.41
2:2:1235:U:H2'	2:2:1236:A:O4'	2.20	0.41
2:2:216:U:H2'	2:2:217:C:C6	2.55	0.41
28:X:37:ARG:HG2	28:X:48:THR:HG23	2.00	0.41
2:2:1333:A:H2'	2:2:1334:G:O4'	2.19	0.41
2:2:502:A:H2'	2:2:503:C:O4'	2.20	0.41
2:2:977:A:H1'	2:2:982:U:O4	2.20	0.41
1:1:1668:A:O2'	1:1:1674:G:N7	2.44	0.41
1:1:742:A:N1	1:1:755:U:O4	2.53	0.41
6:B:119:GLY:O	6:B:130:LEU:HB3	2.20	0.41
9:E:122:PHE:CZ	9:E:167:ARG:HA	2.55	0.41
11:G:9:VAL:HG11	11:G:12:LEU:HD21	2.03	0.41
12:H:35:VAL:O	12:H:39:THR:HG23	2.20	0.41
25:U:39:ILE:HG22	25:U:40:ASN:N	2.34	0.41
1:1:984:A:N3	1:1:984:A:H2'	2.35	0.41
2:2:860:A:H2'	2:2:861:G:O4'	2.21	0.41
9:E:171:ALA:O	9:E:174:ASP:N	2.54	0.41
10:F:25:THR:HG22	10:F:34:THR:HG23	2.02	0.41
1:1:1548:A:H2'	1:1:1549:A:C8	2.55	0.41
1:1:17:G:H2'	1:1:18:U:C6	2.56	0.41
1:1:548:G:H3'	1:1:549:G:O4'	2.20	0.41
2:2:791:G:N2	2:2:1497:G:O3'	2.53	0.41
8:D:145:ASP:HA	8:D:166:LYS:HB3	2.01	0.41
1:1:1082:U:H3	1:1:1086:A:N6	2.15	0.41
1:1:1169:A:H5''	1:1:1169:A:N3	2.36	0.41
1:1:1182:G:H2'	1:1:1183:U:O4'	2.20	0.41
1:1:2273:A:H2'	1:1:2274:A:C8	2.56	0.41
2:2:429:U:O2	2:2:430:A:C8	2.72	0.41
18:N:67:PHE:O	18:N:71:ARG:HG2	2.21	0.41
18:N:9:GLN:O	18:N:17:ARG:NH2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:197:A:N6	1:1:2430:A:H2'	2.36	0.41
1:1:5:A:H2'	1:1:6:A:C8	2.56	0.41
1:1:851:C:H2'	1:1:852:U:C6	2.56	0.41
6:B:76:ALA:HB2	6:B:96:TYR:CE1	2.55	0.41
7:C:175:LEU:CD1	7:C:193:VAL:HG12	2.51	0.41
23:S:92:ARG:NE	23:S:94:ASP:OD1	2.53	0.41
1:1:2683:C:O2	15:K:70:ARG:NH2	2.53	0.41
1:1:493:G:H2'	1:1:494:G:O4'	2.21	0.41
2:2:662:U:O2'	2:2:836:G:OP1	2.32	0.41
19:O:53:THR:HG23	19:O:74:VAL:HG21	2.03	0.41
2:2:548:G:C6	2:2:549:C:C4	3.08	0.41
1:1:2311:A:C2	9:E:85:ILE:HD11	2.55	0.41
21:Q:66:ASN:OD1	21:Q:70:ARG:NE	2.54	0.41
30:Z:25:LEU:HD13	30:Z:25:LEU:C	2.41	0.41
2:2:218:U:H2'	2:2:219:U:O4'	2.21	0.41
1:1:871:U:H2'	1:1:872:U:C6	2.56	0.41
2:2:915:A:C3'	2:2:915:A:C8	3.04	0.41
12:H:118:ILE:HD12	12:H:118:ILE:N	2.36	0.41
12:H:23:LEU:HD22	12:H:93:ALA:N	2.36	0.41
23:S:75:PHE:CZ	23:S:104:THR:HG21	2.56	0.41
1:1:2572:A:N7	7:C:150:GLN:NE2	2.69	0.40
2:2:712:A:H2'	2:2:713:G:O4'	2.21	0.40
24:T:46:ALA:O	24:T:50:LEU:HB2	2.21	0.40
27:W:59:LEU:HD12	27:W:80:ILE:HD12	2.03	0.40
28:X:33:LEU:O	28:X:34:HIS:CG	2.75	0.40
1:1:1406:U:C2'	1:1:1407:G:OP2	2.69	0.40
1:1:1421:G:C2	1:1:1422:G:C8	3.09	0.40
1:1:476:G:H4'	1:1:502:A:N1	2.35	0.40
11:G:57:LYS:O	11:G:61:VAL:HG13	2.21	0.40
16:L:109:LYS:HG2	16:L:126:ARG:HB2	2.02	0.40
17:M:73:ILE:HG21	17:M:91:TYR:CZ	2.56	0.40
18:N:29:VAL:HG11	18:N:75:ILE:HG23	2.03	0.40
1:1:207:A:H2'	1:1:208:C:O4'	2.21	0.40
2:2:1189:U:OP1	23:S:98:LYS:NZ	162.23	0.40
1:1:2298:A:C5	1:1:2321:U:C4	3.09	0.40
1:1:2006:C:O2'	1:1:2823:A:N3	2.47	0.40
1:1:67:U:C4	1:1:74:A:C6	3.04	0.40
2:2:915:A:C6	2:2:916:U:C4	3.09	0.40
13:I:105:LEU:HD22	13:I:128:ILE:CG2	2.51	0.40
1:1:1406:U:O2'	1:1:1407:G:OP2	2.39	0.40
1:1:2806:C:H2'	1:1:2807:U:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:753:A:C5	1:1:754:U:C5	3.09	0.40
2:2:1225:A:H2'	2:2:1226:C:C5	2.56	0.40
2:2:152:A:N6	2:2:170:U:C2	2.89	0.40
2:2:580:C:H2'	2:2:581:G:O4'	2.21	0.40
6:B:232:HIS:CG	6:B:240:PHE:HE1	2.40	0.40
13:I:83:ALA:HB2	13:I:100:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	B	269/273 (98%)	259 (96%)	9 (3%)	1 (0%)	39	75
7	C	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
8	D	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	34	72
9	E	175/179 (98%)	164 (94%)	10 (6%)	1 (1%)	30	68
10	F	173/177 (98%)	161 (93%)	12 (7%)	0	100	100
11	G	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
12	H	128/165 (78%)	106 (83%)	18 (14%)	4 (3%)	5	27
13	I	133/142 (94%)	119 (90%)	13 (10%)	1 (1%)	24	63
14	J	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
15	K	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
16	L	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
17	M	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
18	N	117/127 (92%)	107 (92%)	10 (8%)	0	100	100
19	O	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
20	P	112/115 (97%)	105 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	Q	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	21	61
22	R	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	19	58
23	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
24	T	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
25	U	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	19	58
26	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
27	W	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
28	X	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
29	Y	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
30	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
31	a	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
32	b	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
33	c	50/55 (91%)	50 (100%)	0	0	100	100
34	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
35	e	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
36	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
37	g	223/241 (92%)	210 (94%)	13 (6%)	0	100	100
38	h	206/233 (88%)	196 (95%)	9 (4%)	1 (0%)	34	72
39	i	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
40	j	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	30	68
41	k	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	19	58
42	l	149/179 (83%)	144 (97%)	4 (3%)	1 (1%)	26	65
43	m	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	24	63
44	n	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	24	63
45	o	97/103 (94%)	89 (92%)	7 (7%)	1 (1%)	19	58
46	p	115/129 (89%)	104 (90%)	9 (8%)	2 (2%)	11	43
47	q	120/124 (97%)	119 (99%)	1 (1%)	0	100	100
48	r	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
49	s	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
50	t	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
51	u	80/82 (98%)	75 (94%)	4 (5%)	1 (1%)	15	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	v	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
53	w	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
54	x	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
55	y	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
56	z	68/71 (96%)	68 (100%)	0	0	100	100
All	All	5869/6220 (94%)	5572 (95%)	276 (5%)	21 (0%)	43	75

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	n	56	ASP
6	B	158	ALA
8	D	142	ALA
12	H	51	TYR
12	H	117	LEU
21	Q	3	ARG
42	l	130	ASN
45	o	58	ASN
46	p	119	ASN
9	E	40	VAL
38	h	80	LYS
25	U	39	ILE
12	H	108	VAL
41	k	96	VAL
22	R	44	GLY
40	j	44	GLY
13	I	136	GLY
46	p	74	VAL
51	u	64	GLY
12	H	55	VAL
43	m	75	ILE

