Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Dec 19, 2016 – 05:23 PM EST

PDB ID	:	5MDW
EMDB ID:	:	EMD-3490
Title	:	Structure of ArfA(A18T) and RF2 bound to the 70S ribosome (pre-accommodated state)
Authors	:	James, N.R.; Brown, A.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on	:	2016-11-13
Resolution	:	3.06 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 (i) symbol.

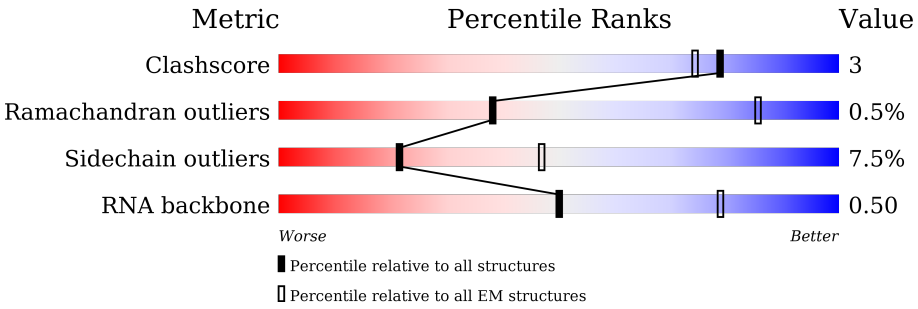
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 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 <=5%

Mol	Chain	Length	Quality of chain
1	1	2904	72% 25% ·
2	2	1534	70% 25% · ·
3	3	120	79% 19% ·
4	4	18	22% 6% 72%
5	5	78	68% 27% · ·
6	6	61	34% 15% · 48%
7	7	365	72% 19% · 7%
8	B	273	84% 14% · ·

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Mol	Chain	Length	Quality of chain
9	C	209	86% 13%
10	D	201	85% 13%
11	E	179	82% 16%
12	F	177	91% 8%
13	G	149	85% 13%
14	H	165	64% 15% 21%
15	I	142	82% 11% 5%
16	J	142	83% 16%
17	K	123	85% 14%
18	L	144	89% 10%
19	M	136	85% 13%
20	N	127	77% 16% 6%
21	O	117	82% 15%
22	P	115	83% 16%
23	Q	118	84% 14%
24	R	103	83% 17%
25	S	110	80% 20%
26	T	100	83% 11% 6%
27	U	104	80% 19%
28	V	94	91% 9%
29	W	85	80% 9% 11%
30	X	78	87% 12%
31	Y	63	86% 11%
32	Z	59	80% 19%
33	a	70	84% 10% 6%

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Mol	Chain	Length	Quality of chain
34	b	57	89% 9%
35	c	55	91% 5%
36	d	46	85% 15%
37	e	65	91% 8%
38	f	38	89% 11%
39	g	241	90% 7%
40	h	233	84% 5% 11%
41	i	206	95%
42	j	167	87% 7% 7%
43	k	135	70% 6% 23%
44	l	179	78% 5% 16%
45	m	130	95% 5%
46	n	130	90% 8%
47	o	103	87% 8%
48	p	129	86% 5% 9%
49	q	124	94% 6%
50	r	118	92% 6%
51	s	101	95%
52	t	89	83% 16%
53	u	82	94% 6%
54	v	84	92% 5%
55	w	75	85% 12%
56	x	92	83% 8% 10%
57	y	87	95%
58	z	71	89% 10%

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 149607 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
			Total	C	N	O	P		
1	1	2903	62336	27816	11470	20147	2903	0	0

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
			Total	C	N	O	P		
2	2	1534	32929	14693	6041	10661	1534	0	0

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

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

- Molecule 4 is a RNA chain called mRNA.

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

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

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

- Molecule 6 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	32	Total	C	N	O	S	0	0
			261	164	53	43	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	0	HIS	-	expression tag	UNP P36675
6	18	THR	ALA	engineered mutation	UNP P36675

- Molecule 7 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	341	Total	C	N	O	S	0	0
			2706	1669	470	558	9		

- Molecule 8 is a protein called 50S ribosomal protein L2.

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

- Molecule 9 is a protein called 50S ribosomal protein L3.

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

- Molecule 10 is a protein called 50S ribosomal protein L4.

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

- Molecule 11 is a protein called 50S ribosomal protein L5.

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

- Molecule 12 is a protein called 50S ribosomal protein L6.

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

- Molecule 13 is a protein called 50S ribosomal protein L9.

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

- Molecule 14 is a protein called 50S ribosomal protein L10.

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

- Molecule 15 is a protein called 50S ribosomal protein L11.

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

- Molecule 16 is a protein called 50S ribosomal protein L13.

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

- Molecule 17 is a protein called 50S ribosomal protein L14.

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

- Molecule 18 is a protein called 50S ribosomal protein L15.

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

- Molecule 19 is a protein called 50S ribosomal protein L16.

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

- Molecule 20 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 21 is a protein called 50S ribosomal protein L18.

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

- Molecule 22 is a protein called 50S ribosomal protein L19.

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

- Molecule 23 is a protein called 50S ribosomal protein L20.

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

- Molecule 24 is a protein called 50S ribosomal protein L21.

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

- Molecule 25 is a protein called 50S ribosomal protein L22.

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

- Molecule 26 is a protein called 50S ribosomal protein L23.

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

- Molecule 27 is a protein called 50S ribosomal protein L24.

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

- Molecule 28 is a protein called 50S ribosomal protein L25.

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

- Molecule 29 is a protein called 50S ribosomal protein L27.

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

- Molecule 30 is a protein called 50S ribosomal protein L28.

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

- Molecule 31 is a protein called 50S ribosomal protein L29.

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

- Molecule 32 is a protein called 50S ribosomal protein L30.

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

- Molecule 33 is a protein called 50S ribosomal protein L31.

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

- Molecule 34 is a protein called 50S ribosomal protein L32.

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

- Molecule 35 is a protein called 50S ribosomal protein L33.

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

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L35.

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

- Molecule 38 is a protein called 50S ribosomal protein L36.

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

- Molecule 39 is a protein called 30S ribosomal protein S2.

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

- Molecule 40 is a protein called 30S ribosomal protein S3.

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

- Molecule 41 is a protein called 30S ribosomal protein S4.

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

- Molecule 42 is a protein called 30S ribosomal protein S5.

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

- Molecule 43 is a protein called 30S ribosomal protein S6.

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

- Molecule 44 is a protein called 30S ribosomal protein S7.

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

- Molecule 45 is a protein called 30S ribosomal protein S8.

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

- Molecule 46 is a protein called 30S ribosomal protein S9.

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

- Molecule 47 is a protein called 30S ribosomal protein S10.

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

- Molecule 48 is a protein called 30S ribosomal protein S11.

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

- Molecule 49 is a protein called 30S ribosomal protein S12.

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

- Molecule 50 is a protein called 30S ribosomal protein S13.

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

- Molecule 51 is a protein called 30S ribosomal protein S14.

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

- Molecule 52 is a protein called 30S ribosomal protein S15.

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

- Molecule 53 is a protein called 30S ribosomal protein S16.

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

- Molecule 54 is a protein called 30S ribosomal protein S17.

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

- Molecule 55 is a protein called 30S ribosomal protein S18.

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

- Molecule 56 is a protein called 30S ribosomal protein S19.

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

- Molecule 57 is a protein called 30S ribosomal protein S20.

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

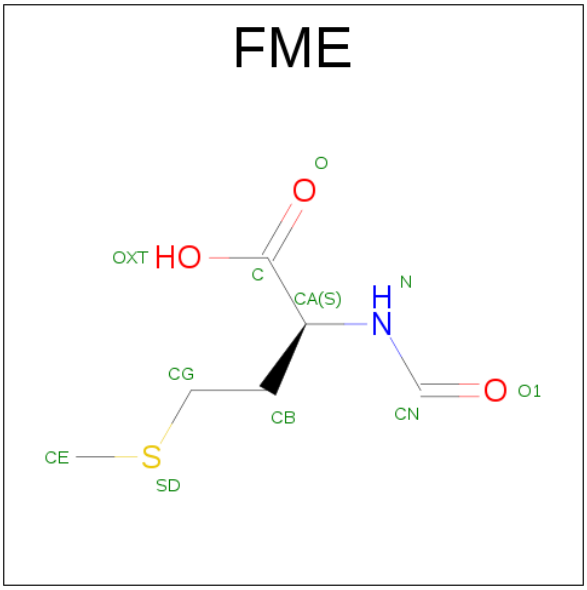
- Molecule 58 is a protein called 30S ribosomal protein S21.

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

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	1	295	Total 295	Mg 295	0
59	b	1	Total 1	Mg 1	0
59	i	1	Total 1	Mg 1	0
59	5	2	Total 2	Mg 2	0
59	2	133	Total 133	Mg 133	0
59	3	6	Total 6	Mg 6	0

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
60	5	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 62 is water.

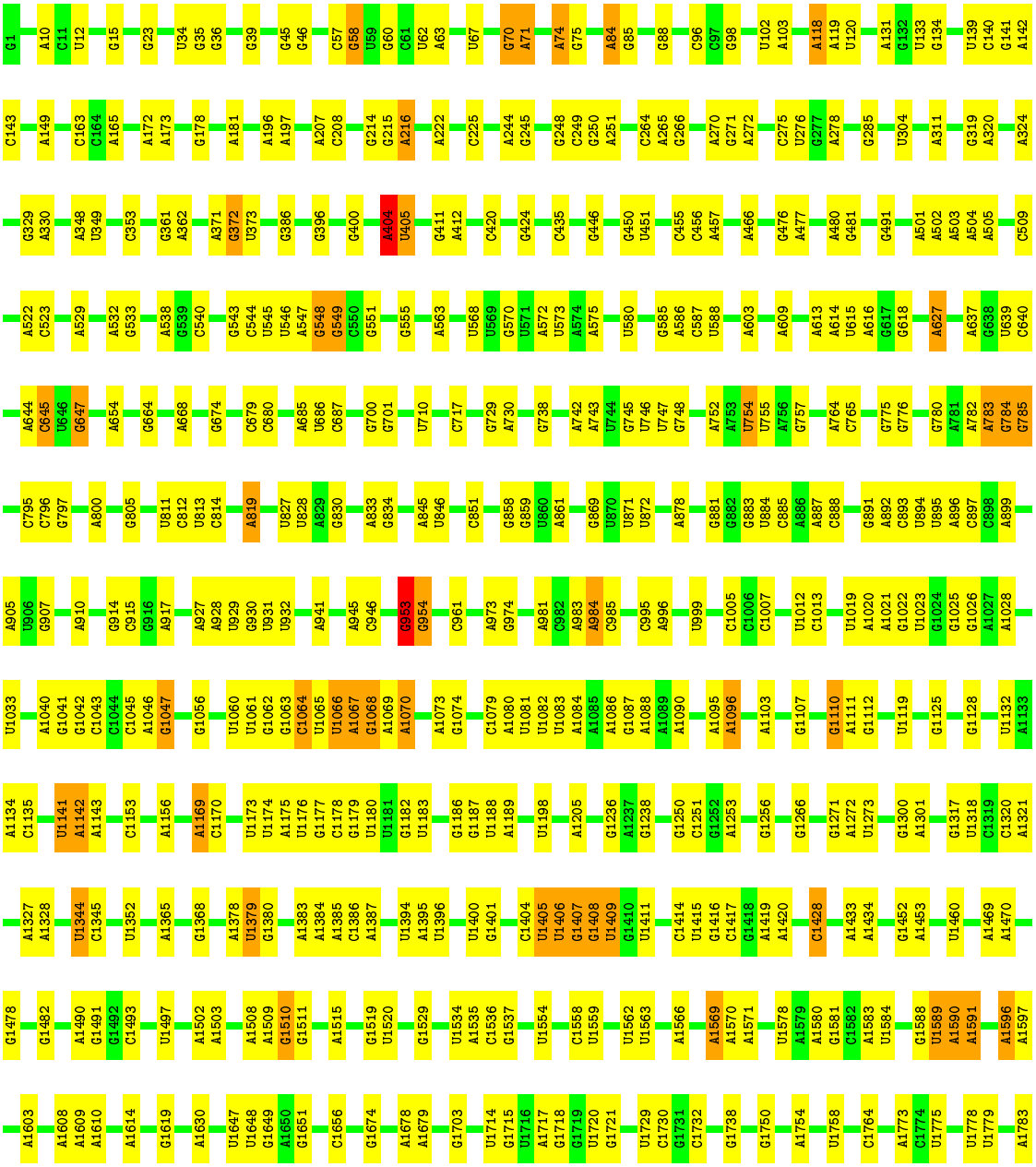
Mol	Chain	Residues	Atoms		AltConf
62	B	2	Total	O	0
			2	2	

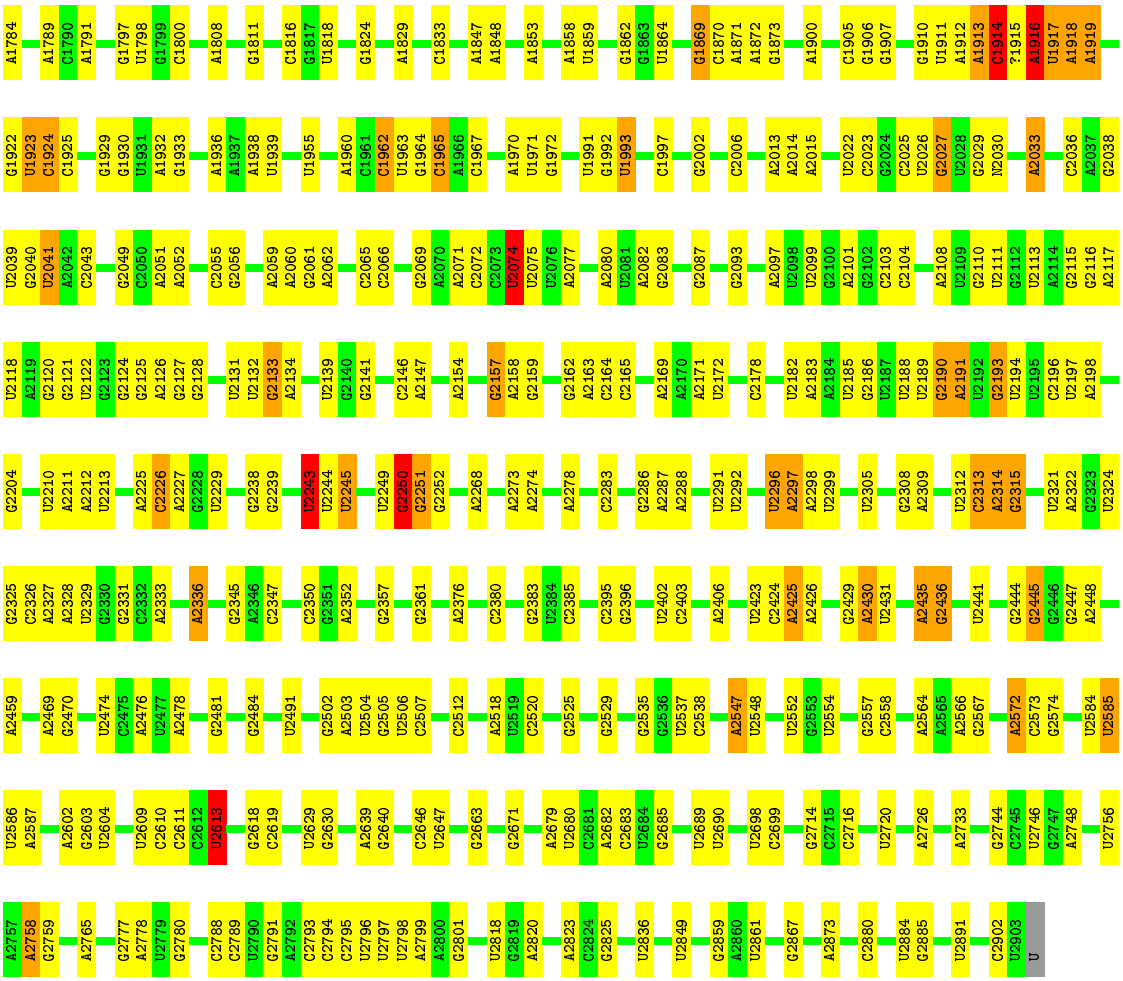
3 Residue-property plots (i)