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	
6	B	216/218 (99%)	199 (92%)	17 (8%)	15	49
7	C	164/164 (100%)	157 (96%)	7 (4%)	35	72
8	D	165/165 (100%)	151 (92%)	14 (8%)	13	45
9	E	148/150 (99%)	134 (90%)	14 (10%)	11	38
10	F	136/138 (99%)	132 (97%)	4 (3%)	50	81
11	G	114/114 (100%)	104 (91%)	10 (9%)	12	43
12	H	99/123 (80%)	88 (89%)	11 (11%)	8	29
13	I	104/110 (94%)	91 (88%)	13 (12%)	6	22
14	J	116/116 (100%)	110 (95%)	6 (5%)	29	65
15	K	104/104 (100%)	98 (94%)	6 (6%)	25	61
16	L	103/103 (100%)	97 (94%)	6 (6%)	25	61
17	M	109/109 (100%)	104 (95%)	5 (5%)	33	70
18	N	99/103 (96%)	91 (92%)	8 (8%)	15	47
19	O	86/87 (99%)	80 (93%)	6 (7%)	19	54
20	P	99/100 (99%)	95 (96%)	4 (4%)	38	75
21	Q	89/90 (99%)	87 (98%)	2 (2%)	60	85
22	R	84/84 (100%)	78 (93%)	6 (7%)	18	54
23	S	93/93 (100%)	84 (90%)	9 (10%)	10	36
24	T	81/84 (96%)	76 (94%)	5 (6%)	23	59
25	U	84/85 (99%)	78 (93%)	6 (7%)	18	54
26	V	78/78 (100%)	74 (95%)	4 (5%)	29	66
27	W	58/63 (92%)	57 (98%)	1 (2%)	68	89
28	X	67/68 (98%)	64 (96%)	3 (4%)	34	70
29	Y	54/55 (98%)	53 (98%)	1 (2%)	65	87
30	Z	48/49 (98%)	46 (96%)	2 (4%)	36	73
31	a	59/62 (95%)	53 (90%)	6 (10%)	9	33
32	b	47/48 (98%)	41 (87%)	6 (13%)	5	21
33	c	47/49 (96%)	44 (94%)	3 (6%)	22	57
34	d	38/38 (100%)	35 (92%)	3 (8%)	15	49
35	e	51/52 (98%)	46 (90%)	5 (10%)	10	36
36	f	34/34 (100%)	32 (94%)	2 (6%)	24	60
37	g	187/199 (94%)	180 (96%)	7 (4%)	41	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	h	171/190 (90%)	166 (97%)	5 (3%)	50	81
39	i	172/173 (99%)	166 (96%)	6 (4%)	43	78
40	j	119/126 (94%)	112 (94%)	7 (6%)	24	60
41	k	91/116 (78%)	85 (93%)	6 (7%)	21	56
42	l	124/147 (84%)	115 (93%)	9 (7%)	17	52
43	m	104/105 (99%)	102 (98%)	2 (2%)	65	87
44	n	105/107 (98%)	100 (95%)	5 (5%)	31	69
45	o	86/90 (96%)	80 (93%)	6 (7%)	19	54
46	p	90/99 (91%)	87 (97%)	3 (3%)	45	79
47	q	102/103 (99%)	95 (93%)	7 (7%)	19	55
48	r	94/96 (98%)	85 (90%)	9 (10%)	10	37
49	s	83/84 (99%)	79 (95%)	4 (5%)	31	69
50	t	76/77 (99%)	64 (84%)	12 (16%)	3	13
51	u	65/65 (100%)	61 (94%)	4 (6%)	23	59
52	v	74/78 (95%)	72 (97%)	2 (3%)	52	82
53	w	57/65 (88%)	56 (98%)	1 (2%)	66	88
54	x	72/79 (91%)	68 (94%)	4 (6%)	26	62
55	y	65/66 (98%)	60 (92%)	5 (8%)	16	50
56	z	60/61 (98%)	57 (95%)	3 (5%)	30	67
All	All	4871/5062 (96%)	4569 (94%)	302 (6%)	27	59

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	51	THR
6	B	52	ARG
6	B	118	SER
6	B	125	LYS
6	B	130	LEU
6	B	141	VAL
6	B	156	ARG
6	B	187	ASP
6	B	189	ARG
6	B	195	VAL
6	B	202	LEU

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Mol	Chain	Res	Type
6	B	203	ARG
6	B	204	VAL
6	B	205	LEU
6	B	242	LYS
6	B	258	ARG
6	B	271	ARG
7	C	13	ARG
7	C	18	ASP
7	C	32	ASN
7	C	46	ARG
7	C	91	THR
7	C	103	ASP
7	C	131	ASP
8	D	7	ASP
8	D	17	THR
8	D	22	ASP
8	D	40	ARG
8	D	48	THR
8	D	57	LYS
8	D	69	ARG
8	D	77	ILE
8	D	80	SER
8	D	108	ILE
8	D	109	LEU
8	D	122	GLU
8	D	149	ILE
8	D	179	SER
9	E	6	ASP
9	E	10	ASP
9	E	57	LEU
9	E	80	ARG
9	E	95	ARG
9	E	105	THR
9	E	115	ARG
9	E	117	LEU
9	E	122	PHE
9	E	123	ASP
9	E	133	ARG
9	E	140	GLU
9	E	152	LEU
9	E	163	ASP
10	F	39	ASP

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Mol	Chain	Res	Type
10	F	95	ARG
10	F	125	CYS
10	F	171	THR
11	G	11	ASN
11	G	12	LEU
11	G	15	LEU
11	G	41	LYS
11	G	66	ASN
11	G	72	ILE
11	G	87	GLU
11	G	97	ARG
11	G	101	ASP
11	G	127	GLU
12	H	3	LEU
12	H	9	GLN
12	H	34	THR
12	H	37	LYS
12	H	40	GLU
12	H	54	VAL
12	H	57	ASN
12	H	81	LEU
12	H	109	LYS
12	H	122	GLN
12	H	123	ILE
13	I	10	LEU
13	I	11	GLN
13	I	38	CYS
13	I	42	ASN
13	I	46	ASP
13	I	48	ILE
13	I	67	THR
13	I	78	LEU
13	I	79	LEU
13	I	81	LYS
13	I	91	LYS
13	I	95	ASP
13	I	111	THR
14	J	1	MET
14	J	14	ASP
14	J	30	THR
14	J	40	HIS
14	J	57	LEU

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Mol	Chain	Res	Type
14	J	142	ILE
15	K	32	TYR
15	K	49	ARG
15	K	53	LYS
15	K	80	ASP
15	K	88	ASN
15	K	104	THR
16	L	5	THR
16	L	27	LEU
16	L	48	ARG
16	L	59	ARG
16	L	76	GLU
16	L	78	ARG
17	M	18	ARG
17	M	84	LYS
17	M	110	GLU
17	M	126	ILE
17	M	128	THR
18	N	2	ARG
18	N	20	MET
18	N	24	MET
18	N	51	LEU
18	N	63	ARG
18	N	65	LEU
18	N	69	ARG
18	N	95	THR
19	O	13	ARG
19	O	19	GLN
19	O	31	THR
19	O	47	VAL
19	O	48	LEU
19	O	91	SER
20	P	10	GLN
20	P	27	GLU
20	P	85	SER
20	P	114	LEU
21	Q	18	LEU
21	Q	51	ARG
22	R	10	LYS
22	R	13	ARG
22	R	48	LYS
22	R	51	VAL

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Mol	Chain	Res	Type
22	R	68	ARG
22	R	86	GLN
23	S	7	HIS
23	S	19	LEU
23	S	30	SER
23	S	41	LYS
23	S	69	LEU
23	S	97	LEU
23	S	107	VAL
23	S	109	ASP
23	S	110	ARG
24	T	1	MET
24	T	24	MET
24	T	37	ASP
24	T	59	ASN
24	T	93	LEU
25	U	52	LEU
25	U	68	SER
25	U	72	ILE
25	U	89	ASP
25	U	99	ASN
25	U	101	GLU
26	V	40	ILE
26	V	41	GLU
26	V	69	GLU
26	V	71	LYS
27	W	70	GLU
28	X	48	THR
28	X	54	LYS
28	X	71	LEU
29	Y	58	ASN
30	Z	3	LYS
30	Z	45	ARG
31	a	3	LYS
31	a	16	CYS
31	a	43	PHE
31	a	47	LYS
31	a	59	ARG
31	a	65	ASN
32	b	9	THR
32	b	12	LYS
32	b	26	THR

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Mol	Chain	Res	Type
32	b	27	SER
32	b	29	SER
32	b	40	ARG
33	c	5	ILE
33	c	24	THR
33	c	26	ASN
34	d	22	MET
34	d	41	ARG
34	d	42	LEU
35	e	8	ARG
35	e	30	ARG
35	e	31	HIS
35	e	54	ASP
35	e	55	LEU
36	f	3	VAL
36	f	26	ILE
37	g	8	ASP
37	g	23	TRP
37	g	45	LYS
37	g	105	LYS
37	g	128	LYS
37	g	129	LEU
37	g	132	LYS
38	h	14	ILE
38	h	89	LYS
38	h	164	ARG
38	h	185	ASN
38	h	200	VAL
39	i	47	ARG
39	i	95	GLU
39	i	104	ARG
39	i	116	GLN
39	i	138	SER
39	i	143	VAL
40	j	10	GLU
40	j	15	LEU
40	j	60	ILE
40	j	114	VAL
40	j	115	LEU
40	j	138	ARG
40	j	162	GLU
41	k	16	GLU

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Mol	Chain	Res	Type
41	k	24	ARG
41	k	38	ARG
41	k	54	LEU
41	k	79	ARG
41	k	86	ARG
42	l	7	ILE
42	l	17	LYS
42	l	21	GLU
42	l	23	LEU
42	l	79	ARG
42	l	97	ASN
42	l	109	ARG
42	l	130	ASN
42	l	146	GLU
43	m	96	MET
43	m	121	LEU
44	n	12	ARG
44	n	27	LYS
44	n	60	LYS
44	n	63	LEU
44	n	118	LEU
45	o	5	ARG
45	o	17	LEU
45	o	24	GLU
45	o	25	ILE
45	o	27	GLU
45	o	37	ARG
46	p	15	GLN
46	p	56	ARG
46	p	107	ILE
47	q	5	ASN
47	q	12	ARG
47	q	24	LEU
47	q	56	ARG
47	q	62	GLU
47	q	74	LEU
47	q	102	LEU
48	r	11	ASP
48	r	16	VAL
48	r	25	VAL
48	r	29	ARG
48	r	59	GLU

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Mol	Chain	Res	Type
48	r	92	ARG
48	r	93	ARG
48	r	104	THR
48	r	117	LYS
49	s	45	VAL
49	s	46	LEU
49	s	89	MET
49	s	92	GLU
50	t	10	LYS
50	t	17	ARG
50	t	22	THR
50	t	39	LEU
50	t	40	GLN
50	t	64	ARG
50	t	66	LEU
50	t	67	LEU
50	t	70	LEU
50	t	73	LYS
50	t	84	ARG
50	t	85	LEU
51	u	1	MET
51	u	2	VAL
51	u	6	LEU
51	u	19	VAL
52	v	75	LEU
52	v	81	LYS
53	w	74	HIS
54	x	12	ASP
54	x	21	LYS
54	x	33	THR
54	x	79	THR
55	y	6	SER
55	y	10	ARG
55	y	48	GLN
55	y	54	MET
55	y	64	LYS
56	z	34	ARG
56	z	62	ARG
56	z	67	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2896/2904 (99%)	538 (18%)	81 (2%)
2	2	1522/1534 (99%)	292 (19%)	38 (2%)
3	3	119/120 (99%)	17 (14%)	0
4	4	4/18 (22%)	1 (25%)	0
5	5	73/78 (93%)	23 (31%)	8 (10%)
All	All	4614/4654 (99%)	871 (18%)	127 (2%)

All (871) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	34	U
1	1	35	G
1	1	46	G
1	1	58	G
1	1	60	G
1	1	63	A
1	1	71	A
1	1	74	A
1	1	75	G
1	1	83	A
1	1	84	A
1	1	85	G
1	1	93	G
1	1	96	C
1	1	102	U
1	1	103	A
1	1	110	G
1	1	114	U
1	1	118	A
1	1	119	A
1	1	120	U
1	1	122	G
1	1	131	A
1	1	136	G
1	1	139	U
1	1	140	C
1	1	141	G
1	1	145	C
1	1	163	C

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Mol	Chain	Res	Type
1	1	165	A
1	1	181	A
1	1	196	A
1	1	200	U
1	1	215	G
1	1	216	A
1	1	222	A
1	1	225	C
1	1	248	G
1	1	249	C
1	1	261	G
1	1	264	C
1	1	265	A
1	1	266	G
1	1	267	C
1	1	271	G
1	1	272	A
1	1	275	C
1	1	276	U
1	1	278	A
1	1	285	G
1	1	311	A
1	1	324	A
1	1	329	G
1	1	330	A
1	1	353	C
1	1	359	G
1	1	361	G
1	1	362	A
1	1	371	A
1	1	372	G
1	1	373	U
1	1	375	G
1	1	383	C
1	1	386	G
1	1	396	G
1	1	405	U
1	1	411	G
1	1	412	A
1	1	420	C
1	1	424	G
1	1	435	C

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Mol	Chain	Res	Type
1	1	451	U
1	1	456	C
1	1	457	A
1	1	477	A
1	1	481	G
1	1	491	G
1	1	501	A
1	1	503	A
1	1	504	A
1	1	505	A
1	1	509	C
1	1	522	A
1	1	529	A
1	1	532	A
1	1	543	G
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	551	G
1	1	563	A
1	1	569	U
1	1	573	U
1	1	575	A
1	1	588	U
1	1	603	A
1	1	609	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	618	G
1	1	621	A
1	1	627	A
1	1	637	A
1	1	645	C
1	1	647	G
1	1	654	A
1	1	664	G
1	1	668	A
1	1	685	A
1	1	686	U

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Mol	Chain	Res	Type
1	1	710	U
1	1	717	C
1	1	730	A
1	1	738	G
1	1	746	PSU
1	1	747	5MU
1	1	757	G
1	1	764	A
1	1	765	C
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	800	A
1	1	802	A
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	845	A
1	1	846	U
1	1	858	G
1	1	859	G
1	1	869	G
1	1	878	A
1	1	881	G
1	1	884	U
1	1	885	C
1	1	888	C
1	1	891	G
1	1	892	A
1	1	893	C
1	1	895	U
1	1	896	A
1	1	897	C
1	1	899	A
1	1	907	G
1	1	910	A
1	1	914	G
1	1	915	C

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Mol	Chain	Res	Type
1	1	931	U
1	1	941	A
1	1	945	A
1	1	946	C
1	1	953	G
1	1	961	C
1	1	974	G
1	1	983	A
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1012	U
1	1	1013	C
1	1	1022	G
1	1	1023	U
1	1	1026	G
1	1	1033	U
1	1	1041	G
1	1	1045	C
1	1	1046	A
1	1	1047	G
1	1	1060	U
1	1	1061	U
1	1	1062	G
1	1	1063	G
1	1	1064	C
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1069	A
1	1	1070	A
1	1	1071	G
1	1	1073	A
1	1	1074	G
1	1	1076	C
1	1	1079	C
1	1	1080	A
1	1	1081	U
1	1	1082	U
1	1	1083	U

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Mol	Chain	Res	Type
1	1	1084	A
1	1	1087	G
1	1	1088	A
1	1	1090	A
1	1	1095	A
1	1	1096	A
1	1	1107	G
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1119	U
1	1	1122	G
1	1	1132	U
1	1	1134	A
1	1	1135	C
1	1	1142	A
1	1	1169	A
1	1	1170	C
1	1	1173	U
1	1	1174	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1179	G
1	1	1180	U
1	1	1186	G
1	1	1238	G
1	1	1248	G
1	1	1253	A
1	1	1256	G
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1273	U
1	1	1301	A
1	1	1321	A
1	1	1345	C
1	1	1352	U
1	1	1365	A
1	1	1368	G
1	1	1378	A

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Mol	Chain	Res	Type
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1387	A
1	1	1392	A
1	1	1395	A
1	1	1406	U
1	1	1407	G
1	1	1408	G
1	1	1411	U
1	1	1414	C
1	1	1415	U
1	1	1416	G
1	1	1417	C
1	1	1419	A
1	1	1420	A
1	1	1428	C
1	1	1452	G
1	1	1453	A
1	1	1460	U
1	1	1478	G
1	1	1482	G
1	1	1490	A
1	1	1497	U
1	1	1503	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1529	G
1	1	1534	U
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1554	U
1	1	1559	U
1	1	1566	A
1	1	1569	A
1	1	1578	U
1	1	1580	A
1	1	1581	G
1	1	1582	C