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

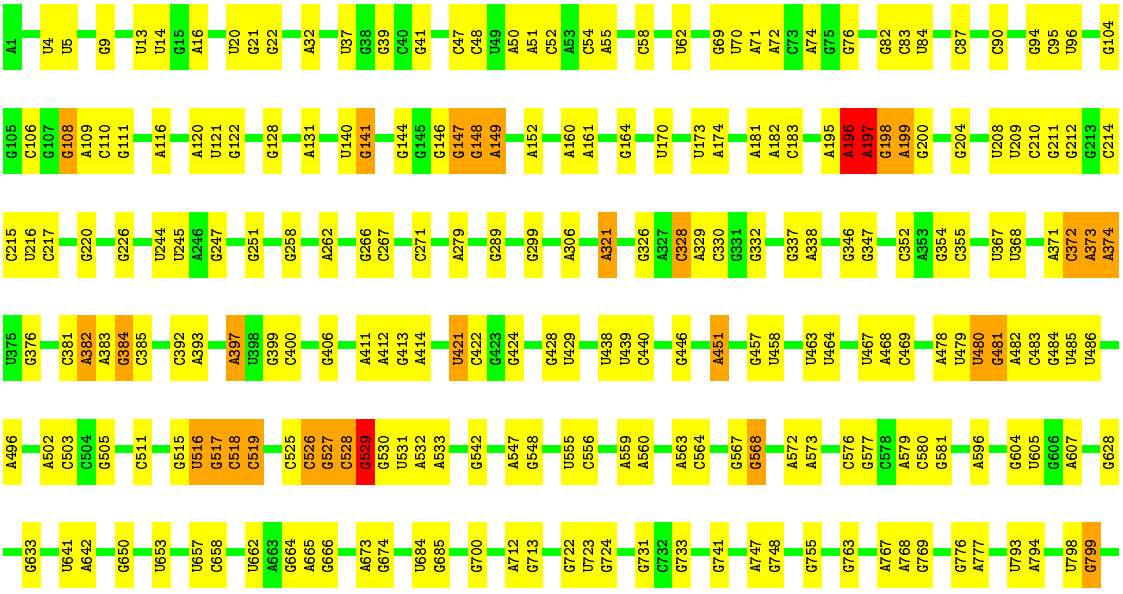
Chain 1: 72% 25%

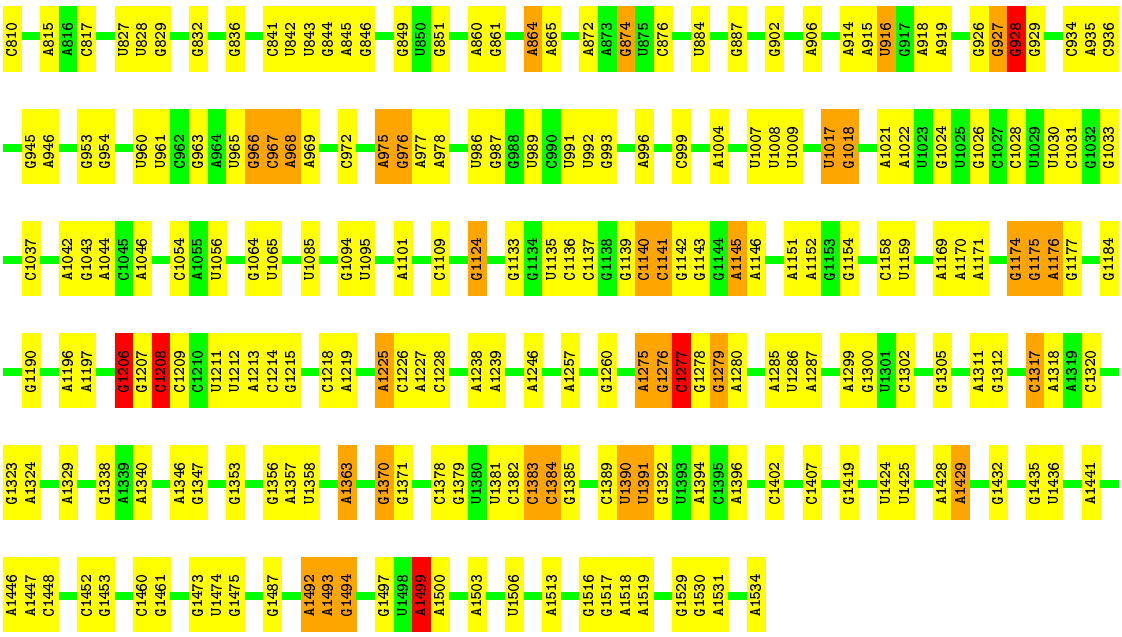




• Molecule 2: 16S ribosomal RNA

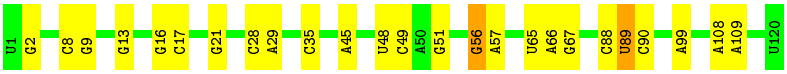
Chain 2:





- Molecule 3: 5S ribosomal RNA

Chain 3:

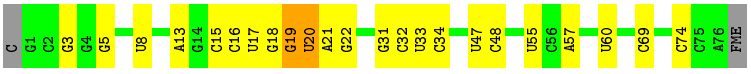


- Molecule 4: mRNA

Chain 4:

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

Chain 5:

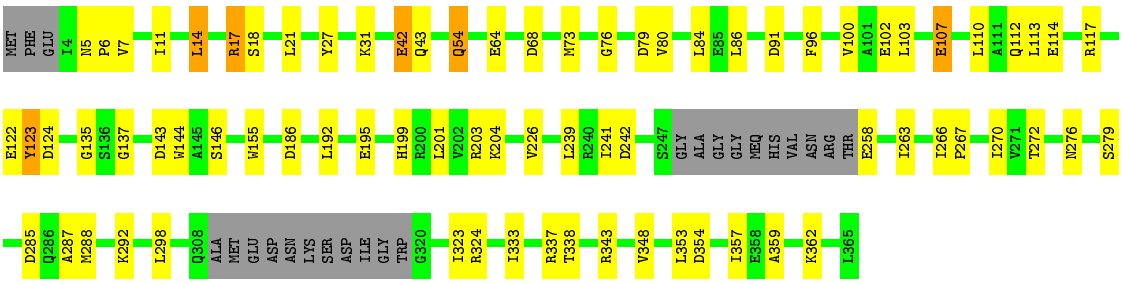


- Molecule 6: Alternative ribosome-rescue factor A

Chain 6:

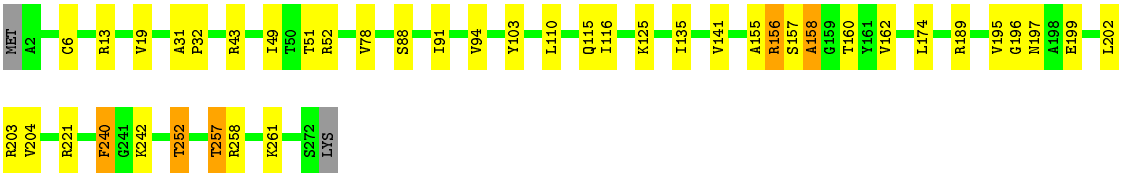
- Molecule 7: Peptide chain release factor 2

Chain 7:



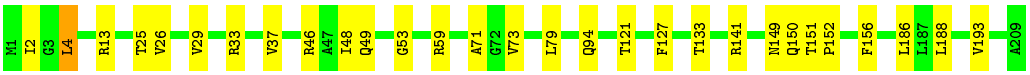
- Molecule 8: 50S ribosomal protein L2

Chain B:



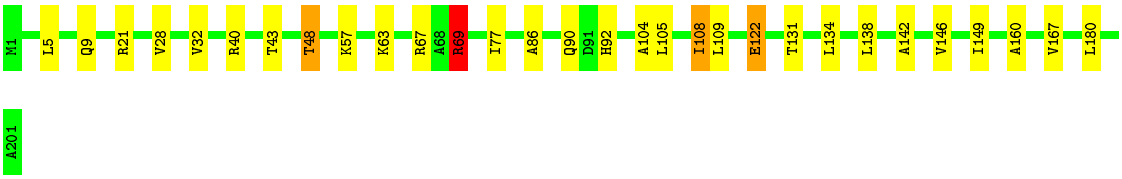
- Molecule 9: 50S ribosomal protein L3

Chain C:



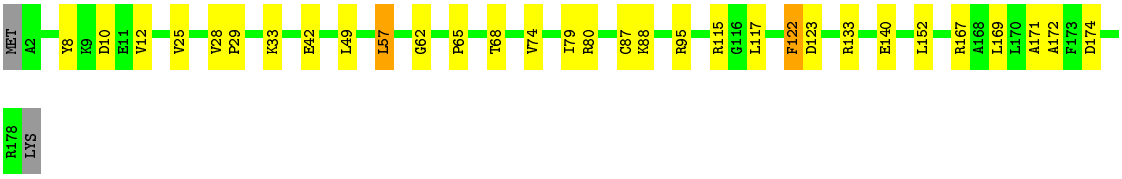
- Molecule 10: 50S ribosomal protein L4

Chain D:



- Molecule 11: 50S ribosomal protein L5

Chain E:

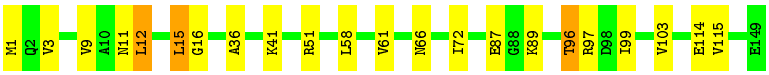


- Molecule 12: 50S ribosomal protein L6

Chain F:

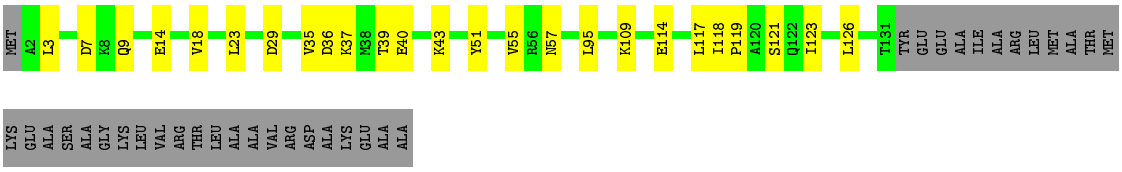
• Molecule 13: 50S ribosomal protein L9

Chain G:



• Molecule 14: 50S ribosomal protein L10

Chain H:

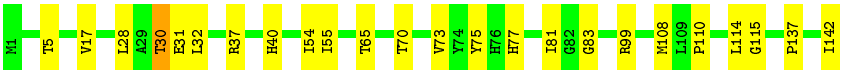


• Molecule 15: 50S ribosomal protein L11

Chain I:

• Molecule 16: 50S ribosomal protein L13

Chain J:

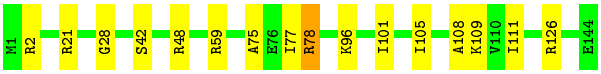


• Molecule 17: 50S ribosomal protein L14

Chain K:

• Molecule 18: 50S ribosomal protein L15

Chain L:



• Molecule 19: 50S ribosomal protein L16

Chain M:

• Molecule 20: 50S ribosomal protein L17

Chain N:

• Molecule 21: 50S ribosomal protein L18

Chain O:

• Molecule 22: 50S ribosomal protein L19

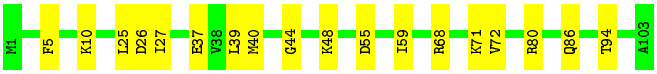
Chain P:

• Molecule 23: 50S ribosomal protein L20

Chain Q:

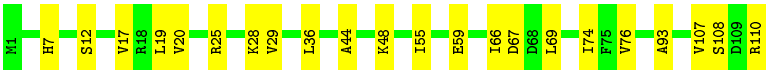
• Molecule 24: 50S ribosomal protein L21

Chain R:



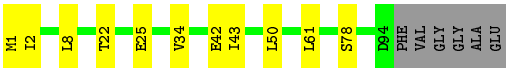
• Molecule 25: 50S ribosomal protein L22

Chain S:



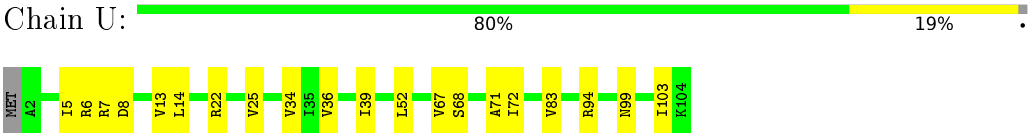
• Molecule 26: 50S ribosomal protein L23

Chain T:



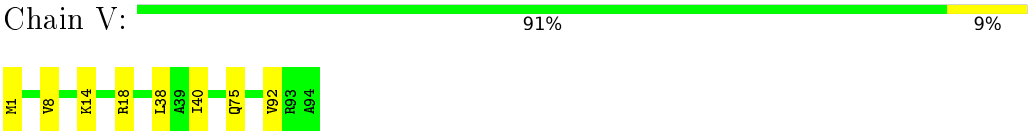
- Molecule 27: 50S ribosomal protein L24

Chain U:



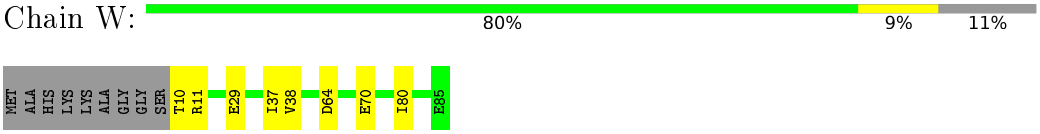
- Molecule 28: 50S ribosomal protein L25

Chain V:



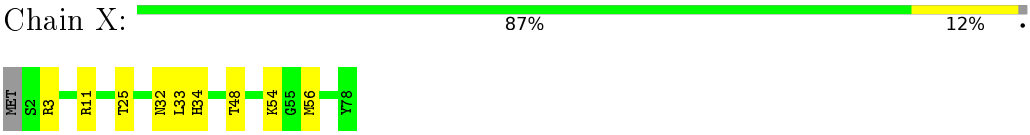
- Molecule 29: 50S ribosomal protein L27

Chain W:



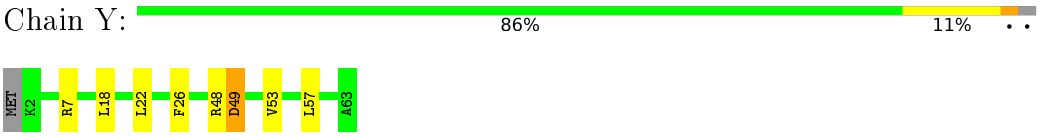
- Molecule 30: 50S ribosomal protein L28

Chain X:



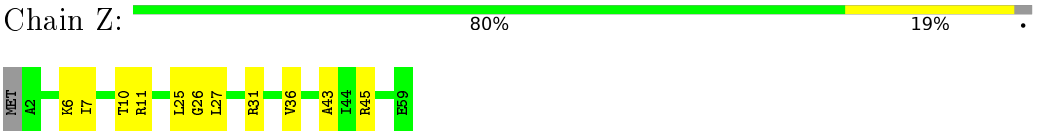
- Molecule 31: 50S ribosomal protein L29

Chain Y:



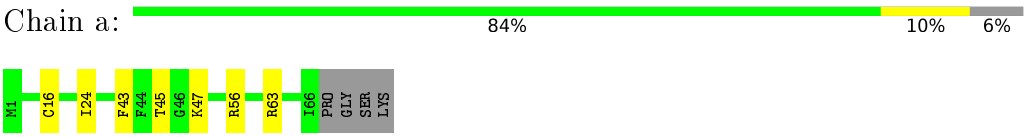
- Molecule 32: 50S ribosomal protein L30

Chain Z:



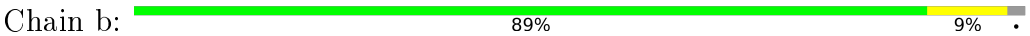
- Molecule 33: 50S ribosomal protein L31

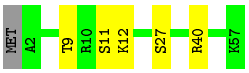
Chain a:



- Molecule 34: 50S ribosomal protein L32

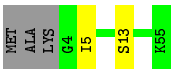
Chain b:





• Molecule 35: 50S ribosomal protein L33

Chain c:



• Molecule 36: 50S ribosomal protein L34

Chain d:

• Molecule 37: 50S ribosomal protein L35

Chain e:

• Molecule 38: 50S ribosomal protein L36

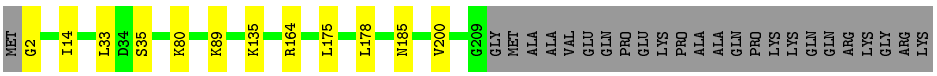
Chain f:

• Molecule 39: 30S ribosomal protein S2

Chain g:

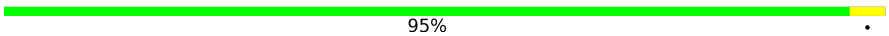
• Molecule 40: 30S ribosomal protein S3

Chain h:



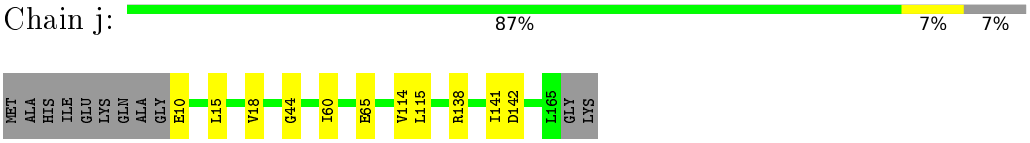
• Molecule 41: 30S ribosomal protein S4

Chain i:



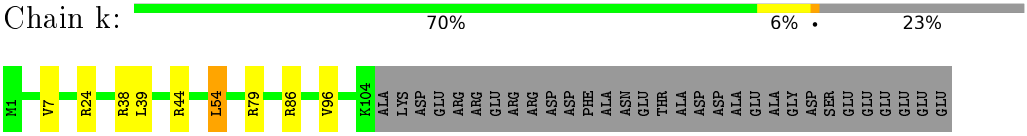
- Molecule 42: 30S ribosomal protein S5

Chain j:



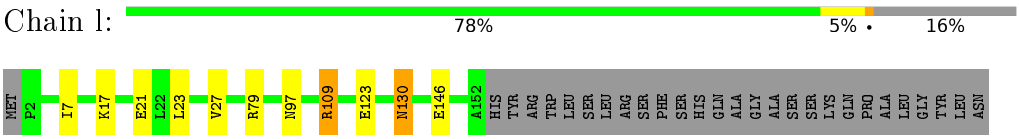
- Molecule 43: 30S ribosomal protein S6

Chain k:



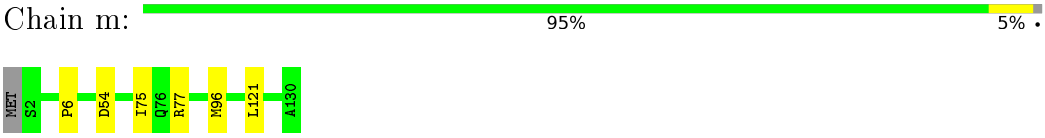
- Molecule 44: 30S ribosomal protein S7

Chain l:



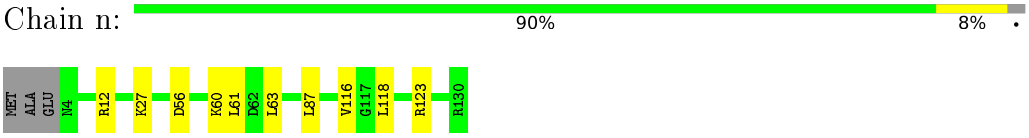
- Molecule 45: 30S ribosomal protein S8

Chain m:



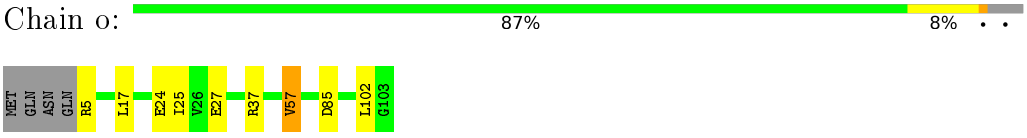
- Molecule 46: 30S ribosomal protein S9

Chain n:



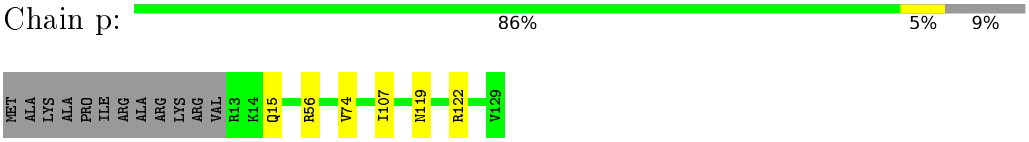
- Molecule 47: 30S ribosomal protein S10

Chain o:



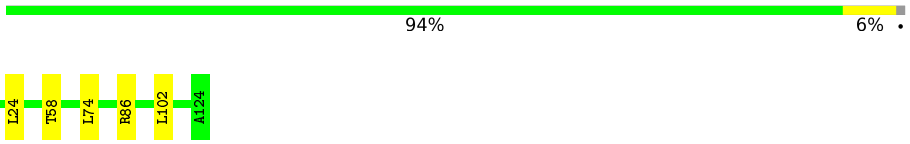
- Molecule 48: 30S ribosomal protein S11

Chain p:



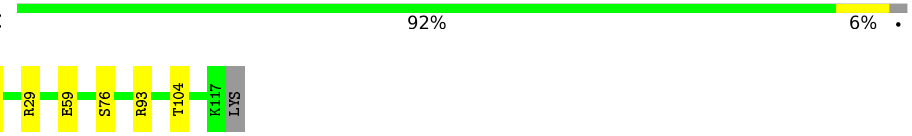
- Molecule 49: 30S ribosomal protein S12

Chain q:



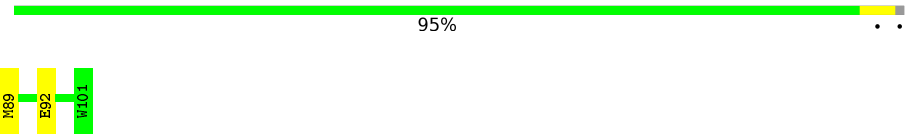
• Molecule 50: 30S ribosomal protein S13

Chain r:



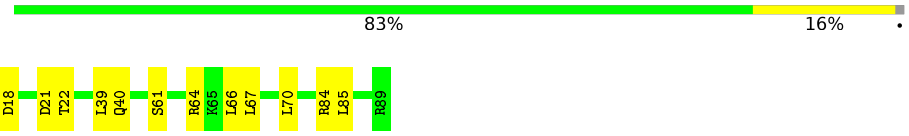
• Molecule 51: 30S ribosomal protein S14

Chain s:



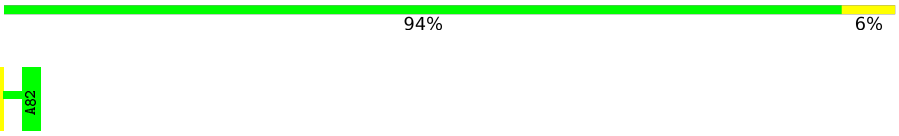
• Molecule 52: 30S ribosomal protein S15

Chain t:



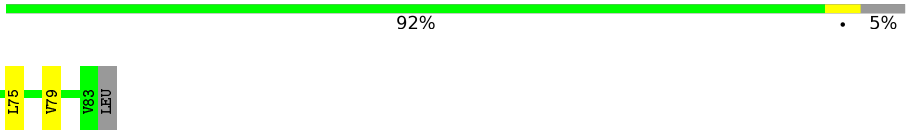
• Molecule 53: 30S ribosomal protein S16

Chain u:



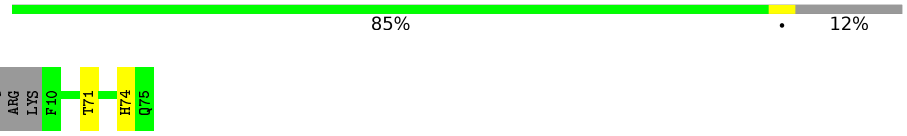
• Molecule 54: 30S ribosomal protein S17

Chain v:



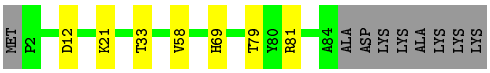
• Molecule 55: 30S ribosomal protein S18

Chain w:



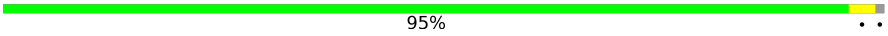
• Molecule 56: 30S ribosomal protein S19

Chain x:



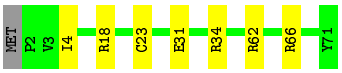
- Molecule 57: 30S ribosomal protein S20

Chain y:



- Molecule 58: 30S ribosomal protein S21

Chain z:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	141950	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 ($e^-/Å^2$)	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	0.42	0/69285	0.74	28/108083 (0.0%)
10	D	0.48	0/1571	0.78	2/2113 (0.1%)
11	E	0.48	0/1434	0.79	0/1926
12	F	0.39	0/1333	0.68	0/1805
13	G	0.43	0/1122	0.68	0/1515
14	H	0.49	0/993	0.73	0/1340
15	I	0.45	0/998	0.69	0/1348
16	J	0.55	0/1152	0.80	0/1551
17	K	0.48	0/955	0.80	0/1279
18	L	0.44	0/1062	0.81	0/1413
19	M	0.54	0/1093	0.82	0/1460
2	2	0.36	0/36590	0.75	34/57074 (0.1%)
20	N	0.52	0/964	0.88	0/1289
21	O	0.49	0/902	0.82	0/1209
22	P	0.50	0/929	0.80	0/1242
23	Q	0.67	0/960	0.96	0/1278
24	R	0.42	0/829	0.73	0/1107
25	S	0.51	0/864	0.83	0/1156
26	T	0.50	0/752	0.76	0/1005
27	U	0.37	0/796	0.66	0/1062
28	V	0.46	0/766	0.72	0/1025
29	W	0.46	0/589	0.78	0/779
3	3	0.33	0/2872	0.70	0/4478
30	X	0.59	0/635	0.90	0/848
31	Y	0.53	0/502	0.86	0/667
32	Z	0.47	0/452	0.80	0/605
33	a	0.41	0/531	0.70	0/709
34	b	0.46	0/450	0.81	0/599
35	c	0.40	0/433	0.69	0/576
36	d	0.59	0/380	1.06	0/498
37	e	0.47	0/513	0.84	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
38	f	0.44	0/303	0.82	1/397 (0.3%)
39	g	0.47	0/1791	0.70	0/2413
4	4	0.49	0/122	0.65	0/188
40	h	0.45	0/1663	0.79	1/2241 (0.0%)
41	i	0.48	0/1665	0.79	0/2227
42	j	0.49	0/1165	0.79	0/1568
43	k	0.48	0/867	0.78	1/1171 (0.1%)
44	l	0.50	0/1195	0.83	1/1602 (0.1%)
45	m	0.44	0/989	0.72	0/1326
46	n	0.43	0/1034	0.78	0/1375
47	o	0.40	0/800	0.76	0/1082
48	p	0.45	0/893	0.74	0/1205
49	q	0.46	0/960	0.80	0/1286
5	5	0.28	0/1672	0.71	0/2603
50	r	0.47	0/909	0.85	0/1215
51	s	0.53	0/817	0.84	0/1088
52	t	0.56	0/722	0.91	0/964
53	u	0.46	0/659	0.76	0/884
54	v	0.35	0/657	0.66	0/881
55	w	0.51	0/553	0.83	0/743
56	x	0.41	0/680	0.65	0/915
57	y	0.58	0/675	0.86	0/895
58	z	0.57	0/597	0.89	0/792
6	6	0.36	0/265	0.64	0/348
7	7	0.48	0/2741	0.78	0/3692
8	B	0.52	0/2121	0.82	0/2852
9	C	0.50	0/1586	0.73	0/2134
All	All	0.43	0/160808	0.75	68/239802 (0.0%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	h	2	GLY	N-CA-C	-14.12	77.80	113.10
2	2	928	G	N9-C1'-C2'	-12.87	97.26	114.00
2	2	1384	C	N1-C1'-C2'	-11.95	98.46	114.00
1	1	2252	G	N9-C1'-C2'	-11.10	99.57	114.00
1	1	1914	C	C4'-C3'-O3'	10.98	134.97	113.00
2	2	199	A	N9-C1'-C2'	-10.97	99.73	114.00
2	2	1277	C	N1-C1'-C2'	-10.72	100.06	114.00
2	2	1499	A	N9-C1'-C2'	-10.41	100.47	114.00
1	1	2315	G	N9-C1'-C2'	-9.92	101.09	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	927	G	N9-C1'-C2'	-9.52	101.53	112.00
2	2	148	G	N9-C1'-C2'	-9.21	101.86	112.00
1	1	1407	G	N9-C1'-C2'	-9.03	102.07	112.00
2	2	1206	G	N9-C1'-C2'	-8.91	102.20	112.00
2	2	1383	C	N1-C1'-C2'	-8.53	102.61	112.00
2	2	1391	U	N1-C1'-C2'	-8.44	102.72	112.00
1	1	1916	A	N9-C1'-C2'	-8.41	102.75	112.00
2	2	480	U	N1-C1'-C2'	-8.21	102.97	112.00
2	2	198	G	N9-C1'-C2'	-8.16	103.02	112.00
1	1	2314	A	N9-C1'-C2'	-8.03	103.17	112.00
1	1	2313	C	N1-C1'-C2'	-7.74	103.49	112.00
2	2	1276	G	N9-C1'-C2'	-7.48	103.77	112.00
1	1	2193	G	C2'-C3'-O3'	7.38	125.73	109.50
2	2	1276	G	C1'-C2'-O2'	-7.25	88.84	110.60
2	2	198	G	C4'-C3'-O3'	7.14	127.28	113.00
1	1	2245	U	N1-C1'-C2'	-7.06	104.23	112.00
2	2	147	G	N9-C1'-C2'	-7.06	104.23	112.00
1	1	754	U	N1-C1'-C2'	6.97	123.06	114.00
1	1	2313	C	C1'-C2'-O2'	-6.75	90.34	110.60
2	2	1390	U	N1-C1'-C2'	-6.51	104.84	112.00
10	D	69	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	1	2250	G	C4'-C3'-O3'	-6.44	95.88	109.40
2	2	480	U	C4'-C3'-O3'	6.36	125.72	113.00
2	2	1276	G	C4'-C3'-O3'	6.33	125.65	113.00
1	1	1379	U	C2'-C3'-O3'	6.30	123.78	113.70
10	D	69	ARG	NE-CZ-NH1	6.19	123.40	120.30
2	2	528	C	C1'-C2'-O2'	-6.06	92.42	110.60
1	1	2425	A	C2'-C3'-O3'	6.03	123.34	113.70
1	1	2313	C	C4'-C3'-O3'	5.84	124.68	113.00
1	1	748	G	C1'-O4'-C4'	-5.83	105.23	109.90
2	2	526	C	N1-C1'-C2'	-5.81	105.61	112.00
1	1	2243	U	N1-C1'-C2'	-5.76	105.66	112.00
44	l	109	ARG	NE-CZ-NH1	5.73	123.17	120.30
2	2	927	G	C4'-C3'-O3'	5.73	124.46	113.00
2	2	928	G	C4'-C3'-O3'	5.70	124.39	113.00
2	2	528	C	N1-C1'-C2'	-5.68	105.75	112.00
2	2	776	G	C2'-C3'-O3'	5.67	122.77	113.70
1	1	783	A	C4'-C3'-O3'	5.66	124.31	113.00
2	2	197	A	N9-C1'-C2'	5.66	121.35	114.00
2	2	196	A	N9-C1'-C2'	-5.59	105.85	112.00
1	1	2613	U	O4'-C1'-N1	5.55	112.64	108.20
2	2	528	C	C4'-C3'-O3'	5.49	123.98	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2252	G	C4'-C3'-O3'	5.46	123.92	113.00
1	1	1914	C	N1-C1'-C2'	-5.44	106.01	112.00
2	2	864	A	N9-C1'-C2'	5.42	121.04	114.00
2	2	529	G	N9-C1'-C2'	-5.39	106.07	112.00
1	1	953	G	C2'-C3'-O3'	5.32	122.21	113.70
1	1	1916	A	C4'-C3'-O3'	5.31	123.63	113.00
2	2	1206	G	C4'-C3'-O3'	5.22	123.45	113.00
2	2	526	C	C4'-C3'-O3'	5.20	123.40	113.00
1	1	1141	U	N1-C1'-C2'	5.19	120.75	114.00
1	1	2074	U	N1-C1'-C2'	5.13	120.67	114.00
1	1	2074	U	C2'-C3'-O3'	5.11	121.88	113.70
1	1	2296	U	C4'-C3'-O3'	5.08	123.15	113.00
2	2	198	G	C1'-C2'-O2'	-5.07	95.38	110.60
43	k	54	LEU	CA-CB-CG	5.07	126.96	115.30
2	2	1208	C	N1-C1'-C2'	-5.07	106.42	112.00
1	1	404	A	C2'-C3'-O3'	5.05	121.79	113.70
38	f	4	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	62336	0	31366	256	0
2	2	32929	0	16587	194	0
3	3	2569	0	1301	6	0
4	4	109	0	55	0	0
5	5	1622	0	829	3	0
6	6	261	0	276	17	0
7	7	2706	0	2616	43	0
8	B	2082	0	2154	22	0
9	C	1565	0	1616	16	0
10	D	1552	0	1619	16	0
11	E	1410	0	1444	16	0
12	F	1313	0	1358	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	G	1111	0	1148	6	0
14	H	980	0	1013	8	0
15	I	984	0	1035	9	0
16	J	1129	0	1162	13	0
17	K	946	0	1023	8	0
18	L	1053	0	1129	9	0
19	M	1074	0	1157	8	0
20	N	951	0	994	8	0
21	O	892	0	923	11	0
22	P	917	0	962	8	0
23	Q	947	0	1019	10	0
24	R	816	0	839	4	0
25	S	857	0	922	10	0
26	T	746	0	811	8	0
27	U	788	0	843	12	0
28	V	753	0	780	3	0
29	W	582	0	599	2	0
30	X	625	0	652	2	0
31	Y	501	0	531	4	0
32	Z	448	0	488	5	0
33	a	522	0	520	0	0
34	b	444	0	458	0	0
35	c	426	0	464	0	0
36	d	377	0	418	0	0
37	e	504	0	572	0	0
38	f	302	0	340	0	0
39	g	1760	0	1787	0	0
40	h	1636	0	1710	0	0
41	i	1643	0	1707	0	0
42	j	1152	0	1196	0	0
43	k	848	0	846	0	0
44	l	1181	0	1238	0	0
45	m	979	0	1031	0	0
46	n	1022	0	1070	0	0
47	o	790	0	831	0	0
48	p	877	0	887	0	0
49	q	957	0	1017	0	0
50	r	900	0	965	0	0
51	s	805	0	844	0	0
52	t	714	0	734	0	0
53	u	649	0	666	0	0
54	v	648	0	691	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	w	544	0	560	0	0
56	x	663	0	688	0	0
57	y	669	0	719	0	0
58	z	589	0	629	0	0
59	1	295	0	0	0	0
59	2	133	0	0	0	0
59	3	6	0	0	0	0
59	5	2	0	0	0	0
59	b	1	0	0	0	0
59	i	1	0	0	0	0
60	5	10	0	10	0	0
61	a	1	0	0	0	0
61	f	1	0	0	0	0
62	B	2	0	0	0	0
All	All	149607	0	101849	678	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 (678) 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	1.60	1.34
2:2:827:U:O4	2:2:872:A:N1	1.59	1.34
2:2:37:U:O4	2:2:397:A:N1	1.62	1.33
2:2:1358:U:O4	2:2:1363:A:N1	1.59	1.31
1:1:1914:C:H5"	6:6:21:HIS:CE1	1.70	1.25
2:2:563:A:N1	2:2:884:U:O4	1.71	1.23
1:1:2074:U:N3	1:1:2435:A:N1	1.87	1.20
2:2:195:A:O2'	2:2:196:A:H5'	1.46	1.15
8:B:158:ALA:O	8:B:196:GLY:O	1.63	1.14
1:1:2297:A:N1	1:1:2321:U:C4	2.26	1.04
2:2:13:U:N3	2:2:915:A:C6	2.25	1.04
1:1:1596:A:O2'	1:1:1597:A:C8	2.13	1.01
1:1:1019:U:H3	1:1:1142:A:H61	1.07	0.99
1:1:1914:C:H5"	6:6:21:HIS:HE1	1.03	0.96
1:1:67:U:N3	1:1:74:A:C6	2.34	0.96
1:1:1019:U:H3	1:1:1142:A:N6	1.63	0.95
2:2:13:U:N3	2:2:915:A:N6	2.14	0.95
2:2:13:U:C4	2:2:915:A:N6	2.34	0.94
2:2:37:U:N3	2:2:397:A:N6	2.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1596:A:HO2'	1:1:1597:A:H8	1.08	0.92
1:1:2297:A:N1	1:1:2321:U:O4	2.03	0.92
1:1:1918:A:O2'	1:1:1919:A:N7	2.01	0.92
2:2:481:G:O2'	2:2:483:C:N4	2.03	0.91
1:1:1916:A:O2'	1:1:1917:PSU:O4'	1.89	0.90
2:2:13:U:O4	2:2:20:U:O4	1.90	0.89
1:1:67:U:N3	1:1:74:A:N6	2.21	0.88
6:6:17:GLU:N	6:6:17:GLU:OE1	2.08	0.87
1:1:2298:A:C4	1:1:2321:U:C5	2.62	0.87
1:1:783:A:H2'	1:1:783:A:N3	1.88	0.86
2:2:527:7MG:H3'	2:2:527:7MG:H81	1.55	0.86
1:1:1915:3TD:H2'	1:1:1916:A:C8	2.11	0.85
1:1:1916:A:H2'	1:1:1917:PSU:C6	2.11	0.85
2:2:13:U:C4	2:2:20:U:O4	2.29	0.85
1:1:1021:A:H61	1:1:1141:U:H3	1.24	0.85
1:1:1021:A:N6	1:1:1141:U:H3	1.75	0.84
6:6:22:ASP:OD1	6:6:23:PRO:HD2	1.75	0.84
1:1:1913:A:OP2	1:1:1913:A:H3'	1.77	0.84
1:1:1405:U:O2'	1:1:1406:U:C6	2.30	0.84
2:2:517:G:O2'	2:2:530:G:H4'	1.77	0.83
2:2:13:U:O4	2:2:21:G:C2	2.32	0.83
1:1:1914:C:H2'	1:1:1915:3TD:O4	1.77	0.83
1:1:2298:A:C4	1:1:2321:U:H5	1.93	0.83
1:1:585:G:N7	23:Q:6:ARG:NH1	2.27	0.82
27:U:36:VAL:HG11	27:U:39:ILE:HD12	1.61	0.82
1:1:1916:A:H2'	1:1:1917:PSU:H6	1.44	0.82
1:1:2013:A:N6	1:1:2613:U:H3	1.78	0.82
2:2:37:U:H3	2:2:397:A:N6	1.77	0.82
1:1:1405:U:H2'	1:1:1406:U:C5	2.15	0.81
2:2:37:U:C4	2:2:397:A:N1	2.48	0.81
2:2:915:A:N6	2:2:916:U:C4	2.48	0.81
1:1:1405:U:H2'	1:1:1406:U:C6	2.15	0.81
1:1:572:A:OP2	24:R:80:ARG:NH2	2.13	0.81
2:2:827:U:H3	2:2:872:A:N6	1.80	0.80
1:1:1915:3TD:O4	1:1:1915:3TD:OP2	1.98	0.80
1:1:2756:U:N3	1:1:2758:A:N6	2.30	0.79
1:1:2756:U:N3	1:1:2758:A:C6	2.50	0.79
2:2:1208:C:O2'	2:2:1209:C:O4'	2.01	0.78
1:1:1405:U:C2'	1:1:1406:U:C6	2.67	0.78
1:1:1914:C:C5'	6:6:21:HIS:HE1	1.92	0.77
7:7:64:GLU:O	7:7:68:ASP:N	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1021:A:N1	1:1:1141:U:C4	2.53	0.76
1:1:742:A:H2'	1:1:743:A:C8	2.21	0.76
2:2:1358:U:C4	2:2:1363:A:N1	2.52	0.76
2:2:146:G:C2'	2:2:147:G:H5'	2.16	0.75
7:7:11:ILE:HA	7:7:103:LEU:HD21	1.68	0.75
2:2:1358:U:H3	2:2:1363:A:N6	1.85	0.74
1:1:67:U:C4	1:1:74:A:N6	2.55	0.74
2:2:927:G:C2'	2:2:928:G:H5'	2.18	0.73
21:O:31:THR:O	21:O:102:ARG:NH1	2.21	0.73
2:2:515:G:O2'	2:2:516:PSU:O4'	2.05	0.73
1:1:1779:U:H5	1:1:1784:A:N7	1.86	0.73
2:2:827:U:C4	2:2:872:A:N1	2.53	0.73
2:2:527:7MG:H3'	2:2:527:7MG:C8	2.23	0.73
28:V:75:GLN:HB2	28:V:92:VAL:HG23	1.70	0.72
1:1:2756:U:C4	1:1:2758:A:N6	2.58	0.72
2:2:197:A:O2'	2:2:220:G:N2	2.22	0.72
1:1:2312:U:H2'	1:1:2313:C:H5'	1.71	0.72
14:H:36:ASP:O	14:H:39:THR:OG1	2.05	0.72
1:1:2298:A:N3	1:1:2321:U:C5	2.59	0.71
8:B:158:ALA:O	8:B:195:VAL:HG13	1.90	0.71
1:1:2312:U:C2'	1:1:2313:C:H5'	2.21	0.71
2:2:927:G:H4'	2:2:927:G:OP2	1.91	0.71
7:7:14:LEU:HD11	7:7:107:GLU:HB2	1.71	0.71
1:1:1962:5MC:O2'	1:1:1964:G:OP2	2.08	0.70
2:2:1358:U:N3	2:2:1363:A:N6	2.40	0.69
2:2:827:U:N3	2:2:872:A:N6	2.40	0.69
2:2:827:U:O4	2:2:872:A:C2	2.45	0.69
1:1:1021:A:H3'	1:1:1021:A:N3	2.08	0.69
1:1:2013:A:N6	1:1:2613:U:N3	2.39	0.68
2:2:563:A:N1	2:2:884:U:C4	2.60	0.68
9:C:33:ARG:NH1	9:C:53:GLY:O	2.27	0.68
7:7:64:GLU:O	7:7:68:ASP:HB2	1.93	0.68
15:I:109:ALA:HB2	15:I:128:ILE:HD12	1.76	0.67
1:1:1818:U:OP2	8:B:156:ARG:NH1	2.27	0.67
9:C:4:LEU:HD23	9:C:29:VAL:HG11	1.77	0.67
7:7:298:LEU:C	7:7:298:LEU:HD23	2.15	0.66
2:2:1358:U:O4	2:2:1363:A:C2	2.46	0.65
8:B:6:CYS:SG	8:B:13:ARG:NH1	2.69	0.65
19:M:66:ARG:NH1	19:M:104:GLU:OE1	2.29	0.65
1:1:2297:A:C2	1:1:2321:U:C4	2.84	0.65
1:1:2196:C:O3'	1:1:2197:U:P	2.55	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:146:G:H2'	2:2:147:G:H5'	1.79	0.64
16:J:17:VAL:HG23	16:J:137:PRO:HB2	1.79	0.64
1:1:1021:A:C2	1:1:1141:U:O4	2.46	0.64
1:1:2435:A:O2'	1:1:2436:G:O5'	2.14	0.64
1:1:2315:G:OP1	11:E:33:LYS:NZ	2.31	0.64
15:I:82:ALA:HB2	15:I:108:ILE:HD11	1.79	0.64
2:2:37:U:O4	2:2:397:A:C2	2.48	0.63
7:7:21:LEU:HD21	7:7:113:LEU:HD12	1.80	0.63
27:U:34:VAL:HG13	27:U:67:VAL:HG22	1.80	0.63
1:1:2298:A:C5	1:1:2321:U:O4	2.51	0.63
1:1:1824:G:O2'	8:B:252:THR:HG21	1.99	0.63
1:1:754:U:H2'	1:1:755:U:C6	2.34	0.63
2:2:439:U:O2	2:2:440:C:C5	2.51	0.63
1:1:2683:C:OP1	22:P:51:ARG:NH2	2.31	0.62
2:2:517:G:O2'	2:2:530:G:C5'	2.47	0.62
2:2:658:C:H1'	26:T:22:THR:HG21	118.45	0.62
1:1:1914:C:C5'	6:6:21:HIS:CE1	2.65	0.62
1:1:927:A:H2'	1:1:928:A:C8	2.34	0.62
1:1:1067:A:C6	7:7:54:GLN:HG3	2.35	0.62
6:6:20:LEU:HD11	7:7:135:GLY:HA2	1.82	0.61
8:B:135:ILE:HD13	8:B:141:VAL:HG11	1.82	0.61
1:1:1405:U:O2'	1:1:1406:U:O4'	2.17	0.61
1:1:1596:A:O2'	1:1:1597:A:O4'	2.18	0.61
1:1:568:U:H1'	1:1:2030:6MZ:H9C1	1.81	0.61
9:C:37:VAL:HG22	9:C:48:ILE:HG22	1.82	0.61
2:2:517:G:O2'	2:2:530:G:C4'	2.45	0.61
2:2:517:G:O2'	2:2:530:G:H5"	2.00	0.61
2:2:527:7MG:C3'	2:2:527:7MG:H81	2.30	0.61
14:H:23:LEU:HD12	14:H:118:ILE:HG12	1.82	0.61
2:2:13:U:O2	2:2:915:A:N7	2.33	0.60
11:E:42:GLU:HG3	11:E:49:LEU:HD23	1.84	0.60
15:I:105:LEU:HD22	15:I:128:ILE:HG22	1.82	0.60
21:O:18:LEU:HD23	21:O:25:ARG:HD2	1.82	0.60
3:3:48:U:H2'	3:3:49:C:C6	2.37	0.59
2:2:16:A:OP2	6:6:41:ARG:NH1	2.35	0.59
25:S:36:LEU:HD13	25:S:48:LYS:HA	1.84	0.59
2:2:527:7MG:C8	2:2:527:7MG:C3'	2.86	0.59
2:2:1218:C:H2'	2:2:1219:A:C8	2.36	0.59
2:2:563:A:N6	2:2:884:U:N3	2.50	0.59
7:7:338:THR:HG21	7:7:359:ALA:HB1	1.84	0.59
12:F:24:ILE:HD11	12:F:43:VAL:HG11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:13:U:C4	2:2:21:G:C2	2.90	0.59