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Mol	Chain	Res	Type
1	1	1583	A
1	1	1584	U
1	1	1589	U
1	1	1590	A
1	1	1608	A
1	1	1609	A
1	1	1610	A
1	1	1619	G
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G
1	1	1674	G
1	1	1677	A
1	1	1703	G
1	1	1714	U
1	1	1715	G
1	1	1718	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1750	G
1	1	1755	A
1	1	1758	U
1	1	1764	C
1	1	1773	A
1	1	1791	A
1	1	1800	C
1	1	1801	A
1	1	1808	A
1	1	1811	G
1	1	1816	C
1	1	1829	A
1	1	1833	C
1	1	1847	A
1	1	1848	A
1	1	1858	A
1	1	1859	U
1	1	1862	G
1	1	1864	U
1	1	1869	G

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Mol	Chain	Res	Type
1	1	1870	C
1	1	1872	A
1	1	1873	G
1	1	1905	C
1	1	1906	G
1	1	1907	G
1	1	1912	A
1	1	1913	A
1	1	1914	C
1	1	1916	A
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1938	A
1	1	1955	U
1	1	1963	U
1	1	1965	C
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1987	A
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2022	U
1	1	2023	C
1	1	2027	G
1	1	2031	A
1	1	2033	A
1	1	2043	C
1	1	2051	A
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A

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Mol	Chain	Res	Type
1	1	2069	G7M
1	1	2077	A
1	1	2093	G
1	1	2097	A
1	1	2099	U
1	1	2100	G
1	1	2108	A
1	1	2110	G
1	1	2111	U
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2121	G
1	1	2122	U
1	1	2124	G
1	1	2125	G
1	1	2126	A
1	1	2127	G
1	1	2128	G
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2139	U
1	1	2141	G
1	1	2146	C
1	1	2147	A
1	1	2154	A
1	1	2157	G
1	1	2158	A
1	1	2159	G
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2169	A
1	1	2171	A
1	1	2172	U
1	1	2178	C
1	1	2182	U

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Mol	Chain	Res	Type
1	1	2183	A
1	1	2185	U
1	1	2188	U
1	1	2189	U
1	1	2190	G
1	1	2191	A
1	1	2193	G
1	1	2194	U
1	1	2198	A
1	1	2204	G
1	1	2210	U
1	1	2211	A
1	1	2212	A
1	1	2213	U
1	1	2225	A
1	1	2226	C
1	1	2229	U
1	1	2238	G
1	1	2239	G
1	1	2244	U
1	1	2250	G
1	1	2251	OMG
1	1	2268	A
1	1	2278	A
1	1	2283	C
1	1	2287	A
1	1	2297	A
1	1	2305	U
1	1	2308	G
1	1	2309	A
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2339	C
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2361	G
1	1	2372	U
1	1	2376	A
1	1	2383	G

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Mol	Chain	Res	Type
1	1	2385	C
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2426	A
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2434	A
1	1	2435	A
1	1	2441	U
1	1	2445	2MG
1	1	2447	G
1	1	2448	A
1	1	2470	G
1	1	2474	U
1	1	2476	A
1	1	2478	A
1	1	2484	G
1	1	2491	U
1	1	2502	G
1	1	2504	PSU
1	1	2505	G
1	1	2506	U
1	1	2507	C
1	1	2512	C
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2525	G
1	1	2529	G
1	1	2535	G
1	1	2547	A
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2574	G

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Mol	Chain	Res	Type
1	1	2585	U
1	1	2586	U
1	1	2602	A
1	1	2603	G
1	1	2609	U
1	1	2610	C
1	1	2611	C
1	1	2613	U
1	1	2629	U
1	1	2663	G
1	1	2669	G
1	1	2671	G
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2722	G
1	1	2726	A
1	1	2744	G
1	1	2748	A
1	1	2757	A
1	1	2758	A
1	1	2765	A
1	1	2777	G
1	1	2778	A
1	1	2791	G
1	1	2793	C
1	1	2796	U
1	1	2797	U
1	1	2798	U
1	1	2799	A
1	1	2801	G
1	1	2818	U
1	1	2820	A
1	1	2823	A
1	1	2825	G
1	1	2849	U
1	1	2850	A
1	1	2859	G
1	1	2861	U
1	1	2867	G
1	1	2880	C
1	1	2884	U

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Mol	Chain	Res	Type
1	1	2885	G
1	1	2891	U
1	1	2902	C
2	2	4	U
2	2	5	U
2	2	9	G
2	2	22	G
2	2	29	U
2	2	32	A
2	2	39	G
2	2	41	G
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	54	C
2	2	69	G
2	2	70	U
2	2	71	A
2	2	72	A
2	2	74	A
2	2	76	G
2	2	82	G
2	2	83	C
2	2	84	U
2	2	87	C
2	2	90	C
2	2	94	G
2	2	95	C
2	2	96	U
2	2	108	G
2	2	120	A
2	2	122	G
2	2	128	G
2	2	131	A
2	2	141	G
2	2	144	G
2	2	149	A
2	2	160	A
2	2	164	G
2	2	173	U

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Mol	Chain	Res	Type
2	2	181	A
2	2	182	A
2	2	197	A
2	2	204	G
2	2	208	U
2	2	209	U
2	2	210	C
2	2	211	G
2	2	212	G
2	2	216	U
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	253	A
2	2	258	G
2	2	262	A
2	2	266	G
2	2	267	C
2	2	271	C
2	2	279	A
2	2	289	G
2	2	299	G
2	2	306	A
2	2	321	A
2	2	328	C
2	2	329	A
2	2	332	G
2	2	347	G
2	2	352	C
2	2	353	A
2	2	354	G
2	2	355	C
2	2	367	U
2	2	372	C
2	2	373	A
2	2	376	G
2	2	382	A
2	2	384	G
2	2	392	C
2	2	393	A
2	2	397	A

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Mol	Chain	Res	Type
2	2	406	G
2	2	411	A
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	429	U
2	2	446	G
2	2	451	A
2	2	457	G
2	2	458	U
2	2	460	A
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	469	C
2	2	478	A
2	2	479	U
2	2	484	G
2	2	485	U
2	2	486	U
2	2	505	G
2	2	509	A
2	2	511	C
2	2	517	G
2	2	518	C
2	2	519	C
2	2	526	C
2	2	527	7MG
2	2	528	C
2	2	531	U
2	2	532	A
2	2	533	A
2	2	542	G
2	2	547	A
2	2	559	A
2	2	562	U
2	2	568	G
2	2	572	A

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Mol	Chain	Res	Type
2	2	573	A
2	2	576	C
2	2	577	G
2	2	579	A
2	2	596	A
2	2	628	G
2	2	633	G
2	2	642	A
2	2	649	A
2	2	650	G
2	2	653	U
2	2	665	A
2	2	666	G
2	2	687	A
2	2	700	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	747	A
2	2	748	G
2	2	755	G
2	2	760	G
2	2	777	A
2	2	793	U
2	2	794	A
2	2	815	A
2	2	817	C
2	2	828	U
2	2	829	G
2	2	832	G
2	2	841	C
2	2	844	G
2	2	845	A
2	2	849	G
2	2	874	G
2	2	887	G
2	2	902	G
2	2	914	A
2	2	916	U
2	2	926	G
2	2	934	C

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Mol	Chain	Res	Type
2	2	935	A
2	2	954	G
2	2	960	U
2	2	963	G
2	2	966	2MG
2	2	967	5MC
2	2	968	A
2	2	969	A
2	2	972	C
2	2	975	A
2	2	976	G
2	2	991	U
2	2	992	U
2	2	993	G
2	2	996	A
2	2	999	C
2	2	1004	A
2	2	1008	U
2	2	1009	U
2	2	1017	U
2	2	1018	G
2	2	1021	A
2	2	1024	G
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1037	C
2	2	1043	G
2	2	1044	A
2	2	1046	A
2	2	1065	U
2	2	1085	U
2	2	1086	U
2	2	1094	G
2	2	1095	U
2	2	1099	G
2	2	1101	A
2	2	1124	G
2	2	1133	G
2	2	1135	U
2	2	1136	C

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Mol	Chain	Res	Type
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1142	G
2	2	1143	G
2	2	1145	A
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1158	C
2	2	1159	U
2	2	1167	A
2	2	1171	A
2	2	1174	G
2	2	1175	G
2	2	1176	A
2	2	1184	G
2	2	1196	A
2	2	1197	A
2	2	1206	G
2	2	1208	C
2	2	1211	U
2	2	1212	U
2	2	1213	A
2	2	1214	C
2	2	1215	G
2	2	1226	C
2	2	1227	A
2	2	1228	C
2	2	1238	A
2	2	1256	A
2	2	1257	A
2	2	1260	G
2	2	1275	A
2	2	1278	G
2	2	1279	G
2	2	1280	A
2	2	1285	A
2	2	1286	U
2	2	1287	A
2	2	1299	A

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Mol	Chain	Res	Type
2	2	1300	G
2	2	1302	C
2	2	1305	G
2	2	1312	G
2	2	1317	C
2	2	1320	C
2	2	1323	G
2	2	1329	A
2	2	1338	G
2	2	1340	A
2	2	1346	A
2	2	1347	G
2	2	1353	G
2	2	1363	A
2	2	1370	G
2	2	1378	C
2	2	1379	G
2	2	1381	U
2	2	1396	A
2	2	1397	C
2	2	1407	5MC
2	2	1408	A
2	2	1419	G
2	2	1429	A
2	2	1441	A
2	2	1446	A
2	2	1447	A
2	2	1448	C
2	2	1452	C
2	2	1453	G
2	2	1475	G
2	2	1487	G
2	2	1492	A
2	2	1494	G
2	2	1495	U
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1529	G
2	2	1530	G

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Mol	Chain	Res	Type
2	2	1534	A
3	3	2	G
3	3	9	G
3	3	13	G
3	3	16	G
3	3	17	C
3	3	35	C
3	3	36	C
3	3	45	A
3	3	51	G
3	3	56	G
3	3	64	G
3	3	66	A
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	109	A
4	4	15	A
5	5	5	G
5	5	8	4SU
5	5	13	A
5	5	15	C
5	5	16	C
5	5	17	U
5	5	18	G
5	5	19	G
5	5	20	H2U
5	5	21	A
5	5	22	G
5	5	25	C
5	5	37	A
5	5	47	U
5	5	48	C
5	5	49	G
5	5	55	PSU
5	5	58	A
5	5	59	A
5	5	60	U
5	5	64	G
5	5	69	C
5	5	74	C

All (127) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	62	U
1	1	70	G
1	1	101	A
1	1	140	C
1	1	196	A
1	1	199	A
1	1	271	G
1	1	369	U
1	1	404	A
1	1	446	G
1	1	503	A
1	1	512	G
1	1	545	U
1	1	546	U
1	1	548	G
1	1	555	G
1	1	614	A
1	1	620	G
1	1	685	A
1	1	764	A
1	1	784	G
1	1	883	G
1	1	892	A
1	1	894	U
1	1	896	A
1	1	984	A
1	1	995	C
1	1	1041	G
1	1	1045	C
1	1	1061	U
1	1	1063	G
1	1	1064	C
1	1	1069	A
1	1	1070	A
1	1	1110	G
1	1	1128	G
1	1	1142	A
1	1	1173	U
1	1	1174	U
1	1	1177	G
1	1	1286	A
1	1	1320	C

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Mol	Chain	Res	Type
1	1	1344	U
1	1	1379	U
1	1	1405	U
1	1	1406	U
1	1	1415	U
1	1	1420	A
1	1	1490	A
1	1	1509	A
1	1	1582	C
1	1	1583	A
1	1	1584	U
1	1	1608	A
1	1	1847	A
1	1	1913	A
1	1	1918	A
1	1	1962	5MC
1	1	2062	A
1	1	2146	C
1	1	2162	G
1	1	2189	U
1	1	2193	G
1	1	2210	U
1	1	2211	A
1	1	2212	A
1	1	2225	A
1	1	2250	G
1	1	2296	U
1	1	2425	A
1	1	2447	G
1	1	2506	U
1	1	2572	A
1	1	2602	A
1	1	2610	C
1	1	2756	U
1	1	2796	U
1	1	2797	U
1	1	2798	U
1	1	2849	U
1	1	2873	A
2	2	7	A
2	2	70	U
2	2	121	U

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Mol	Chain	Res	Type
2	2	181	A
2	2	183	C
2	2	209	U
2	2	305	G
2	2	328	C
2	2	428	G
2	2	481	G
2	2	496	A
2	2	516	PSU
2	2	517	G
2	2	531	U
2	2	532	A
2	2	559	A
2	2	562	U
2	2	641	U
2	2	722	G
2	2	793	U
2	2	966	2MG
2	2	967	5MC
2	2	991	U
2	2	992	U
2	2	1145	A
2	2	1196	A
2	2	1211	U
2	2	1212	U
2	2	1213	A
2	2	1214	C
2	2	1225	A
2	2	1299	A
2	2	1396	A
2	2	1407	5MC
2	2	1432	G
2	2	1447	A
2	2	1493	A
2	2	1516	2MG
5	5	16	C
5	5	17	U
5	5	18	G
5	5	19	G
5	5	20	H2U
5	5	47	U
5	5	58	A

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Mol	Chain	Res	Type
5	5	60	U

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

40 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	6MZ	1	1618	1	17,25,26	0.91	1 (5%)	15,36,39	1.85	4 (26%)
1	2MG	1	1835	1	18,26,27	1.29	1 (5%)	21,38,41	2.87	6 (28%)
1	PSU	1	1911	1	15,21,22	1.87	4 (26%)	16,30,33	3.21	5 (31%)
1	3TD	1	1915	1	15,22,23	1.13	1 (6%)	17,32,35	1.88	7 (41%)
1	PSU	1	1917	1	15,21,22	1.87	4 (26%)	16,30,33	3.36	4 (25%)
1	5MU	1	1939	1	13,22,23	1.78	2 (15%)	16,32,35	4.02	4 (25%)
1	5MC	1	1962	1	14,22,23	1.57	1 (7%)	17,32,35	1.78	2 (11%)
1	6MZ	1	2030	1	17,25,26	0.93	1 (5%)	15,36,39	2.18	4 (26%)
1	G7M	1	2069	1	18,26,27	1.66	2 (11%)	21,39,42	3.84	10 (47%)
1	OMG	1	2251	1,5	18,26,27	1.29	2 (11%)	21,38,41	2.52	5 (23%)
1	2MG	1	2445	1	18,26,27	1.32	1 (5%)	21,38,41	2.79	6 (28%)
1	PSU	1	2457	1	15,21,22	3.57	4 (26%)	16,30,33	3.64	7 (43%)
1	OMC	1	2498	1,57	15,22,23	1.22	2 (13%)	20,31,34	1.67	4 (20%)
1	2MA	1	2503	1,57	17,25,26	1.44	3 (17%)	18,37,40	3.00	7 (38%)
1	PSU	1	2504	1	15,21,22	3.20	4 (26%)	16,30,33	3.61	7 (43%)
1	OMU	1	2552	1	14,22,23	1.00	1 (7%)	19,31,34	2.34	2 (10%)
1	PSU	1	2580	1,57	15,21,22	2.86	3 (20%)	16,30,33	3.80	7 (43%)
1	PSU	1	2605	1	15,21,22	3.25	4 (26%)	16,30,33	3.70	8 (50%)
1	1MG	1	745	1	17,26,27	1.50	3 (17%)	19,39,42	1.77	4 (21%)
1	PSU	1	746	1,57	15,21,22	3.42	3 (20%)	16,30,33	3.97	7 (43%)
1	5MU	1	747	1	13,22,23	1.61	2 (15%)	16,32,35	4.05	4 (25%)
1	PSU	1	955	1	15,21,22	3.29	4 (26%)	16,30,33	3.64	7 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2MG	2	1207	2	18,26,27	1.70	2 (11%)	21,38,41	2.66	4 (19%)
2	4OC	2	1402	2	15,23,24	0.86	0	21,32,35	1.34	4 (19%)
2	5MC	2	1407	2	14,22,23	0.70	0	17,32,35	1.60	2 (11%)
2	UR3	2	1498	2	13,22,23	1.18	1 (7%)	18,32,35	1.02	1 (5%)
2	2MG	2	1516	2	18,26,27	1.30	1 (5%)	21,38,41	2.84	7 (33%)
2	MA6	2	1518	2	18,26,27	0.52	0	15,38,41	1.42	2 (13%)
2	MA6	2	1519	2	18,26,27	0.50	0	15,38,41	1.53	4 (26%)
2	PSU	2	516	57,2	15,21,22	1.89	4 (26%)	16,30,33	3.19	5 (31%)
2	7MG	2	527	2	20,26,27	1.34	2 (10%)	23,39,42	3.27	7 (30%)
2	2MG	2	966	2	18,26,27	1.34	1 (5%)	21,38,41	3.23	8 (38%)
2	5MC	2	967	2	14,22,23	1.41	1 (7%)	17,32,35	1.75	3 (17%)
5	H2U	5	20	5	17,21,22	0.72	0	23,30,33	1.84	4 (17%)
5	4OC	5	32	5	15,23,24	0.67	0	21,32,35	1.80	5 (23%)
5	5MU	5	54	5	13,22,23	1.40	2 (15%)	16,32,35	4.11	5 (31%)
5	PSU	5	55	5	15,21,22	3.06	4 (26%)	16,30,33	3.59	5 (31%)
5	8AN	5	76	57,5,58	18,24,25	0.67	0	10,35,38	0.51	0
5	4SU	5	8	5	12,21,22	0.76	0	15,30,33	1.37	3 (20%)
47	0TD	q	89	47	4,9,10	4.31	3 (75%)	4,11,13	5.61	4 (100%)