31:Y:49:ASP:O	31:Y:53:VAL:HG23	2.03	0.59
2:2:13:U:C5	2:2:20:U:O4	2.54	0.58
7:7:11:ILE:HD12	7:7:84:LEU:HD22	1.83	0.58
10:D:146:VAL:HG12	10:D:167:VAL:HG22	1.85	0.58
1:1:570:G:H2'	1:1:2030:6MZ:N7	2.18	0.58
1:1:1405:U:HO2'	1:1:1406:U:H6	1.49	0.58
2:2:515:G:O2'	2:2:516:PSU:O5'	2.21	0.58
2:2:13:U:C2	2:2:915:A:N6	2.70	0.58
2:2:563:A:N6	2:2:884:U:H3	2.02	0.58
20:N:67:PHE:O	20:N:71:ARG:N	2.36	0.58
24:R:5:PHE:HB3	24:R:59:ILE:HD12	1.86	0.58
2:2:966:2MG:HM22	5:5:34:C:H5"	1.84	0.58
26:T:50:LEU:HD23	31:Y:26:PHE:CZ	2.38	0.58
27:U:14:LEU:HD11	27:U:71:ALA:HB2	1.84	0.57
1:1:2297:A:C2	1:1:2321:U:C5	2.92	0.57
2:2:146:G:O2'	2:2:147:G:H5'	2.05	0.57
1:1:1614:A:C2	25:S:93:ALA:HB2	2.39	0.57
2:2:1499:A:O2'	2:2:1500:A:H5'	2.04	0.57
26:T:61:LEU:C	26:T:61:LEU:HD12	2.25	0.57
1:1:627:A:OP1	18:L:78:ARG:NH2	2.38	0.56
2:2:966:2MG:H5"	2:2:967:5MC:OP2	2.05	0.56
25:S:20:VAL:HG11	25:S:44:ALA:HA	1.87	0.56
1:1:1590:A:H2'	1:1:1591:A:C8	2.40	0.56
21:O:35:ILE:HG21	21:O:71:ALA:HA	1.86	0.56
1:1:1020:A:C2	1:1:1141:U:C2	2.93	0.56
2:2:927:G:H2'	2:2:928:G:H5'	1.87	0.56
15:I:78:LEU:HD22	15:I:108:ILE:HG23	1.86	0.56
22:P:14:LYS:NZ	22:P:76:THR:O	2.39	0.56
1:1:929:U:H1'	32:Z:26:GLY:O	2.05	0.56
7:7:96:PHE:O	7:7:100:VAL:HG23	2.05	0.56
1:1:1433:A:H2'	1:1:1434:A:O4'	2.05	0.56
1:1:1082:U:N3	1:1:1086:A:N6	2.54	0.56
1:1:2646:C:O5'	1:1:2646:C:H6	1.89	0.56
1:1:404:A:O2'	1:1:405:U:OP2	2.25	0.56
2:2:1169:A:H2'	2:2:1170:A:C8	2.40	0.55
1:1:1797:G:O2'	8:B:257:THR:OG1	2.24	0.55
1:1:1250:G:OP2	18:L:21:ARG:NH2	2.39	0.55
2:2:1275:A:H2'	2:2:1276:G:H5'	1.87	0.55
2:2:13:U:O4	2:2:21:G:N3	2.39	0.55
2:2:928:G:O2'	2:2:929:G:C5'	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1070:A:N7	1:1:1096:A:O2'	2.40	0.55
2:2:769:G:H4'	2:2:1513:A:H4'	1.87	0.55
16:J:17:VAL:HG22	16:J:55:ILE:HB	1.88	0.55
1:1:2328:A:H2'	1:1:2329:U:C6	2.41	0.55
2:2:515:G:H2'	2:2:516:PSU:C6	2.41	0.55
1:1:2245:U:O2'	1:1:2436:G:OP2	2.24	0.55
1:1:2249:U:H3'	1:1:2250:G:H5'	1.89	0.55
12:F:35:ARG:HD3	12:F:71:LEU:HD13	1.88	0.55
10:D:108:ILE:HD11	10:D:180:LEU:HD13	1.87	0.55
2:2:1208:C:H2'	2:2:1209:C:C6	2.42	0.55
2:2:1394:A:N1	2:2:1500:A:O2'	2.37	0.55
2:2:1518:MA6:N6	2:2:1519:MA6:H93	2.22	0.54
2:2:673:A:H2'	2:2:674:G:C8	2.42	0.54
2:2:915:A:C6	2:2:916:U:C4	2.94	0.54
7:7:14:LEU:HD13	7:7:103:LEU:CD1	2.38	0.54
1:1:2082:A:H2'	1:1:2083:G:O4'	2.07	0.54
1:1:2006:C:O2'	1:1:2823:A:N3	2.40	0.54
2:2:13:U:C4	2:2:915:A:C6	2.88	0.54
13:G:9:VAL:HG11	13:G:12:LEU:HD21	1.88	0.54
2:2:195:A:O2'	2:2:196:A:C5'	2.37	0.54
5:5:32:4OC:HM43	5:5:33:U:C4	2.43	0.54
15:I:82:ALA:CB	15:I:108:ILE:HD11	2.36	0.54
1:1:1327:A:H2'	1:1:1328:A:O4'	2.08	0.54
2:2:1206:G:H2'	2:2:1207:2MG:C8	2.42	0.54
2:2:13:U:C2	2:2:915:A:C6	2.96	0.54
11:E:25:VAL:O	11:E:28:VAL:HG12	2.08	0.54
13:G:58:LEU:O	13:G:61:VAL:HG22	2.08	0.54
28:V:14:LYS:O	28:V:18:ARG:HG2	2.08	0.54
1:1:1570:A:H2'	1:1:1571:A:C8	2.43	0.54
7:7:155:TRP:CZ3	7:7:192:LEU:HD21	2.43	0.54
2:2:1175:G:N3	2:2:1176:A:C8	2.76	0.54
7:7:11:ILE:CD1	7:7:84:LEU:HD22	2.38	0.54
8:B:78:VAL:HG21	8:B:110:LEU:HD21	1.89	0.54
1:1:1717:A:H2'	1:1:1718:G:O4'	2.07	0.54
2:2:915:A:C8	2:2:915:A:H3'	2.43	0.54
27:U:94:ARG:HB3	27:U:103:ILE:HD12	1.88	0.54
25:S:59:GLU:CG	25:S:66:ILE:HD11	2.38	0.54
10:D:104:ALA:O	10:D:108:ILE:HG23	2.08	0.53
22:P:33:VAL:HG22	22:P:38:LYS:HG2	1.91	0.53
2:2:195:A:C2'	2:2:196:A:H5'	2.35	0.53
8:B:155:ALA:HB2	8:B:162:VAL:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:77:ILE:HD11	18:L:108:ALA:HB1	1.89	0.53
2:2:62:U:OP1	2:2:385:C:O2'	2.25	0.53
1:1:1596:A:O2'	1:1:1597:A:H8	1.72	0.53
2:2:1275:A:C2'	2:2:1276:G:H5'	2.38	0.53
32:Z:7:ILE:HD13	32:Z:27:LEU:HD22	1.91	0.53
1:1:2298:A:C2	1:1:2321:U:C5	2.96	0.53
1:1:1153:C:OP1	23:Q:92:ARG:NH1	2.42	0.53
1:1:811:U:H2'	18:L:21:ARG:HA	1.90	0.53
2:2:1389:C:C2'	2:2:1390:U:H5'	2.39	0.53
2:2:397:A:N3	2:2:397:A:H3'	2.23	0.53
17:K:123:LEU:HD21	22:P:70:VAL:HG11	1.91	0.53
1:1:1588:G:C6	1:1:1589:U:O4	2.62	0.53
2:2:1174:G:H2'	2:2:1175:G:H5'	1.89	0.53
8:B:240:PHE:CD2	8:B:240:PHE:O	2.61	0.53
1:1:1047:G:HO2'	1:1:1110:G:H1	1.57	0.53
2:2:915:A:N6	2:2:916:U:O4	2.42	0.53
2:2:928:G:HO2'	2:2:929:G:C5'	2.21	0.52
1:1:1869:G:N2	1:1:1871:A:O2'	2.42	0.52
2:2:13:U:O4	2:2:20:U:C4	2.61	0.52
2:2:712:A:H2'	2:2:713:G:O4'	2.09	0.52
21:O:53:THR:HG23	21:O:74:VAL:CG2	2.39	0.52
2:2:37:U:O2	2:2:548:G:C2	2.62	0.52
27:U:36:VAL:CG1	27:U:39:ILE:HD12	2.38	0.52
1:1:2029:G:N1	1:1:2033:A:OP2	2.33	0.52
8:B:160:THR:H	8:B:195:VAL:HG12	1.75	0.52
17:K:107:LEU:HD21	17:K:115:ILE:HG21	1.92	0.52
2:2:109:A:H2'	2:2:326:G:N2	2.24	0.52
1:1:2557:G:H2'	1:1:2558:C:C6	2.45	0.52
7:7:17:ARG:HD3	7:7:110:LEU:HD22	1.92	0.52
7:7:239:LEU:HD11	7:7:241:ILE:HD11	1.91	0.52
7:7:80:VAL:HG11	7:7:103:LEU:HD13	1.91	0.52
2:2:864:A:H2'	2:2:865:A:C8	2.45	0.51
27:U:94:ARG:CB	27:U:103:ILE:HD12	2.40	0.51
16:J:32:LEU:CD2	16:J:54:ILE:HG21	2.39	0.51
1:1:783:A:N3	1:1:783:A:C2'	2.70	0.51
2:2:966:2MG:H2'	2:2:966:2MG:N3	2.26	0.51
12:F:121:ILE:HD12	12:F:141:ILE:CG2	2.40	0.51
1:1:1020:A:C6	1:1:1141:U:O2	2.63	0.51
1:1:2683:C:O2	17:K:70:ARG:NH2	2.41	0.51
2:2:1225:A:N3	2:2:1225:A:C2'	2.72	0.51
2:2:439:U:O2	2:2:440:C:C6	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:516:PSU:O2'	2:2:519:C:N3	2.42	0.51
21:O:51:ALA:HB3	21:O:78:VAL:HB	1.92	0.51
2:2:518:C:C5	2:2:529:G:H2'	2.46	0.51
1:1:1596:A:C2'	1:1:1597:A:C8	2.94	0.50
7:7:73:MET:CE	7:7:110:LEU:HD12	2.41	0.50
7:7:144:TRP:CE3	7:7:201:LEU:HD22	2.47	0.50
1:1:2547:A:H2'	1:1:2548:U:C6	2.46	0.50
1:1:476:G:H4'	1:1:502:A:N1	2.27	0.50
2:2:664:G:H22	2:2:741:G:H1	1.59	0.50
1:1:1385:A:O2'	1:1:1396:U:O2	2.26	0.50
2:2:496:A:N3	2:2:496:A:H2'	2.27	0.50
2:2:975:A:H8	2:2:1357:A:HO2'	1.58	0.50
7:7:73:MET:HE2	7:7:110:LEU:HD12	1.94	0.50
1:1:1408:G:H2'	1:1:1409:U:C6	2.47	0.50
2:2:371:A:H2'	2:2:372:C:O4'	2.11	0.50
2:2:563:A:C2	2:2:884:U:O4	2.59	0.50
11:E:12:VAL:HG13	11:E:172:ALA:CB	2.42	0.49
25:S:59:GLU:HG3	25:S:66:ILE:HD11	1.94	0.49
1:1:2298:A:C6	1:1:2299:U:C2	3.00	0.49
15:I:38:CYS:SG	15:I:39:LYS:N	2.85	0.49
1:1:2585:U:O2	1:1:2585:U:O4'	2.30	0.49
2:2:346:G:OP1	22:P:39:ARG:NH2	2.43	0.49
2:2:14:U:OP2	6:6:41:ARG:NH2	2.46	0.49
7:7:353:LEU:HD12	7:7:357:ILE:HD11	1.94	0.49
2:2:604:G:H2'	2:2:605:U:O4'	2.12	0.49
10:D:90:GLN:HG3	10:D:92:HIS:CE1	2.48	0.49
1:1:2297:A:C6	1:1:2321:U:O4	2.64	0.49
1:1:39:G:H1'	10:D:43:THR:HG21	1.95	0.49
2:2:1064:G:O2'	2:2:1190:G:N2	2.45	0.49
1:1:2291:U:H2'	1:1:2292:U:C6	2.47	0.49
9:C:26:VAL:HG22	9:C:188:LEU:CD2	2.43	0.49
13:G:3:VAL:HG22	13:G:36:ALA:HB1	1.95	0.49
2:2:1140:C:HO2'	2:2:1141:C:P	2.36	0.49
21:O:27:VAL:HG21	21:O:40:ILE:HD12	1.94	0.49
26:T:34:VAL:HG21	26:T:43:ILE:HD11	1.95	0.49
1:1:207:A:H2'	1:1:208:C:O4'	2.13	0.49
1:1:2059:A:N6	1:1:2503:2MA:O2'	2.46	0.49
2:2:555:U:H2'	2:2:556:C:C6	2.48	0.49
29:W:37:ILE:HG22	29:W:38:VAL:HG23	1.95	0.49
7:7:64:GLU:O	7:7:68:ASP:CB	2.60	0.48
16:J:30:THR:HG22	16:J:31:GLU:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:70:G:H4'	1:1:71:A:OP1	2.13	0.48
2:2:13:U:C2	2:2:915:A:C5	3.01	0.48
2:2:373:A:O2'	2:2:451:A:N7	2.46	0.48
2:2:767:A:H2'	2:2:768:A:O4'	2.14	0.48
27:U:13:VAL:CG2	27:U:39:ILE:HD13	2.42	0.48
1:1:2298:A:C6	1:1:2321:U:O4	2.66	0.48
1:1:1789:A:OP2	8:B:221:ARG:NH1	2.47	0.48
21:O:53:THR:HG23	21:O:74:VAL:HG21	1.94	0.48
1:1:1469:A:H2'	1:1:1470:A:C8	2.49	0.48
1:1:2243:U:H2'	1:1:2244:U:C6	2.49	0.48
1:1:2291:U:OP1	1:1:2380:C:O2'	2.28	0.48
2:2:1054:C:O2'	7:7:204:LYS:NZ	2.46	0.48
8:B:88:SER:O	8:B:197:ASN:ND2	2.40	0.48
1:1:2065:C:H4'	1:1:2251:OMG:CM2	2.43	0.48
1:1:1914:C:O2'	1:1:1915:3TD:H5'A	2.14	0.48
11:E:57:LEU:HD12	11:E:87:CYS:SG	2.54	0.48
8:B:157:SER:O	8:B:195:VAL:HG11	2.14	0.48
2:2:108:G:N3	2:2:108:G:H5"	2.29	0.48
7:7:239:LEU:HD11	7:7:241:ILE:CD1	2.44	0.48
16:J:73:VAL:HG11	16:J:75:TYR:CZ	2.48	0.48
1:1:214:G:N2	1:1:216:A:N3	2.62	0.47
2:2:1473:G:H2'	2:2:1474:U:O4'	2.14	0.47
2:2:55:A:N1	2:2:368:U:H5	2.12	0.47
7:7:263:ILE:HD13	7:7:287:ALA:CB	2.44	0.47
12:F:121:ILE:HD12	12:F:141:ILE:HG22	1.96	0.47
25:S:29:VAL:HB	25:S:55:ILE:HD11	1.96	0.47
1:1:2038:G:H2'	1:1:2039:U:O4'	2.14	0.47
1:1:1720:U:H2'	1:1:1721:G:O4'	2.15	0.47
2:2:37:U:N3	2:2:397:A:C6	2.83	0.47
2:2:195:A:HO2'	2:2:196:A:H5'	1.69	0.47
8:B:43:ARG:NH2	8:B:49:ILE:HD11	2.29	0.47
9:C:25:THR:HG21	9:C:193:VAL:HG22	1.96	0.47
1:1:851:C:O2'	32:Z:43:ALA:O	2.30	0.47
1:1:1853:A:N1	1:1:2087:G:H1'	2.29	0.47
1:1:2014:A:H2'	1:1:2015:A:C8	2.50	0.47
10:D:48:THR:HG23	10:D:86:ALA:HB3	1.97	0.47
13:G:99:ILE:O	13:G:103:VAL:HG23	2.15	0.47
2:2:1318:A:OP1	30:X:3:ARG:NH1	145.45	0.47
2:2:148:G:O2'	2:2:149:A:C5'	2.62	0.47
2:2:5:U:O4'	2:2:5:U:O2	2.33	0.47
23:Q:41:LYS:HE2	23:Q:45:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:13:VAL:HG23	27:U:39:ILE:HD13	1.96	0.47
1:1:244:A:H2'	1:1:245:G:O4'	2.15	0.47
1:1:2572:A:N7	9:C:150:GLN:NE2	2.63	0.47
16:J:77:HIS:HA	16:J:83:GLY:O	2.15	0.47
24:R:26:ASP:O	24:R:27:ILE:HD13	2.14	0.47
2:2:1208:C:H2'	2:2:1209:C:H6	1.80	0.47
1:1:1317:G:H2'	1:1:1318:U:O4'	2.15	0.47
1:1:2314:A:OP1	11:E:88:LYS:NZ	2.42	0.47
6:6:20:LEU:HD13	6:6:20:LEU:O	2.15	0.47
7:7:201:LEU:HD21	7:7:203:ARG:HD3	1.96	0.47
27:U:72:ILE:HD12	27:U:83:VAL:HG21	1.96	0.47
1:1:548:G:H3'	1:1:549:G:O4'	2.14	0.46
1:1:819:A:C4	1:1:1189:A:C2	3.03	0.46
8:B:158:ALA:HB1	8:B:197:ASN:O	2.15	0.46
11:E:171:ALA:O	11:E:174:ASP:N	2.49	0.46
18:L:75:ALA:HB2	18:L:105:ILE:HD12	1.95	0.46
1:1:639:U:H2'	1:1:640:C:C6	2.50	0.46
1:1:700:G:H2'	1:1:701:G:O4'	2.15	0.46
2:2:1402:4OC:O2	2:2:1500:A:N1	2.47	0.46
2:2:1317:C:OP2	25:S:28:LYS:CE	197.32	0.46
1:1:1067:A:O2'	1:1:1068:G:O4'	2.33	0.46
1:1:2469:A:N6	1:1:2481:G:O2'	2.48	0.46
2:2:1225:A:N3	2:2:1225:A:H2'	2.30	0.46
1:1:2788:C:H2'	1:1:2789:C:C6	2.51	0.46
1:1:813:U:H2'	1:1:814:C:C6	2.50	0.46
1:1:84:A:N1	1:1:98:G:O2'	2.37	0.46
1:1:1824:G:O2'	8:B:252:THR:CG2	2.64	0.46
1:1:2074:U:C2	1:1:2435:A:N1	2.76	0.46
1:1:2245:U:O2	1:1:2435:A:H2'	2.15	0.46
2:2:1356:G:H2'	2:2:1357:A:C8	2.51	0.46
14:H:118:ILE:HB	14:H:119:PRO:HD3	1.98	0.46
11:E:8:TYR:HA	11:E:12:VAL:HB	1.97	0.46
20:N:38:LEU:N	20:N:39:PRO:CD	2.79	0.46
25:S:25:ARG:NH1	25:S:74:ILE:O	2.49	0.46
32:Z:25:LEU:HD13	32:Z:25:LEU:C	2.36	0.46
1:1:1141:U:H4'	1:1:1142:A:O4'	2.16	0.46
1:1:2315:G:OP1	11:E:33:LYS:CE	2.64	0.46
2:2:915:A:C3'	2:2:915:A:C8	2.99	0.46
7:7:144:TRP:CD2	7:7:201:LEU:HB2	2.51	0.46
9:C:49:GLN:OE1	9:C:79:LEU:HD13	2.16	0.46
1:1:1614:A:N1	25:S:93:ALA:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:131:THR:HG22	10:D:160:ALA:O	2.16	0.46
1:1:1056:G:O2'	1:1:1103:A:N6	2.49	0.45
2:2:517:G:HO2'	2:2:530:G:H5"	1.79	0.45
7:7:14:LEU:HD13	7:7:103:LEU:HD11	1.97	0.45
21:O:27:VAL:CG2	21:O:40:ILE:HD12	2.46	0.45
1:1:1344:U:H5'	1:1:1384:A:C6	2.51	0.45
1:1:2445:2MG:P	10:D:69:ARG:HH22	2.38	0.45
2:2:1017:U:O2'	2:2:1018:G:O4'	2.34	0.45
2:2:945:G:C2	2:2:946:A:C8	3.05	0.45
1:1:1394:U:H4'	1:1:1603:A:H4'	1.97	0.45
7:7:76:GLY:O	7:7:80:VAL:HG23	2.17	0.45
8:B:91:ILE:HD12	8:B:103:TYR:CD1	2.51	0.45
8:B:94:VAL:HG11	8:B:116:ILE:HD11	1.98	0.45
9:C:121:THR:HB	9:C:127:PHE:CD2	2.50	0.45
1:1:320:A:H2'	10:D:131:THR:HG21	1.99	0.45
23:Q:58:ARG:HA	23:Q:61:TRP:CE3	2.52	0.45
1:1:784:G:H5'	1:1:785:G:OP1	2.16	0.45
7:7:298:LEU:O	7:7:298:LEU:HD23	2.15	0.45
23:Q:76:TYR:CZ	23:Q:80:ILE:HG13	2.51	0.45
1:1:1047:G:N2	1:1:1110:G:O2'	2.49	0.45
1:1:2313:C:H5"	11:E:68:THR:HG21	1.97	0.45
1:1:67:U:C2	1:1:74:A:N6	2.84	0.45
7:7:353:LEU:CD1	7:7:357:ILE:HD11	2.45	0.45
8:B:158:ALA:C	8:B:195:VAL:HG13	2.37	0.45
9:C:152:PRO:HG3	9:C:156:PHE:CZ	2.51	0.45
10:D:5:LEU:HD23	10:D:122:GLU:OE1	2.17	0.45
26:T:2:ILE:HD13	26:T:42:GLU:HA	1.99	0.45
6:6:16:ILE:N	6:6:17:GLU:OE1	2.49	0.45
10:D:138:LEU:HD13	10:D:167:VAL:HG21	1.98	0.45
1:1:1510:G:H2'	1:1:1511:G:O4'	2.16	0.45
1:1:1783:A:N1	1:1:2587:A:H2'	2.31	0.45
1:1:1922:G:C2'	1:1:1923:U:H5'	2.47	0.45
1:1:1939:5MU:OP1	1:1:2604:U:O2'	2.35	0.45
2:2:1435:G:H2'	2:2:1436:U:C6	2.51	0.45
2:2:1493:A:O2'	2:2:1494:G:P	2.74	0.45
2:2:1499:A:O2'	2:2:1500:A:C5'	2.65	0.45
11:E:42:GLU:CG	11:E:49:LEU:HD23	2.47	0.45
16:J:110:PRO:O	16:J:115:GLY:HA3	2.17	0.45
1:1:2552:OMU:O5'	1:1:2552:OMU:H6	2.17	0.45
16:J:114:LEU:HD12	16:J:114:LEU:HA	1.81	0.45
1:1:729:G:H2'	1:1:1775:U:H1'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:197:A:N6	1:1:2430:A:H2'	2.32	0.45
1:1:348:A:H2'	1:1:349:U:O4'	2.17	0.45
13:G:96:THR:HG22	13:G:115:VAL:HB	1.99	0.45
1:1:1797:G:C5	1:1:1798:U:C5	3.05	0.44
7:7:199:HIS:CE1	7:7:323:ILE:HD11	2.52	0.44
7:7:5:ASN:N	7:7:6:PRO:CD	2.80	0.44
18:L:96:LYS:HG3	18:L:101:ILE:HD11	1.99	0.44
1:1:319:G:H2'	1:1:320:A:O4'	2.17	0.44
2:2:1382:C:O2'	2:2:1383:C:H5'	2.17	0.44
3:3:28:C:H2'	3:3:29:A:O4'	2.17	0.44
23:Q:92:ARG:HA	23:Q:95:LEU:HD12	1.98	0.44
10:D:28:VAL:O	10:D:32:VAL:HG23	2.18	0.44
1:1:981:A:H2	1:1:2027:G:N3	2.15	0.44
2:2:1323:G:H2'	2:2:1324:A:C8	2.53	0.44