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	6MZ	1	1618	1	-	0/5/27/28	0/3/3/3
1	2MG	1	1835	1	-	0/5/27/28	0/3/3/3
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
1	3TD	1	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	1	1939	1	-	0/3/25/26	0/2/2/2
1	5MC	1	1962	1	-	0/3/25/26	0/2/2/2
1	6MZ	1	2030	1	-	0/5/27/28	0/3/3/3
1	G7M	1	2069	1	-	0/3/25/26	0/3/3/3
1	OMG	1	2251	1,5	-	0/5/27/28	0/3/3/3
1	2MG	1	2445	1	-	0/5/27/28	0/3/3/3
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2498	1,57	-	0/5/27/28	0/2/2/2
1	2MA	1	2503	1,57	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	2504	1	-	0/7/25/26	0/2/2/2
1	OMU	1	2552	1	-	0/5/27/28	0/2/2/2
1	PSU	1	2580	1,57	-	0/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
1	PSU	1	746	1,57	-	0/7/25/26	0/2/2/2
1	5MU	1	747	1	-	0/3/25/26	0/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
2	4OC	2	1402	2	-	0/7/29/30	0/2/2/2
2	5MC	2	1407	2	-	0/3/25/26	0/2/2/2
2	UR3	2	1498	2	-	0/3/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
2	MA6	2	1518	2	-	0/7/29/30	0/3/3/3
2	MA6	2	1519	2	-	0/7/29/30	0/3/3/3
2	PSU	2	516	57,2	-	0/7/25/26	0/2/2/2
2	7MG	2	527	2	-	0/7/37/38	0/3/3/3
2	2MG	2	966	2	-	0/5/27/28	0/3/3/3
2	5MC	2	967	2	-	0/3/25/26	0/2/2/2
5	H2U	5	20	5	-	0/7/38/39	0/2/2/2
5	4OC	5	32	5	-	0/7/29/30	0/2/2/2
5	5MU	5	54	5	-	0/3/25/26	0/2/2/2
5	PSU	5	55	5	-	0/7/25/26	0/2/2/2
5	8AN	5	76	57,5,58	-	0/3/25/26	0/3/3/3
5	4SU	5	8	5	-	0/3/25/26	0/2/2/2
47	0TD	q	89	47	-	0/2/12/14	0/0/0/0

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2457	PSU	C2'-C1'	-12.52	1.42	1.53
1	1	746	PSU	C2'-C1'	-12.25	1.42	1.53
1	1	2605	PSU	C2'-C1'	-11.24	1.43	1.53
1	1	2504	PSU	C2'-C1'	-11.05	1.43	1.53
1	1	955	PSU	C2'-C1'	-11.02	1.43	1.53
5	5	55	PSU	C2'-C1'	-10.69	1.43	1.53
1	1	2580	PSU	C2'-C1'	-9.86	1.44	1.53
47	q	89	0TD	CB-SB	-7.53	1.65	1.84
1	1	1962	5MC	C2'-C1'	-5.35	1.45	1.53
1	1	2069	G7M	C2'-C1'	-5.29	1.45	1.53
1	1	1939	5MU	C2'-C1'	-5.26	1.45	1.53
2	2	967	5MC	C2'-C1'	-4.66	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	747	5MU	C2'-C1'	-4.62	1.46	1.53
1	1	1917	PSU	C5-C1'	-4.51	1.48	1.52
1	1	745	1MG	C2'-C1'	-4.22	1.46	1.53
2	2	516	PSU	C5-C1'	-3.98	1.48	1.52
1	1	955	PSU	C5-C1'	-3.94	1.48	1.52
1	1	1911	PSU	C5-C1'	-3.84	1.48	1.52
1	1	1911	PSU	C2'-C1'	-3.76	1.50	1.53
2	2	516	PSU	C2'-C1'	-3.74	1.50	1.53
5	5	54	5MU	C2'-C1'	-3.68	1.47	1.53
1	1	2498	OMC	C3'-C2'	-3.43	1.45	1.53
47	q	89	0TD	CA-N	-3.38	1.37	1.47
2	2	1207	2MG	C2'-C1'	-3.37	1.48	1.53
1	1	2457	PSU	C5-C1'	-3.21	1.49	1.52
1	1	2504	PSU	C5-C1'	-3.13	1.49	1.52
1	1	1915	3TD	C6-C5	-3.12	1.34	1.38
1	1	2457	PSU	C6-C5	-3.11	1.34	1.38
1	1	1917	PSU	C2'-C1'	-3.06	1.50	1.53
1	1	746	PSU	C6-C5	-3.01	1.34	1.38
2	2	516	PSU	C6-C5	-3.00	1.34	1.38
1	1	955	PSU	C6-C5	-2.98	1.34	1.38
1	1	2605	PSU	C5-C1'	-2.96	1.49	1.52
1	1	2605	PSU	C6-C5	-2.95	1.34	1.38
1	1	1911	PSU	C6-C5	-2.94	1.34	1.38
1	1	1917	PSU	C6-C5	-2.90	1.34	1.38
1	1	2504	PSU	C6-C5	-2.82	1.34	1.38
1	1	2580	PSU	C6-C5	-2.81	1.34	1.38
2	2	1498	UR3	C2'-C1'	-2.74	1.49	1.53
1	1	2030	6MZ	C2'-C1'	-2.65	1.49	1.53
5	5	55	PSU	C6-C5	-2.54	1.34	1.38
47	q	89	0TD	CSB-SB	-2.47	1.74	1.79
1	1	2503	2MA	C2'-C3'	-2.44	1.46	1.53
1	1	1618	6MZ	C2'-C1'	-2.38	1.49	1.53
1	1	2251	OMG	C5-C4	-2.35	1.35	1.40
5	5	55	PSU	C5-C1'	-2.33	1.50	1.52
1	1	2498	OMC	C2'-C1'	-2.21	1.47	1.53
1	1	745	1MG	C2'-C3'	-2.06	1.47	1.53
1	1	2503	2MA	C6-N1	2.27	1.39	1.34
1	1	745	1MG	C6-N1	2.38	1.41	1.38
1	1	2457	PSU	C4-N3	2.65	1.37	1.33
1	1	2580	PSU	C4-N3	2.69	1.37	1.33
1	1	2504	PSU	C4-N3	2.71	1.37	1.33
2	2	527	7MG	C5-C4	2.75	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	516	PSU	C4-N3	2.77	1.38	1.33
1	1	955	PSU	C4-N3	2.77	1.38	1.33
1	1	746	PSU	C4-N3	2.78	1.38	1.33
1	1	1911	PSU	C4-N3	2.80	1.38	1.33
1	1	2605	PSU	C4-N3	2.80	1.38	1.33
1	1	1917	PSU	C4-N3	2.87	1.38	1.33
5	5	55	PSU	C4-N3	2.93	1.38	1.33
1	1	2552	OMU	C4-N3	3.00	1.38	1.33
1	1	747	5MU	C4-N3	3.07	1.38	1.33
1	1	2069	G7M	C6-N1	3.10	1.38	1.33
5	5	54	5MU	C4-N3	3.16	1.38	1.33
1	1	1939	5MU	C4-N3	3.16	1.38	1.33
1	1	2251	OMG	C6-N1	3.57	1.39	1.33
2	2	527	7MG	C6-C5	3.62	1.46	1.41
1	1	2503	2MA	C2-N1	3.77	1.41	1.34
1	1	2445	2MG	C6-N1	4.39	1.41	1.33
1	1	1835	2MG	C6-N1	4.69	1.41	1.33
2	2	1516	2MG	C6-N1	4.69	1.41	1.33
2	2	966	2MG	C6-N1	5.00	1.42	1.33
2	2	1207	2MG	C6-N1	5.06	1.42	1.33