2:2:481:G:HO2'	2:2:483:C:H41	1.60	0.44
2:2:529:G:O2'	2:2:530:G:H5'	2.17	0.44
2:2:798:U:H2'	2:2:799:G:O4'	2.16	0.44
2:2:244:U:O4	2:2:906:A:H1'	2.17	0.44
2:2:928:G:O2'	2:2:929:G:O5'	2.36	0.44
7:7:298:LEU:C	7:7:298:LEU:CD2	2.85	0.44
1:1:1993:U:H4'	9:C:133:THR:HG22	1.99	0.44
1:1:2537:U:H2'	1:1:2538:C:C6	2.52	0.44
2:2:1176:A:H2'	2:2:1177:G:O4'	2.17	0.44
2:2:140:U:H2'	2:2:141:G:O4'	2.18	0.44
2:2:515:G:H2'	2:2:516:PSU:H6	1.82	0.44
25:S:17:VAL:HG12	25:S:76:VAL:HG21	1.99	0.44
1:1:1064:C:H2'	1:1:1065:U:C6	2.51	0.44
1:1:1141:U:O2	1:1:1142:A:N6	2.51	0.44
1:1:1519:G:H2'	1:1:1520:U:O4'	2.18	0.44
2:2:1207:2MG:C2'	2:2:1208:C:H5'	2.48	0.44
2:2:872:A:N3	2:2:872:A:H2'	2.33	0.44
3:3:65:U:C4	3:3:108:A:C4	3.06	0.44
7:7:18:SER:HA	7:7:110:LEU:HD11	2.00	0.44
11:E:57:LEU:HD13	11:E:65:PRO:HB3	1.99	0.44
1:1:1028:A:N6	1:1:1125:G:H2'	2.32	0.44
1:1:2065:C:H2'	1:1:2066:C:O4'	2.18	0.44
1:1:2298:A:C5	1:1:2321:U:C4	3.06	0.44
2:2:399:G:H2'	2:2:400:C:C6	2.52	0.44
2:2:515:G:O2'	2:2:516:PSU:C5'	2.66	0.44
2:2:915:A:C5	2:2:916:U:C5	3.05	0.44
2:2:967:5MC:H5"	2:2:968:A:P	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:19:VAL:HG13	8:B:199:GLU:HG3	1.99	0.44
14:H:35:VAL:O	14:H:39:THR:HG23	2.18	0.44
19:M:24:THR:O	19:M:24:THR:HG22	2.17	0.44
23:Q:14:HIS:O	23:Q:18:LEU:HD23	2.17	0.44
24:R:25:LEU:HD12	24:R:94:THR:HG21	2.00	0.44
27:U:13:VAL:HG21	27:U:39:ILE:HG21	1.98	0.44
1:1:1386:C:H2'	1:1:1387:A:C8	2.53	0.44
2:2:321:A:N7	2:2:328:C:O2'	2.45	0.44
2:2:986:U:H2'	2:2:987:G:O4'	2.18	0.44
7:7:266:ILE:HB	7:7:267:PRO:HD3	2.00	0.44
16:J:28:LEU:HD12	16:J:142:ILE:HG21	1.99	0.44
1:1:754:U:O2	1:1:755:U:C2	2.71	0.44
2:2:1382:C:C2'	2:2:1383:C:H5'	2.48	0.44
2:2:37:U:C4	2:2:397:A:N6	2.82	0.44
2:2:860:A:H2'	2:2:861:G:O4'	2.18	0.44
6:6:22:ASP:OD1	6:6:23:PRO:CD	2.57	0.44
9:C:71:ALA:HB3	9:C:73:VAL:HG12	1.99	0.44
1:1:1169:A:H5"	1:1:1169:A:N3	2.33	0.43
1:1:973:A:O4'	1:1:1188:U:C6	2.71	0.43
1:1:57:C:H2'	1:1:58:G:O4'	2.18	0.43
1:1:783:A:H8	1:1:1778:U:HO2'	1.65	0.43
2:2:1370:G:C2	2:2:1371:G:C8	3.06	0.43
1:1:1062:G:O2'	15:I:131:THR:HG23	2.19	0.43
1:1:36:G:N3	1:1:450:G:O2'	2.52	0.43
19:M:53:MET:HG3	19:M:63:ILE:HD13	2.00	0.43
2:2:1518:MA6:C9	2:2:1519:MA6:H93	2.48	0.43
2:2:421:U:O4'	2:2:421:U:O2	2.37	0.43
2:2:580:C:H2'	2:2:581:G:O4'	2.18	0.43
1:1:2698:U:H2'	1:1:2699:C:C6	2.53	0.43
1:1:1656:C:OP1	9:C:141:ARG:NH1	2.52	0.43
1:1:2273:A:H2'	1:1:2274:A:C8	2.53	0.43
1:1:2314:A:H2'	1:1:2315:G:C8	2.53	0.43
1:1:745:1MG:HN21	1:1:745:1MG:HM11	1.65	0.43
17:K:113:MET:O	17:K:116:ILE:HG13	2.17	0.43
17:K:42:THR:HG23	17:K:44:LYS:HE2	2.01	0.43
1:1:2133:G:O2'	1:1:2157:G:N2	2.50	0.43
2:2:1175:G:O2'	2:2:1176:A:P	2.76	0.43
2:2:1460:C:H2'	2:2:1461:G:O4'	2.18	0.43
14:H:14:GLU:O	14:H:18:VAL:HG23	2.18	0.43
1:1:1182:G:H2'	1:1:1183:U:O4'	2.18	0.43
1:1:679:C:H2'	1:1:680:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1109:C:C3'	2:2:1109:C:C5'	2.97	0.43
2:2:657:U:O2	26:T:22:THR:HG23	119.77	0.43
3:3:8:C:O3'	21:O:25:ARG:NH1	2.47	0.43
15:I:105:LEU:HD22	15:I:128:ILE:CG2	2.49	0.43
18:L:111:ILE:HD12	18:L:111:ILE:N	2.34	0.43
19:M:41:LEU:HD21	19:M:126:ILE:HD13	2.00	0.43
1:1:372:G:O2'	1:1:400:G:O6	2.28	0.43
3:3:29:A:C2	3:3:56:G:C2	3.06	0.43
1:1:12:U:O2	1:1:12:U:H2'	2.18	0.43
12:F:140:VAL:O	12:F:144:VAL:HG23	2.19	0.43
1:1:1021:A:N6	1:1:1141:U:N3	2.45	0.43
1:1:1141:U:O2	1:1:1142:A:C6	2.72	0.43
1:1:2395:C:H2'	1:1:2396:G:O4'	2.19	0.43
2:2:148:G:O2'	2:2:149:A:O4'	2.31	0.43
2:2:382:A:H2'	2:2:383:A:C8	2.54	0.43
11:E:12:VAL:HG13	11:E:172:ALA:HB1	2.00	0.43
18:L:109:LYS:HA	18:L:126:ARG:O	2.19	0.43
20:N:28:LEU:HD23	20:N:48:VAL:HG21	1.99	0.43
22:P:106:LYS:HA	22:P:109:ARG:HD3	2.00	0.43
1:1:2445:2MG:OP1	10:D:69:ARG:NH2	2.42	0.42
2:2:1124:G:O2'	2:2:1145:A:N6	2.52	0.42
11:E:122:PHE:CZ	11:E:167:ARG:HA	2.53	0.42
21:O:28:VAL:HG11	21:O:103:VAL:HG13	2.01	0.42
21:O:75:GLY:O	21:O:78:VAL:HG12	2.19	0.42
2:2:827:U:C2	2:2:874:G:N2	2.87	0.42
9:C:26:VAL:HG22	9:C:188:LEU:HD22	2.00	0.42
15:I:10:LEU:HD22	15:I:26:ALA:HB1	2.00	0.42
29:W:37:ILE:HG21	29:W:80:ILE:HG21	2.01	0.42
1:1:118:A:N3	1:1:178:G:H1'	2.34	0.42
1:1:2074:U:C4	1:1:2435:A:N1	2.79	0.42
2:2:110:C:H2'	2:2:111:G:O4'	2.19	0.42
2:2:842:U:H3'	2:2:843:U:C5'	2.48	0.42
2:2:928:G:O2'	2:2:929:G:H5'	2.19	0.42
6:6:19:LEU:C	6:6:19:LEU:HD23	2.40	0.42
1:1:1428:C:C5	1:1:1569:A:H5'	2.54	0.42
1:1:2071:A:H2'	1:1:2072:C:C6	2.55	0.42
1:1:2226:C:H2'	1:1:2227:A:O4'	2.19	0.42
1:1:67:U:O2	1:1:74:A:N7	2.52	0.42
2:2:373:A:C2	2:2:374:A:C8	3.08	0.42
26:T:50:LEU:HD23	31:Y:26:PHE:CE1	2.53	0.42
1:1:587:C:OP2	18:L:21:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:953:G:C2'	1:1:954:G:O5'	2.68	0.42
2:2:37:U:C4	2:2:397:A:C6	3.07	0.42
1:1:1007:C:OP1	16:J:37:ARG:NH2	2.52	0.42
1:1:74:A:N7	1:1:88:G:C5	2.87	0.42
1:1:796:C:H2'	1:1:797:G:C8	2.54	0.42
1:1:861:A:C2	1:1:917:A:C4	3.08	0.42
1:1:984:A:H2'	1:1:984:A:N3	2.34	0.42
2:2:1389:C:O2'	2:2:1390:U:H5'	2.19	0.42
2:2:337:G:H2'	2:2:338:A:C8	2.54	0.42
27:U:7:ARG:O	27:U:25:VAL:O	2.38	0.42
26:T:8:LEU:HD13	31:Y:22:LEU:HB3	2.01	0.42
2:2:199:A:H2'	2:2:200:G:H8	1.84	0.42
14:H:43:LYS:HE3	14:H:95:LEU:HD22	2.02	0.42
1:1:2618:G:C6	1:1:2619:C:C4	3.08	0.42
2:2:216:U:H2'	2:2:217:C:C6	2.55	0.42
27:U:5:ILE:HD12	27:U:5:ILE:N	2.34	0.42
28:V:8:VAL:HG22	28:V:38:LEU:HD11	2.00	0.42
2:2:1428:A:H2'	2:2:1429:A:O4'	2.20	0.42
7:7:7:VAL:HG22	7:7:100:VAL:HG13	2.01	0.42
9:C:156:PHE:CE1	16:J:81:ILE:HD13	2.54	0.42
19:M:74:THR:HA	19:M:88:ASN:O	2.19	0.42
1:1:1678:A:H2'	1:1:1679:A:O4'	2.20	0.42
1:1:580:U:O3'	23:Q:31:VAL:HG13	2.20	0.42
1:1:780:G:O2'	1:1:783:A:N6	2.53	0.42
2:2:381:C:H2'	2:2:382:A:O4'	2.19	0.42
7:7:17:ARG:CD	7:7:110:LEU:HD22	2.50	0.42
13:G:15:LEU:HD22	13:G:16:GLY:N	2.34	0.42
1:1:2190:G:H2'	1:1:2191:A:O4'	2.20	0.41
1:1:523:C:H4'	1:1:540:C:O2	2.20	0.41
2:2:104:G:H4'	2:2:174:A:O4'	2.20	0.41
1:1:2639:A:H2'	1:1:2640:G:O4'	2.20	0.41
1:1:644:A:H2'	1:1:645:C:O4'	2.20	0.41
14:H:121:SER:OG	14:H:126:LEU:HD11	2.20	0.41
1:1:1589:U:C2	1:1:1590:A:C8	3.08	0.41
1:1:674:G:O2'	10:D:69:ARG:HD3	2.20	0.41
2:2:1493:A:HO2'	2:2:1494:G:P	2.43	0.41
2:2:918:A:H2'	2:2:919:A:O4'	2.20	0.41
3:3:89:U:O2	3:3:89:U:O4'	2.35	0.41
7:7:123:TYR:CZ	7:7:226:VAL:HG12	2.55	0.41
19:M:109:PRO:HD2	19:M:112:LEU:HD23	2.02	0.41
1:1:1198:U:H5'	23:Q:9:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2297:A:H2	1:1:2321:U:C5	2.37	0.41
1:1:250:G:C6	1:1:251:A:C6	3.08	0.41
1:1:2780:G:O6	16:J:99:ARG:NH1	2.53	0.41
2:2:976:G:C8	2:2:1358:U:C2	3.08	0.41
7:7:143:ASP:O	7:7:146:SER:OG	2.37	0.41
7:7:333:ILE:HD13	7:7:348:VAL:HG11	2.02	0.41
17:K:38:ILE:HD11	17:K:112:PHE:CZ	2.55	0.41
1:1:930:G:H1'	32:Z:25:LEU:HD11	2.03	0.41
1:1:2103:C:HO2'	1:1:2104:C:H6	1.67	0.41
1:1:2249:U:H3'	1:1:2250:G:C5'	2.49	0.41
1:1:2286:G:C8	1:1:2286:G:H5'	2.56	0.41
1:1:2331:G:O2'	1:1:2336:A:N1	2.48	0.41
2:2:1391:U:O2'	2:2:1392:G:O5'	2.38	0.41
9:C:186:LEU:HD21	22:P:4:ILE:HG21	2.03	0.41
1:1:133:U:H2'	1:1:134:G:O4'	2.20	0.41
1:1:2040:G:H2'	1:1:2041:U:O4'	2.21	0.41
1:1:2756:U:C4	1:1:2759:G:C6	3.08	0.41
1:1:74:A:N7	1:1:88:G:N7	2.68	0.41
2:2:502:A:H2'	2:2:503:C:O4'	2.20	0.41
2:2:662:U:O2'	2:2:836:G:OP1	2.36	0.41
7:7:14:LEU:O	7:7:17:ARG:HG3	2.20	0.41
11:E:29:PRO:HB2	11:E:169:LEU:HD22	2.02	0.41
2:2:152:A:N6	2:2:170:U:C2	2.88	0.41
2:2:384:G:H2'	2:2:385:C:C6	2.55	0.41
11:E:74:VAL:HG22	11:E:79:ILE:HD11	2.02	0.41
1:1:2679:A:H2'	1:1:2680:U:O4'	2.21	0.41
1:1:811:U:C2	1:1:1251:C:C5	3.08	0.41
1:1:1913:A:H1'	2:2:1492:A:N1	2.36	0.41
2:2:525:C:C2'	2:2:526:C:H5'	2.51	0.41
2:2:16:A:OP1	6:6:41:ARG:HG3	2.20	0.41
1:1:2564:A:C2	1:1:2647:U:H4'	2.56	0.41
1:1:2794:C:H2'	1:1:2795:C:C6	2.55	0.41
1:1:466:A:H2	1:1:795:C:O2	2.04	0.41
2:2:1499:A:H3'	2:2:1499:A:OP2	2.21	0.41
5:5:19:G:H3'	5:5:20:H2U:H5"	2.03	0.41
20:N:67:PHE:O	20:N:71:ARG:HG2	2.20	0.41
1:1:172:A:H2'	1:1:173:A:C8	2.56	0.41
1:1:645:C:H2'	1:1:647:G:C8	2.56	0.41
2:2:1007:U:N3	2:2:1022:A:N1	2.67	0.41
2:2:1277:C:O2'	2:2:1279:G:H8	2.04	0.41
1:1:2444:G:OP2	10:D:63:LYS:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:23:LEU:HA	14:H:118:ILE:HG12	2.03	0.41
22:P:43:PHE:CZ	22:P:63:LYS:HG2	2.56	0.41
1:1:1065:U:HO2'	1:1:1066:U:C5'	2.32	0.41
1:1:1562:U:H2'	1:1:1563:U:O4'	2.21	0.41
2:2:684:U:H2'	2:2:685:G:O4'	2.20	0.41
20:N:90:ARG:CZ	20:N:116:VAL:HG11	2.51	0.41
20:N:2:ARG:O	20:N:2:ARG:NH1	2.54	0.41
1:1:1198:U:C5'	23:Q:9:ILE:HD11	2.51	0.41
1:1:833:A:H2'	1:1:834:G:C8	2.56	0.40
2:2:1384:C:H2'	2:2:1385:G:C8	2.56	0.40
1:1:1400:U:H2'	1:1:1401:G:O4'	2.21	0.40
1:1:1964:G:H4'	1:1:1965:C:OP2	2.21	0.40
1:1:742:A:C2	1:1:743:A:C6	3.09	0.40
2:2:215:C:H2'	2:2:216:U:O4'	2.21	0.40
2:2:915:A:H8	2:2:915:A:O5'	2.04	0.40
6:6:22:ASP:CG	6:6:23:PRO:HD2	2.41	0.40
7:7:42:GLU:HG3	7:7:43:GLN:N	2.35	0.40
20:N:55:ALA:HA	20:N:80:PHE:CE1	2.56	0.40
1:1:1932:A:H2'	1:1:1933:G:O4'	2.22	0.40
6:6:23:PRO:O	6:6:24:LEU:C	2.60	0.40
8:B:31:ALA:N	8:B:32:PRO:CD	2.84	0.40
10:D:134:LEU:HB2	10:D:160:ALA:HB1	2.03	0.40
19:M:14:LYS:O	19:M:71:LYS:NZ	2.48	0.40
20:N:14:SER:HA	20:N:17:ARG:NH1	2.36	0.40
1:1:1797:G:C6	1:1:1798:U:C4	3.09	0.40
1:1:1924:C:H2'	1:1:1925:C:O4'	2.21	0.40
1:1:2025:C:H2'	1:1:2026:U:C6	2.56	0.40
1:1:2074:U:H2'	1:1:2075:U:C6	2.57	0.40
1:1:2685:G:OP1	17:K:78:ARG:NH2	2.53	0.40
2:2:1424:U:H2'	2:2:1425:U:O4'	2.21	0.40
2:2:567:G:H2'	2:2:568:G:O4'	2.22	0.40
16:J:30:THR:CG2	16:J:31:GLU:N	2.85	0.40
19:M:41:LEU:HD21	19:M:126:ILE:CD1	2.51	0.40
30:X:32:ASN:OD1	30:X:34:HIS:NE2	2.55	0.40
1:1:1021:A:C3'	1:1:1021:A:N3	2.79	0.40
1:1:1754:A:N1	1:1:2716:C:O2'	2.38	0.40
1:1:1910:G:H2'	1:1:1911:PSU:C6	2.57	0.40
1:1:1910:G:H2'	1:1:1911:PSU:H6	1.86	0.40
1:1:871:U:H2'	1:1:872:U:C6	2.56	0.40
1:1:74:A:N6	1:1:88:G:O6	2.54	0.40
2:2:953:G:H2'	2:2:954:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:530:G:C5	6:6:30:GLU:HG3	2.57	0.40
9:C:149:ASN:O	9:C:151:THR:N	2.54	0.40
17:K:33:ALA:HB1	17:K:37:ASP:HB2	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	6	30/61 (49%)	24 (80%)	6 (20%)	0	100	100
7	7	335/365 (92%)	322 (96%)	11 (3%)	2 (1%)	30	66
8	B	269/273 (98%)	249 (93%)	18 (7%)	2 (1%)	26	64
9	C	207/209 (99%)	196 (95%)	10 (5%)	1 (0%)	34	70
10	D	199/201 (99%)	188 (94%)	10 (5%)	1 (0%)	34	70
11	E	175/179 (98%)	164 (94%)	10 (6%)	1 (1%)	30	66
12	F	173/177 (98%)	165 (95%)	8 (5%)	0	100	100
13	G	147/149 (99%)	132 (90%)	14 (10%)	1 (1%)	26	64
14	H	128/165 (78%)	106 (83%)	19 (15%)	3 (2%)	8	32
15	I	133/142 (94%)	116 (87%)	15 (11%)	2 (2%)	13	44
16	J	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
17	K	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
18	L	142/144 (99%)	135 (95%)	6 (4%)	1 (1%)	26	64
19	M	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
20	N	117/127 (92%)	106 (91%)	11 (9%)	0	100	100
21	O	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
22	P	112/115 (97%)	106 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
23	Q	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	21 58
24	R	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	9 36
25	S	108/110 (98%)	103 (95%)	5 (5%)	0	100 100
26	T	92/100 (92%)	87 (95%)	5 (5%)	0	100 100
27	U	101/104 (97%)	96 (95%)	5 (5%)	0	100 100
28	V	92/94 (98%)	89 (97%)	3 (3%)	0	100 100
29	W	74/85 (87%)	68 (92%)	5 (7%)	1 (1%)	14 46
30	X	75/78 (96%)	71 (95%)	4 (5%)	0	100 100
31	Y	60/63 (95%)	57 (95%)	3 (5%)	0	100 100
32	Z	56/59 (95%)	52 (93%)	4 (7%)	0	100 100
33	a	64/70 (91%)	58 (91%)	6 (9%)	0	100 100
34	b	54/57 (95%)	51 (94%)	3 (6%)	0	100 100
35	c	50/55 (91%)	47 (94%)	3 (6%)	0	100 100
36	d	44/46 (96%)	40 (91%)	4 (9%)	0	100 100
37	e	62/65 (95%)	56 (90%)	6 (10%)	0	100 100
38	f	36/38 (95%)	33 (92%)	3 (8%)	0	100 100
39	g	223/241 (92%)	208 (93%)	14 (6%)	1 (0%)	39 74
40	h	206/233 (88%)	193 (94%)	12 (6%)	1 (0%)	34 70
41	i	203/206 (98%)	196 (97%)	7 (3%)	0	100 100
42	j	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	30 66
43	k	102/135 (76%)	98 (96%)	3 (3%)	1 (1%)	19 56
44	l	149/179 (83%)	142 (95%)	6 (4%)	1 (1%)	26 64
45	m	127/130 (98%)	120 (94%)	5 (4%)	2 (2%)	12 42
46	n	125/130 (96%)	113 (90%)	11 (9%)	1 (1%)	24 61
47	o	97/103 (94%)	90 (93%)	6 (6%)	1 (1%)	19 56
48	p	115/129 (89%)	103 (90%)	10 (9%)	2 (2%)	11 41
49	q	120/124 (97%)	115 (96%)	5 (4%)	0	100 100
50	r	114/118 (97%)	110 (96%)	4 (4%)	0	100 100
51	s	98/101 (97%)	95 (97%)	3 (3%)	0	100 100
52	t	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	16 50
53	u	80/82 (98%)	76 (95%)	4 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	v	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
55	w	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
56	x	81/92 (88%)	77 (95%)	4 (5%)	0	100	100
57	y	84/87 (97%)	84 (100%)	0	0	100	100
58	z	68/71 (96%)	68 (100%)	0	0	100	100
All	All	6234/6646 (94%)	5854 (94%)	350 (6%)	30 (0%)	38	70