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	54	5MU	C5-C4-N3	-10.80	116.28	125.35
1	1	747	5MU	C5-C4-N3	-10.79	116.29	125.35
1	1	1939	5MU	C5-C4-N3	-10.75	116.32	125.35
1	1	2069	G7M	C4'-O4'-C1'	-10.03	99.01	109.64
1	1	1835	2MG	C5-C6-N1	-9.05	111.69	123.52
2	2	1516	2MG	C5-C6-N1	-9.02	111.73	123.52
2	2	1207	2MG	C5-C6-N1	-9.01	111.75	123.52
2	2	966	2MG	C5-C6-N1	-9.00	111.75	123.52
1	1	2445	2MG	C5-C6-N1	-9.00	111.76	123.52
47	q	89	0TD	CB-CA-N	-8.37	93.08	109.83
1	1	2503	2MA	C4'-O4'-C1'	-8.34	100.81	109.64
2	2	527	7MG	C5-C4-N3	-8.10	118.48	126.74
1	1	2251	OMG	C5-C6-N1	-8.07	112.97	123.52
1	1	2069	G7M	C5-C6-N1	-7.84	113.27	123.52
2	2	527	7MG	C5-C6-N1	-5.19	115.67	123.39
1	1	1917	PSU	C5-C1'-C2'	-5.08	106.81	115.44
1	1	2030	6MZ	C4'-O4'-C1'	-4.15	105.24	109.64
1	1	1915	3TD	C5'-C4'-C3'	-4.13	99.24	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2605	PSU	C4'-O4'-C1'	-3.63	105.80	109.54
1	1	955	PSU	C4'-O4'-C1'	-3.62	105.81	109.54
2	2	966	2MG	C2'-C3'-C4'	-3.58	95.31	102.64
2	2	966	2MG	C4'-O4'-C1'	-3.37	106.07	109.64
1	1	2503	2MA	O4'-C1'-N9	-3.25	101.97	108.11
1	1	1915	3TD	C5-C1'-C2'	-3.18	110.03	115.44
1	1	745	1MG	C5-C6-N1	-3.18	114.19	118.35
5	5	8	4SU	C5-C4-N3	-2.99	120.39	123.56
2	2	1207	2MG	O2'-C2'-C1'	-2.91	102.52	111.61
1	1	2069	G7M	N3-C2-N1	-2.89	123.62	127.56
1	1	2251	OMG	N3-C2-N1	-2.88	123.64	127.56
1	1	2504	PSU	C4'-O4'-C1'	-2.87	106.59	109.54
2	2	527	7MG	O4'-C4'-C3'	-2.85	99.39	105.16
1	1	2552	OMU	C5-C4-N3	-2.76	116.50	123.28
2	2	1519	MA6	C4'-O4'-C1'	-2.71	106.77	109.64
2	2	527	7MG	C8-N9-C1'	-2.70	114.32	122.43
1	1	2504	PSU	C2'-C3'-C4'	-2.61	97.30	102.64
1	1	2457	PSU	C4'-O4'-C1'	-2.55	106.91	109.54
2	2	1402	4OC	O4'-C4'-C3'	-2.54	100.00	105.16
1	1	1915	3TD	C4'-O4'-C1'	-2.48	106.98	109.54
1	1	2251	OMG	C2'-C1'-N9	-2.42	106.56	113.48
1	1	2605	PSU	C2'-C3'-C4'	-2.42	97.69	102.64
1	1	2069	G7M	C2'-C3'-C4'	-2.38	97.76	102.64
2	2	1519	MA6	C2'-C3'-C4'	-2.34	97.84	102.64
1	1	2457	PSU	C2'-C3'-C4'	-2.31	97.91	102.64
1	1	955	PSU	C2'-C3'-C4'	-2.26	98.00	102.64
1	1	1911	PSU	O2'-C2'-C1'	-2.25	107.02	111.93
2	2	1518	MA6	C1'-N9-C4	-2.25	124.29	126.81
2	2	516	PSU	O2'-C2'-C1'	-2.24	107.05	111.93
1	1	2580	PSU	C4-C5-C1'	-2.20	117.51	121.22
2	2	1519	MA6	C1'-N9-C4	-2.18	124.37	126.81
2	2	516	PSU	C5-C6-N1	-2.14	121.39	124.38
1	1	2504	PSU	C5-C6-N1	-2.13	121.41	124.38
2	2	1516	2MG	N3-C2-N1	-2.12	123.02	126.19
1	1	1915	3TD	C5-C6-N1	-2.11	121.43	124.38
5	5	8	4SU	C4'-O4'-C1'	-2.11	107.40	109.64
1	1	1917	PSU	C5-C6-N1	-2.11	121.44	124.38
1	1	1911	PSU	C5-C6-N1	-2.10	121.45	124.38
1	1	2605	PSU	C5-C6-N1	-2.10	121.46	124.38
1	1	1835	2MG	N3-C2-N1	-2.10	123.05	126.19
1	1	2580	PSU	C5-C6-N1	-2.09	121.46	124.38
47	q	89	0TD	O-C-CA	-2.09	119.97	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	54	5MU	C4'-O4'-C1'	-2.09	107.43	109.64
5	5	32	4OC	O2'-C2'-C3'	-2.08	105.86	111.23
2	2	1516	2MG	C1'-N9-C4	-2.08	124.48	126.81
1	1	746	PSU	C5-C6-N1	-2.08	121.48	124.38
2	2	966	2MG	N3-C2-N1	-2.07	123.08	126.19
1	1	1618	6MZ	C4'-O4'-C1'	-2.07	107.45	109.64
1	1	955	PSU	C5-C6-N1	-2.07	121.50	124.38
1	1	2457	PSU	C5-C6-N1	-2.06	121.51	124.38
1	1	2445	2MG	N3-C2-N1	-2.05	123.13	126.19
2	2	967	5MC	C4'-O4'-C1'	-2.03	107.49	109.64
5	5	55	PSU	C5-C6-N1	-2.03	121.55	124.38
2	2	527	7MG	C5-C4-N9	-2.00	103.01	106.25
1	1	1915	3TD	O5'-C5'-C4'	2.01	116.30	109.09
2	2	1498	UR3	C4'-O4'-C1'	2.01	111.78	109.64
1	1	1915	3TD	C3'-C2'-C1'	2.04	104.13	101.71
2	2	966	2MG	O3'-C3'-C2'	2.06	118.52	111.86
2	2	1516	2MG	N2-C2-N3	2.09	119.37	116.94
1	1	747	5MU	C5M-C5-C6	2.12	122.92	118.63
1	1	1939	5MU	C5M-C5-C6	2.13	122.94	118.63
2	2	1402	4OC	C4'-O4'-C1'	2.14	111.92	109.64
5	5	54	5MU	C5M-C5-C6	2.15	122.98	118.63
1	1	955	PSU	C5-C1'-C2'	2.18	119.14	115.44
2	2	1207	2MG	N2-C2-N3	2.25	119.55	116.94
1	1	2069	G7M	O3'-C3'-C2'	2.25	119.14	111.86
1	1	2498	OMC	C3'-C2'-C1'	2.31	107.05	102.63
2	2	1402	4OC	C6-C5-C4	2.33	118.34	117.42
1	1	746	PSU	O4'-C1'-C2'	2.36	107.25	104.69
1	1	1618	6MZ	C2'-C1'-N9	2.36	119.79	113.47
1	1	2605	PSU	O4'-C1'-C2'	2.39	107.27	104.69
1	1	2445	2MG	O3'-C3'-C4'	2.40	118.19	111.01
1	1	1915	3TD	O4'-C1'-C2'	2.41	107.29	104.69
1	1	2580	PSU	C3'-C2'-C1'	2.44	104.61	101.71
5	5	8	4SU	O4'-C1'-N1	2.48	112.82	108.10
1	1	2498	OMC	O3'-C3'-C4'	2.49	118.43	111.01
1	1	2069	G7M	O4'-C1'-N9	2.50	112.83	108.11
2	2	966	2MG	N2-C2-N3	2.50	119.84	116.94
2	2	967	5MC	C2'-C1'-N1	2.52	120.24	113.46
2	2	1407	5MC	C5'-C4'-C3'	2.56	125.13	115.20
1	1	1962	5MC	O3'-C3'-C2'	2.59	120.24	111.86
1	1	2251	OMG	C4'-O4'-C1'	2.60	112.40	109.64
1	1	1835	2MG	N2-C2-N3	2.62	119.98	116.94
5	5	54	5MU	C2'-C1'-N1	2.63	120.53	113.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	747	5MU	C2'-C1'-N1	2.63	120.53	113.46
1	1	1939	5MU	C2'-C1'-N1	2.63	120.53	113.46
1	1	1911	PSU	C3'-C2'-C1'	2.73	104.95	101.71
2	2	516	PSU	C3'-C2'-C1'	2.74	104.97	101.71
5	5	32	4OC	O3'-C3'-C4'	2.77	119.28	111.01
1	1	745	1MG	O2'-C2'-C3'	2.79	120.86	111.86