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	B	158	ALA
46	n	56	ASP
7	7	137	GLY
11	E	62	GLY
14	H	117	LEU
23	Q	3	ARG
42	j	44	GLY
43	k	96	VAL
47	o	57	VAL
7	7	91	ASP
15	I	113	ALA
40	h	80	LYS
44	l	130	ASN
52	t	21	ASP
8	B	240	PHE
10	D	142	ALA
14	H	51	TYR
24	R	37	GLU
48	p	119	ASN
13	G	89	LYS
14	H	55	VAL
9	C	94	GLN
29	W	29	GLU
39	g	74	ARG
45	m	6	PRO
15	I	136	GLY
48	p	74	VAL
18	L	28	GLY
24	R	44	GLY
45	m	75	ILE

5.3.2 Protein sidechains (i)

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	6	27/52 (52%)	24 (89%)	3 (11%)	8 28
7	7	292/310 (94%)	260 (89%)	32 (11%)	8 29
8	B	216/218 (99%)	201 (93%)	15 (7%)	19 52
9	C	164/164 (100%)	159 (97%)	5 (3%)	48 80
10	D	165/165 (100%)	152 (92%)	13 (8%)	15 46
11	E	148/150 (99%)	137 (93%)	11 (7%)	17 49
12	F	136/138 (99%)	130 (96%)	6 (4%)	35 70
13	G	114/114 (100%)	102 (90%)	12 (10%)	8 30
14	H	99/123 (80%)	89 (90%)	10 (10%)	9 32
15	I	104/110 (94%)	95 (91%)	9 (9%)	13 42
16	J	116/116 (100%)	110 (95%)	6 (5%)	29 64
17	K	104/104 (100%)	98 (94%)	6 (6%)	25 59
18	L	103/103 (100%)	98 (95%)	5 (5%)	31 67
19	M	109/109 (100%)	100 (92%)	9 (8%)	14 44
20	N	99/103 (96%)	90 (91%)	9 (9%)	12 38
21	O	86/87 (99%)	79 (92%)	7 (8%)	15 45
22	P	99/100 (99%)	91 (92%)	8 (8%)	15 45
23	Q	89/90 (99%)	84 (94%)	5 (6%)	26 61
24	R	84/84 (100%)	75 (89%)	9 (11%)	8 30
25	S	93/93 (100%)	85 (91%)	8 (9%)	13 43
26	T	81/84 (96%)	78 (96%)	3 (4%)	41 76
27	U	84/85 (99%)	78 (93%)	6 (7%)	18 52
28	V	78/78 (100%)	76 (97%)	2 (3%)	54 83
29	W	58/63 (92%)	54 (93%)	4 (7%)	19 52
30	X	67/68 (98%)	61 (91%)	6 (9%)	12 39
31	Y	54/55 (98%)	49 (91%)	5 (9%)	11 37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
32	Z	48/49 (98%)	42 (88%)	6 (12%)	6 21
33	a	59/62 (95%)	52 (88%)	7 (12%)	6 23
34	b	47/48 (98%)	42 (89%)	5 (11%)	8 30
35	c	47/49 (96%)	45 (96%)	2 (4%)	35 71
36	d	38/38 (100%)	31 (82%)	7 (18%)	2 8
37	e	51/52 (98%)	46 (90%)	5 (10%)	10 34
38	f	34/34 (100%)	31 (91%)	3 (9%)	12 41
39	g	187/199 (94%)	180 (96%)	7 (4%)	41 76
40	h	171/190 (90%)	161 (94%)	10 (6%)	25 59
41	i	172/173 (99%)	163 (95%)	9 (5%)	29 64
42	j	119/126 (94%)	109 (92%)	10 (8%)	14 43
43	k	91/116 (78%)	83 (91%)	8 (9%)	12 41
44	l	124/147 (84%)	113 (91%)	11 (9%)	12 39
45	m	104/105 (99%)	100 (96%)	4 (4%)	40 75
46	n	105/107 (98%)	96 (91%)	9 (9%)	13 43
47	o	86/90 (96%)	77 (90%)	9 (10%)	8 30
48	p	90/99 (91%)	86 (96%)	4 (4%)	35 70
49	q	102/103 (99%)	95 (93%)	7 (7%)	19 52
50	r	94/96 (98%)	87 (93%)	7 (7%)	17 49
51	s	83/84 (99%)	79 (95%)	4 (5%)	31 67
52	t	76/77 (99%)	63 (83%)	13 (17%)	2 10
53	u	65/65 (100%)	60 (92%)	5 (8%)	16 48
54	v	74/78 (95%)	71 (96%)	3 (4%)	37 73
55	w	57/65 (88%)	55 (96%)	2 (4%)	43 78
56	x	72/79 (91%)	65 (90%)	7 (10%)	10 34
57	y	65/66 (98%)	62 (95%)	3 (5%)	33 69
58	z	60/61 (98%)	53 (88%)	7 (12%)	7 25
All	All	5190/5424 (96%)	4802 (92%)	388 (8%)	21 49

All (388) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	17	GLU

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Mol	Chain	Res	Type
6	6	18	THR
6	6	20	LEU
7	7	14	LEU
7	7	17	ARG
7	7	27	TYR
7	7	31	LYS
7	7	42	GLU
7	7	54	GLN
7	7	79	ASP
7	7	86	LEU
7	7	102	GLU
7	7	107	GLU
7	7	112	GLN
7	7	114	GLU
7	7	117	ARG
7	7	122	GLU
7	7	123	TYR
7	7	124	ASP
7	7	186	ASP
7	7	195	GLU
7	7	242	ASP
7	7	258	GLU
7	7	270	ILE
7	7	272	THR
7	7	276	ASN
7	7	279	SER
7	7	285	ASP
7	7	288	MET
7	7	292	LYS
7	7	324	ARG
7	7	337	ARG
7	7	343	ARG
7	7	354	ASP
7	7	362	LYS
8	B	51	THR
8	B	52	ARG
8	B	115	GLN
8	B	125	LYS
8	B	156	ARG
8	B	174	LEU
8	B	189	ARG
8	B	202	LEU

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Mol	Chain	Res	Type
8	B	203	ARG
8	B	204	VAL
8	B	242	LYS
8	B	252	THR
8	B	257	THR
8	B	258	ARG
8	B	261	LYS
9	C	2	ILE
9	C	4	LEU
9	C	13	ARG
9	C	46	ARG
9	C	59	ARG
10	D	9	GLN
10	D	21	ARG
10	D	40	ARG
10	D	48	THR
10	D	57	LYS
10	D	67	ARG
10	D	69	ARG
10	D	77	ILE
10	D	105	LEU
10	D	108	ILE
10	D	109	LEU
10	D	122	GLU
10	D	149	ILE
11	E	10	ASP
11	E	57	LEU
11	E	80	ARG
11	E	95	ARG
11	E	115	ARG
11	E	117	LEU
11	E	122	PHE
11	E	123	ASP
11	E	133	ARG
11	E	140	GLU
11	E	152	LEU
12	F	32	GLU
12	F	95	ARG
12	F	104	ASN
12	F	114	ASP
12	F	152	ARG
12	F	176	LYS

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Mol	Chain	Res	Type
13	G	1	MET
13	G	11	ASN
13	G	12	LEU
13	G	15	LEU
13	G	41	LYS
13	G	51	ARG
13	G	66	ASN
13	G	72	ILE
13	G	87	GLU
13	G	96	THR
13	G	97	ARG
13	G	114	GLU
14	H	3	LEU
14	H	7	ASP
14	H	9	GLN
14	H	29	ASP
14	H	37	LYS
14	H	40	GLU
14	H	57	ASN
14	H	109	LYS
14	H	114	GLU
14	H	123	ILE
15	I	10	LEU
15	I	11	GLN
15	I	38	CYS
15	I	44	LYS
15	I	71	LYS
15	I	78	LEU
15	I	79	LEU
15	I	95	ASP
15	I	137	LEU
16	J	5	THR
16	J	30	THR
16	J	40	HIS
16	J	65	THR
16	J	70	THR
16	J	108	MET
17	K	17	ARG
17	K	49	ARG
17	K	53	LYS
17	K	70	ARG
17	K	91	SER

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Mol	Chain	Res	Type
17	K	99	ILE
18	L	2	ARG
18	L	42	SER
18	L	48	ARG
18	L	59	ARG
18	L	78	ARG
19	M	6	ARG
19	M	14	LYS
19	M	18	ARG
19	M	40	ARG
19	M	95	LEU
19	M	110	GLU
19	M	115	GLU
19	M	126	ILE
19	M	134	THR
20	N	1	MET
20	N	2	ARG
20	N	20	MET
20	N	46	ARG
20	N	51	LEU
20	N	59	SER
20	N	63	ARG
20	N	69	ARG
20	N	95	THR
21	O	8	ILE
21	O	19	GLN
21	O	20	GLU
21	O	31	THR
21	O	48	LEU
21	O	94	ARG
21	O	102	ARG
22	P	8	LEU
22	P	11	GLU
22	P	26	VAL
22	P	27	GLU
22	P	81	VAL
22	P	109	ARG
22	P	110	ILE
22	P	114	LEU
23	Q	3	ARG
23	Q	51	ARG
23	Q	75	SER

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Mol	Chain	Res	Type
23	Q	91	ASP
23	Q	117	LEU
24	R	10	LYS
24	R	39	LEU
24	R	40	MET
24	R	48	LYS
24	R	55	ASP
24	R	68	ARG
24	R	71	LYS
24	R	72	VAL
24	R	86	GLN
25	S	7	HIS
25	S	12	SER
25	S	19	LEU
25	S	67	ASP
25	S	69	LEU
25	S	107	VAL
25	S	108	SER
25	S	110	ARG
26	T	1	MET
26	T	25	GLU
26	T	78	SER
27	U	6	ARG
27	U	8	ASP
27	U	22	ARG
27	U	52	LEU
27	U	68	SER
27	U	99	ASN
28	V	1	MET
28	V	40	ILE
29	W	10	THR
29	W	11	ARG
29	W	64	ASP
29	W	70	GLU
30	X	11	ARG
30	X	25	THR
30	X	33	LEU
30	X	48	THR
30	X	54	LYS
30	X	56	MET
31	Y	7	ARG
31	Y	18	LEU

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Mol	Chain	Res	Type
31	Y	48	ARG
31	Y	49	ASP
31	Y	57	LEU
32	Z	6	LYS
32	Z	10	THR
32	Z	11	ARG
32	Z	31	ARG
32	Z	36	VAL
32	Z	45	ARG
33	a	16	CYS
33	a	24	ILE
33	a	43	PHE
33	a	45	THR
33	a	47	LYS
33	a	56	ARG
33	a	63	ARG
34	b	9	THR
34	b	11	SER
34	b	12	LYS
34	b	27	SER
34	b	40	ARG
35	c	5	ILE
35	c	13	SER
36	d	3	ARG
36	d	12	ARG
36	d	24	THR
36	d	41	ARG
36	d	42	LEU
36	d	43	THR
36	d	45	SER
37	e	16	LYS
37	e	30	ARG
37	e	31	HIS
37	e	54	ASP
37	e	55	LEU
38	f	3	VAL
38	f	6	SER
38	f	26	ILE
39	g	23	TRP
39	g	105	LYS
39	g	117	LEU
39	g	128	LYS

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Mol	Chain	Res	Type
39	g	129	LEU
39	g	132	LYS
39	g	220	THR
40	h	14	ILE
40	h	33	LEU
40	h	35	SER
40	h	89	LYS
40	h	135	LYS
40	h	164	ARG
40	h	175	LEU
40	h	178	LEU
40	h	185	ASN
40	h	200	VAL
41	i	5	LEU
41	i	47	ARG
41	i	95	GLU
41	i	104	ARG
41	i	116	GLN
41	i	138	SER
41	i	143	VAL
41	i	197	GLU
41	i	206	LYS
42	j	10	GLU
42	j	15	LEU
42	j	18	VAL
42	j	60	ILE
42	j	65	GLU
42	j	114	VAL
42	j	115	LEU
42	j	138	ARG
42	j	141	ILE
42	j	142	ASP
43	k	7	VAL
43	k	24	ARG
43	k	38	ARG
43	k	39	LEU
43	k	44	ARG
43	k	54	LEU
43	k	79	ARG
43	k	86	ARG
44	l	7	ILE
44	l	17	LYS

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Mol	Chain	Res	Type
44	l	21	GLU
44	l	23	LEU
44	l	27	VAL
44	l	79	ARG
44	l	97	ASN
44	l	109	ARG
44	l	123	GLU
44	l	130	ASN
44	l	146	GLU
45	m	54	ASP
45	m	77	ARG
45	m	96	MET
45	m	121	LEU
46	n	12	ARG
46	n	27	LYS
46	n	60	LYS
46	n	61	LEU
46	n	63	LEU
46	n	87	LEU
46	n	116	VAL
46	n	118	LEU
46	n	123	ARG
47	o	5	ARG
47	o	17	LEU
47	o	24	GLU
47	o	25	ILE
47	o	27	GLU
47	o	37	ARG
47	o	57	VAL
47	o	85	ASP
47	o	102	LEU
48	p	15	GLN
48	p	56	ARG
48	p	107	ILE
48	p	122	ARG
49	q	5	ASN
49	q	21	VAL
49	q	24	LEU
49	q	58	THR
49	q	74	LEU
49	q	86	ARG
49	q	102	LEU

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Mol	Chain	Res	Type
50	r	16	VAL
50	r	25	VAL
50	r	29	ARG
50	r	59	GLU
50	r	76	SER
50	r	93	ARG
50	r	104	THR
51	s	45	VAL
51	s	46	LEU
51	s	89	MET
51	s	92	GLU
52	t	10	LYS
52	t	17	ARG
52	t	18	ASP
52	t	22	THR
52	t	39	LEU
52	t	40	GLN
52	t	61	SER
52	t	64	ARG
52	t	66	LEU
52	t	67	LEU
52	t	70	LEU
52	t	84	ARG
52	t	85	LEU
53	u	1	MET
53	u	18	GLN
53	u	19	VAL
53	u	20	VAL
53	u	35	ARG
54	v	67	LEU
54	v	75	LEU
54	v	79	VAL
55	w	71	THR
55	w	74	HIS
56	x	12	ASP
56	x	21	LYS
56	x	33	THR
56	x	58	VAL
56	x	69	HIS
56	x	79	THR
56	x	81	ARG
57	y	6	SER

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Mol	Chain	Res	Type
57	y	10	ARG
57	y	54	MET
58	z	4	ILE
58	z	18	ARG
58	z	23	CYS
58	z	31	GLU
58	z	34	ARG
58	z	62	ARG
58	z	66	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	2897/2904 (99%)	559 (19%)	70 (2%)
2	2	1528/1534 (99%)	309 (20%)	34 (2%)
3	3	119/120 (99%)	18 (15%)	0
4	4	4/18 (22%)	1 (25%)	0
5	5	73/78 (93%)	20 (27%)	8 (10%)
All	All	4621/4654 (99%)	907 (19%)	112 (2%)

All (907) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	23	G
1	1	34	U
1	1	35	G
1	1	45	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	84	A
1	1	85	G