1	1	2445	2MG	N2-C2-N3	2.83	120.23	116.94
1	1	2504	PSU	C5-C1'-C2'	2.88	120.33	115.44
1	1	746	PSU	O2'-C2'-C1'	2.95	118.34	111.93
47	q	89	0TD	C-CA-N	2.97	116.50	109.95
5	5	32	4OC	C6-C5-C4	2.98	118.59	117.42
1	1	1917	PSU	C3'-C2'-C1'	3.07	105.35	101.71
1	1	2503	2MA	C1'-N9-C4	3.09	130.26	126.81
1	1	2503	2MA	O2'-C2'-C3'	3.13	121.98	111.86
1	1	1911	PSU	C4'-O4'-C1'	3.14	112.78	109.54
1	1	2498	OMC	C6-C5-C4	3.19	118.68	117.44
2	2	516	PSU	C4'-O4'-C1'	3.19	112.83	109.54
2	2	1516	2MG	O3'-C3'-C4'	3.22	120.62	111.01
5	5	20	H2U	O2'-C2'-C1'	3.24	121.23	109.98
1	1	2605	PSU	C5-C1'-C2'	3.34	121.11	115.44
1	1	1835	2MG	O3'-C3'-C4'	3.47	121.36	111.01
2	2	1519	MA6	C2-N1-C6	3.48	119.85	111.64
1	1	745	1MG	O3'-C3'-C4'	3.62	121.82	111.01
1	1	2030	6MZ	O3'-C3'-C4'	3.65	121.92	111.01
2	2	1402	4OC	C2-N3-C4	3.71	120.14	115.43
1	1	1618	6MZ	C2-N1-C6	3.71	119.14	116.47
1	1	2445	2MG	O3'-C3'-C2'	3.72	123.89	111.86
2	2	1518	MA6	C2-N1-C6	3.73	120.44	111.64
5	5	32	4OC	C2-N3-C4	3.76	120.22	115.43
1	1	2457	PSU	O2'-C2'-C1'	3.77	120.11	111.93
1	1	2030	6MZ	O3'-C3'-C2'	3.88	124.39	111.86
1	1	2030	6MZ	C2-N1-C6	3.95	119.31	116.47
5	5	20	H2U	O3'-C3'-C4'	4.03	123.06	111.01
1	1	1835	2MG	O3'-C3'-C2'	4.07	125.00	111.86
5	5	55	PSU	C5-C1'-C2'	4.13	122.45	115.44
5	5	55	PSU	O2'-C2'-C1'	4.20	121.06	111.93
1	1	2457	PSU	C5-C1'-C2'	4.21	122.58	115.44
5	5	20	H2U	O3'-C3'-C2'	4.29	125.71	111.86
1	1	2580	PSU	O2'-C2'-C3'	4.29	125.72	111.86
1	1	746	PSU	O2'-C2'-C3'	4.29	125.73	111.86
1	1	2503	2MA	O3'-C3'-C4'	4.34	123.97	111.01
1	1	955	PSU	O2'-C2'-C1'	4.34	121.36	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2504	PSU	O2'-C2'-C1'	4.38	121.46	111.93
1	1	745	1MG	O3'-C3'-C2'	4.39	126.03	111.86
1	1	2580	PSU	O2'-C2'-C1'	4.41	121.51	111.93
1	1	2605	PSU	O2'-C2'-C1'	4.41	121.52	111.93
2	2	1516	2MG	O3'-C3'-C2'	4.43	126.16	111.86
1	1	2503	2MA	O3'-C3'-C2'	4.44	126.21	111.86
1	1	2503	2MA	O2'-C2'-C1'	4.62	126.07	111.61
1	1	2605	PSU	O2'-C2'-C3'	4.62	126.80	111.86
1	1	2457	PSU	O2'-C2'-C3'	4.64	126.85	111.86
2	2	1407	5MC	O3'-C3'-C2'	4.67	126.96	111.86
1	1	2504	PSU	O2'-C2'-C3'	4.70	127.06	111.86
5	5	20	H2U	O2'-C2'-C3'	4.73	127.13	111.86
5	5	32	4OC	O3'-C3'-C2'	4.77	124.89	111.13
1	1	746	PSU	C5-C1'-C2'	4.81	123.61	115.44
1	1	1618	6MZ	O3'-C3'-C4'	4.82	125.41	111.01
1	1	955	PSU	O2'-C2'-C3'	5.14	128.45	111.86
1	1	2069	G7M	O2'-C2'-C3'	5.20	128.67	111.86
5	5	55	PSU	O2'-C2'-C3'	5.21	128.70	111.86
1	1	2069	G7M	C6-N1-C2	5.22	122.00	115.88
1	1	2069	G7M	O2'-C2'-C1'	5.32	128.27	111.61
1	1	2498	OMC	O3'-C3'-C2'	5.44	126.84	111.13
1	1	2069	G7M	C2'-C1'-N9	5.48	128.13	113.47
2	2	967	5MC	O3'-C3'-C4'	5.54	127.55	111.01
1	1	2251	OMG	C6-N1-C2	5.89	122.78	115.88
2	2	527	7MG	C6-N1-C2	6.01	122.92	115.88
1	1	2580	PSU	C5-C1'-C2'	6.01	125.64	115.44
2	2	1207	2MG	C6-N1-C2	6.07	123.94	115.24
1	1	1962	5MC	O3'-C3'-C4'	6.14	129.33	111.01
2	2	966	2MG	C6-N1-C2	6.15	124.05	115.24
2	2	1516	2MG	C6-N1-C2	6.22	124.15	115.24
1	1	2445	2MG	C6-N1-C2	6.28	124.24	115.24
1	1	1835	2MG	C6-N1-C2	6.33	124.30	115.24
47	q	89	0TD	CSB-SB-CB	6.52	113.63	101.44
2	2	966	2MG	O3'-C3'-C4'	7.23	132.61	111.01
1	1	746	PSU	C3'-C2'-C1'	7.57	110.69	101.71
2	2	527	7MG	N3-C4-N9	8.90	138.49	126.98
1	1	2552	OMU	C4-N3-C2	9.43	124.15	114.21
1	1	1939	5MU	C4-N3-C2	11.17	124.47	115.16
1	1	747	5MU	C4-N3-C2	11.38	124.65	115.16
2	2	516	PSU	C4-N3-C2	11.40	124.67	115.16
1	1	1917	PSU	C4-N3-C2	11.41	124.68	115.16
1	1	1911	PSU	C4-N3-C2	11.48	124.74	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	54	5MU	C4-N3-C2	11.52	124.77	115.16
1	1	746	PSU	C4-N3-C2	11.52	124.77	115.16
1	1	955	PSU	C4-N3-C2	11.54	124.79	115.16
1	1	2605	PSU	C4-N3-C2	11.55	124.80	115.16
1	1	2504	PSU	C4-N3-C2	11.60	124.84	115.16
5	5	55	PSU	C4-N3-C2	11.61	124.85	115.16
1	1	2457	PSU	C4-N3-C2	11.67	124.90	115.16
1	1	2580	PSU	C4-N3-C2	11.70	124.92	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1915	3TD	3	0
1	1	1939	5MU	1	0
1	1	1962	5MC	2	0
1	1	2030	6MZ	2	0
1	1	2251	OMG	2	0
1	1	2445	2MG	4	0
1	1	2457	PSU	1	0
1	1	2503	2MA	1	0
1	1	2552	OMU	1	0
1	1	745	1MG	1	0
2	2	1207	2MG	2	0
2	2	1407	5MC	2	0
2	2	1498	UR3	2	0
2	2	1516	2MG	1	0
2	2	1518	MA6	1	0
2	2	1519	MA6	4	0
2	2	516	PSU	3	0
2	2	966	2MG	3	0
2	2	967	5MC	1	0
5	5	20	H2U	2	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 440 ligands modelled in this entry, 439 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	$\# Z > 2$
58	FME	5	101	5	8,9,10	0.47	0	5,9,11	1.41	1 (20%)

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
58	FME	5	101	5	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
58	5	101	FME	O-C-CA	-3.14	117.10	125.69

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	7
1	1	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1276:G	O3'	1277:C	P	3.19
1	1	2314:A	O3'	2315:G	P	3.10
1	2	147:G	O3'	148:G	P	3.07
1	2	1383:C	O3'	1384:C	P	3.06
1	2	480:U	O3'	481:G	P	2.98
1	2	1390:U	O3'	1391:U	P	2.82
1	1	2196:C	O3'	2197:U	P	2.67
1	2	197:A	O3'	198:G	P	2.67
1	2	927:G	O3'	928:G	P	2.61