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Mol	Chain	Res	Type
1	1	96	C
1	1	102	U
1	1	103	A
1	1	118	A
1	1	119	A
1	1	120	U
1	1	131	A
1	1	139	U
1	1	140	C
1	1	141	G
1	1	142	A
1	1	143	C
1	1	149	A
1	1	163	C
1	1	165	A
1	1	181	A
1	1	196	A
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	264	C
1	1	265	A
1	1	266	G
1	1	270	A
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	304	U
1	1	311	A
1	1	324	A
1	1	329	G
1	1	330	A
1	1	353	C
1	1	361	G
1	1	362	A
1	1	371	A

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Mol	Chain	Res	Type
1	1	372	G
1	1	373	U
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
1	1	451	U
1	1	455	C
1	1	456	C
1	1	457	A
1	1	477	A
1	1	480	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	533	G
1	1	538	A
1	1	543	G
1	1	544	C
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	573	U
1	1	575	A
1	1	586	A
1	1	588	U
1	1	603	A
1	1	609	A

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Mol	Chain	Res	Type
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	618	G
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
1	1	687	C
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	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	830	G
1	1	845	A
1	1	846	U
1	1	858	G
1	1	859	G
1	1	869	G
1	1	878	A

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Mol	Chain	Res	Type
1	1	881	G
1	1	884	U
1	1	885	C
1	1	887	A
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	905	A
1	1	907	G
1	1	910	A
1	1	914	G
1	1	915	C
1	1	931	U
1	1	932	U
1	1	941	A
1	1	945	A
1	1	946	C
1	1	953	G
1	1	954	G
1	1	961	C
1	1	974	G
1	1	983	A
1	1	984	A
1	1	985	C
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	1025	G
1	1	1026	G
1	1	1033	U
1	1	1040	A
1	1	1041	G

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Mol	Chain	Res	Type
1	1	1042	G
1	1	1043	C
1	1	1045	C
1	1	1046	A
1	1	1047	G
1	1	1060	U
1	1	1061	U
1	1	1063	G
1	1	1064	C
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1069	A
1	1	1070	A
1	1	1073	A
1	1	1074	G
1	1	1079	C
1	1	1080	A
1	1	1081	U
1	1	1083	U
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	1132	U
1	1	1134	A
1	1	1135	C
1	1	1142	A
1	1	1143	A
1	1	1156	A
1	1	1169	A
1	1	1170	C
1	1	1173	U
1	1	1174	U
1	1	1175	A

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Mol	Chain	Res	Type
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	1187	G
1	1	1236	G
1	1	1238	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	1300	G
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
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1395	A
1	1	1404	C
1	1	1405	U
1	1	1406	U
1	1	1407	G
1	1	1408	G
1	1	1409	U
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

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Mol	Chain	Res	Type
1	1	1453	A
1	1	1460	U
1	1	1478	G
1	1	1482	G
1	1	1490	A
1	1	1491	G
1	1	1493	C
1	1	1497	U
1	1	1502	A
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	1558	C
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	1583	A
1	1	1584	U
1	1	1589	U
1	1	1590	A
1	1	1591	A
1	1	1596	A
1	1	1608	A
1	1	1609	A
1	1	1610	A
1	1	1619	G
1	1	1630	A
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G

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Mol	Chain	Res	Type
1	1	1674	G
1	1	1703	G
1	1	1714	U
1	1	1715	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1750	G
1	1	1758	U
1	1	1764	C
1	1	1773	A
1	1	1791	A
1	1	1800	C
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
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	1917	PSU
1	1	1918	A
1	1	1919	A
1	1	1923	U
1	1	1924	C
1	1	1929	G

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Mol	Chain	Res	Type
1	1	1930	G
1	1	1936	A
1	1	1938	A
1	1	1955	U
1	1	1960	A
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	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	2033	A
1	1	2036	C
1	1	2041	U
1	1	2043	C
1	1	2049	G
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
1	1	2069	G7M
1	1	2077	A
1	1	2080	A
1	1	2093	G
1	1	2097	A
1	1	2099	U
1	1	2101	A
1	1	2108	A
1	1	2110	G
1	1	2111	U
1	1	2113	U

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Mol	Chain	Res	Type
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2120	G
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
1	1	2183	A
1	1	2185	U
1	1	2186	G
1	1	2188	U
1	1	2189	U
1	1	2190	G
1	1	2191	A
1	1	2193	G
1	1	2194	U

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Mol	Chain	Res	Type
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	2243	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	2288	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	2336	A
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2352	A
1	1	2357	G
1	1	2361	G
1	1	2376	A
1	1	2383	G
1	1	2385	C
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2423	U
1	1	2424	C

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Mol	Chain	Res	Type
1	1	2425	A
1	1	2426	A
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2435	A
1	1	2436	G
1	1	2441	U
1	1	2445	2MG
1	1	2447	G
1	1	2448	A
1	1	2459	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	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
1	1	2584	U
1	1	2585	U
1	1	2586	U
1	1	2602	A
1	1	2603	G
1	1	2609	U

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Mol	Chain	Res	Type
1	1	2610	C
1	1	2611	C
1	1	2613	U
1	1	2629	U
1	1	2630	G
1	1	2663	G
1	1	2671	G
1	1	2682	A
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2720	U
1	1	2726	A
1	1	2733	A
1	1	2744	G
1	1	2746	U
1	1	2748	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	2825	G
1	1	2836	U
1	1	2859	G
1	1	2861	U
1	1	2867	G
1	1	2880	C
1	1	2884	U
1	1	2885	G
1	1	2891	U
1	1	2902	C
2	2	4	U
2	2	9	G

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Mol	Chain	Res	Type
2	2	22	G
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	58	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	116	A
2	2	120	A
2	2	121	U
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	161	A
2	2	164	G
2	2	173	U
2	2	181	A
2	2	182	A
2	2	196	A

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Mol	Chain	Res	Type
2	2	197	A
2	2	198	G
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	214	C
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
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	330	C
2	2	332	G
2	2	347	G
2	2	352	C
2	2	354	G
2	2	355	C
2	2	367	U
2	2	372	C
2	2	373	A
2	2	374	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
2	2	406	G

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Mol	Chain	Res	Type
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	428	G
2	2	429	U
2	2	446	G
2	2	451	A
2	2	457	G
2	2	458	U
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	480	U
2	2	481	G
2	2	482	A
2	2	484	G
2	2	485	U
2	2	486	U
2	2	505	G
2	2	511	C
2	2	516	PSU
2	2	517	G
2	2	518	C
2	2	519	C
2	2	528	C
2	2	529	G
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	564	C
2	2	568	G

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Mol	Chain	Res	Type
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	579	A
2	2	596	A
2	2	607	A
2	2	628	G
2	2	633	G
2	2	642	A
2	2	650	G
2	2	653	U
2	2	665	A
2	2	666	G
2	2	700	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	733	G
2	2	747	A
2	2	748	G
2	2	755	G
2	2	763	G
2	2	777	A
2	2	793	U
2	2	794	A
2	2	799	G
2	2	810	C
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	846	G
2	2	849	G
2	2	851	G
2	2	874	G
2	2	876	C
2	2	887	G

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Mol	Chain	Res	Type
2	2	902	G
2	2	914	A
2	2	916	U
2	2	926	G
2	2	928	G
2	2	934	C
2	2	935	A
2	2	936	C
2	2	960	U
2	2	961	U
2	2	963	G
2	2	965	U
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	977	A
2	2	978	A
2	2	989	U
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	1033	G
2	2	1037	C
2	2	1042	A
2	2	1043	G

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Mol	Chain	Res	Type
2	2	1044	A
2	2	1046	A
2	2	1056	U
2	2	1065	U
2	2	1085	U
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1124	G
2	2	1133	G
2	2	1135	U
2	2	1136	C
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	1154	G
2	2	1158	C
2	2	1159	U
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	1212	U
2	2	1213	A
2	2	1214	C
2	2	1215	G
2	2	1225	A
2	2	1226	C
2	2	1227	A
2	2	1228	C

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Mol	Chain	Res	Type
2	2	1238	A
2	2	1239	A
2	2	1246	A
2	2	1257	A
2	2	1260	G
2	2	1275	A
2	2	1277	C
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
2	2	1300	G
2	2	1302	C
2	2	1305	G
2	2	1311	A
2	2	1312	G
2	2	1317	C
2	2	1320	C
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	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

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Mol	Chain	Res	Type
2	2	1487	G
2	2	1492	A
2	2	1493	A
2	2	1494	G
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
2	2	1531	A
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	21	G
3	3	35	C
3	3	45	A
3	3	51	G
3	3	56	G
3	3	57	A
3	3	66	A
3	3	67	G
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	3	G
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

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Mol	Chain	Res	Type
5	5	21	A
5	5	22	G
5	5	31	G
5	5	47	U
5	5	48	C
5	5	55	PSU
5	5	57	A
5	5	60	U
5	5	69	C
5	5	74	C

All (112) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	62	U
1	1	70	G
1	1	140	C
1	1	142	A
1	1	271	G
1	1	404	A
1	1	446	G
1	1	503	A
1	1	532	A
1	1	545	U
1	1	548	G
1	1	555	G
1	1	685	A
1	1	752	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	1045	C
1	1	1063	G
1	1	1064	C
1	1	1069	A
1	1	1110	G
1	1	1128	G
1	1	1142	A

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Mol	Chain	Res	Type
1	1	1173	U
1	1	1177	G
1	1	1205	A
1	1	1253	A
1	1	1320	C
1	1	1344	U
1	1	1379	U
1	1	1415	U
1	1	1490	A
1	1	1509	A
1	1	1583	A
1	1	1584	U
1	1	1608	A
1	1	1847	A
1	1	1900	A
1	1	1912	A
1	1	1913	A
1	1	1918	A
1	1	1962	5MC
1	1	2062	A
1	1	2074	U
1	1	2146	C
1	1	2162	G
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	2308	G
1	1	2324	U
1	1	2326	C
1	1	2425	A
1	1	2447	G
1	1	2506	U
1	1	2572	A
1	1	2585	U
1	1	2610	C
1	1	2798	U
1	1	2849	U
1	1	2873	A

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Mol	Chain	Res	Type
2	2	70	U
2	2	106	C
2	2	181	A
2	2	183	C
2	2	197	A
2	2	209	U
2	2	428	G
2	2	438	U
2	2	481	G
2	2	517	G
2	2	527	7MG
2	2	531	U
2	2	560	A
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	1213	A
2	2	1214	C
2	2	1225	A
2	2	1299	A
2	2	1363	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	8	4SU
5	5	16	C
5	5	17	U
5	5	18	G
5	5	20	H2U
5	5	21	A
5	5	47	U
5	5	60	U

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

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	0.93	1 (5%)	15,36,39	1.87	3 (20%)
1	2MG	1	1835	1	18,26,27	1.28	1 (5%)	21,38,41	2.84	6 (28%)
1	PSU	1	1911	1	15,21,22	1.83	4 (26%)	16,30,33	2.30	3 (18%)
1	3TD	1	1915	1	15,22,23	6.87	3 (20%)	17,32,35	3.71	8 (47%)
1	PSU	1	1917	1	15,21,22	2.08	4 (26%)	16,30,33	3.39	4 (25%)
1	5MU	1	1939	1,59	13,22,23	1.85	2 (15%)	16,32,35	4.02	4 (25%)
1	5MC	1	1962	1	14,22,23	1.66	1 (7%)	17,32,35	1.71	3 (17%)
1	6MZ	1	2030	1	17,25,26	1.20	1 (5%)	15,36,39	2.30	4 (26%)
1	G7M	1	2069	1	18,26,27	1.76	2 (11%)	21,39,42	3.77	10 (47%)
1	OMG	1	2251	1,5	18,26,27	2.12	3 (16%)	21,38,41	3.21	7 (33%)
1	2MG	1	2445	1	18,26,27	1.24	1 (5%)	21,38,41	2.86	6 (28%)
1	PSU	1	2457	1	15,21,22	3.52	4 (26%)	16,30,33	3.62	8 (50%)
1	OMC	1	2498	1,59	15,22,23	1.28	2 (13%)	20,31,34	1.62	4 (20%)
1	2MA	1	2503	1,59	17,25,26	1.44	3 (17%)	18,37,40	3.16	7 (38%)
1	PSU	1	2504	1	15,21,22	2.77	4 (26%)	16,30,33	3.67	7 (43%)
1	OMU	1	2552	1	14,22,23	1.03	1 (7%)	19,31,34	2.37	2 (10%)
1	PSU	1	2580	1	15,21,22	2.99	4 (26%)	16,30,33	3.78	7 (43%)
1	PSU	1	2605	1	15,21,22	3.25	4 (26%)	16,30,33	3.78	8 (50%)
1	1MG	1	745	1	17,26,27	1.50	1 (5%)	19,39,42	1.82	5 (26%)
1	PSU	1	746	1,59	15,21,22	3.46	3 (20%)	16,30,33	3.99	7 (43%)
1	5MU	1	747	1	13,22,23	1.55	2 (15%)	16,32,35	4.07	4 (25%)
1	PSU	1	955	1	15,21,22	3.54	5 (33%)	16,30,33	3.71	7 (43%)
2	2MG	2	1207	2	18,26,27	1.74	2 (11%)	21,38,41	2.71	6 (28%)
2	4OC	2	1402	2	15,23,24	1.33	2 (13%)	21,32,35	1.89	5 (23%)
2	5MC	2	1407	2	14,22,23	1.51	1 (7%)	17,32,35	1.52	2 (11%)
2	UR3	2	1498	2	13,22,23	1.56	3 (23%)	18,32,35	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	2MG	2	1516	2	18,26,27	1.33	1 (5%)	21,38,41	2.84	7 (33%)
2	MA6	2	1518	2	18,26,27	0.50	0	15,38,41	1.47	2 (13%)
2	MA6	2	1519	2	18,26,27	0.53	0	15,38,41	1.53	3 (20%)
2	PSU	2	516	2,59	15,21,22	2.68	4 (26%)	16,30,33	3.74	6 (37%)
2	7MG	2	527	2,59	20,26,27	1.29	2 (10%)	23,39,42	3.50	9 (39%)
2	2MG	2	966	2	18,26,27	1.32	1 (5%)	21,38,41	3.15	8 (38%)
2	5MC	2	967	2	14,22,23	1.50	1 (7%)	17,32,35	1.70	3 (17%)
5	H2U	5	20	5	17,21,22	0.69	0	23,30,33	1.85	4 (17%)
5	4OC	5	32	5	15,23,24	0.78	0	21,32,35	1.70	4 (19%)
5	5MU	5	54	5	13,22,23	1.45	2 (15%)	16,32,35	4.09	5 (31%)
5	PSU	5	55	5	15,21,22	3.07	4 (26%)	16,30,33	3.59	6 (37%)
5	8AN	5	76	60,59,1,5	18,24,25	0.64	0	10,35,38	0.58	0
5	4SU	5	8	5	12,21,22	0.73	0	15,30,33	1.82	3 (20%)
49	0TD	q	89	49	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	1,59	-	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	1,59	-	0/5/27/28	0/2/2/2
1	2MA	1	2503	1,59	-	0/3/25/26	0/3/3/3
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	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	746	1,59	-	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	2,59	-	0/7/25/26	0/2/2/2
2	7MG	2	527	2,59	-	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	60,59,1,5	-	0/3/25/26	0/3/3/3
5	4SU	5	8	5	-	0/3/25/26	0/2/2/2
49	0TD	q	89	49	-	0/2/12/14	0/0/0/0

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1915	3TD	C5-C1'	-26.27	1.29	1.52
1	1	746	PSU	C2'-C1'	-12.37	1.42	1.53
1	1	955	PSU	C2'-C1'	-12.08	1.42	1.53
1	1	2457	PSU	C2'-C1'	-12.03	1.42	1.53
1	1	2605	PSU	C2'-C1'	-11.13	1.43	1.53
5	5	55	PSU	C2'-C1'	-10.72	1.43	1.53
1	1	2580	PSU	C2'-C1'	-10.38	1.44	1.53
1	1	2504	PSU	C2'-C1'	-9.15	1.45	1.53
2	2	516	PSU	C2'-C1'	-8.82	1.45	1.53
49	q	89	0TD	CB-SB	-7.53	1.65	1.84
1	1	2069	G7M	C2'-C1'	-5.94	1.44	1.53
1	1	1917	PSU	C5-C1'	-5.68	1.47	1.52
1	1	1962	5MC	C2'-C1'	-5.64	1.44	1.53
1	1	1939	5MU	C2'-C1'	-5.64	1.44	1.53
1	1	1911	PSU	C5-C1'	-5.54	1.47	1.52
2	2	967	5MC	C2'-C1'	-5.09	1.45	1.53
2	2	1407	5MC	C2'-C1'	-4.90	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2251	OMG	C2'-C1'	-4.67	1.40	1.53
1	1	2251	OMG	C3'-C2'	-4.41	1.43	1.53
1	1	745	1MG	C2'-C1'	-4.40	1.46	1.53
1	1	747	5MU	C2'-C1'	-4.40	1.46	1.53
1	1	2457	PSU	C5-C1'	-3.87	1.48	1.52
1	1	955	PSU	C5-C1'	-3.87	1.48	1.52
5	5	54	5MU	C2'-C1'	-3.85	1.47	1.53
1	1	2030	6MZ	C2'-C1'	-3.79	1.47	1.53
1	1	2498	OMC	C3'-C2'	-3.49	1.45	1.53
49	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	2605	PSU	C5-C1'	-3.20	1.49	1.52
1	1	2504	PSU	C5-C1'	-3.14	1.49	1.52
1	1	1917	PSU	C2'-C1'	-3.12	1.50	1.53
1	1	2457	PSU	C6-C5	-3.11	1.34	1.38
1	1	955	PSU	C6-C5	-3.10	1.34	1.38
1	1	2605	PSU	C6-C5	-3.04	1.34	1.38
1	1	746	PSU	C6-C5	-3.03	1.34	1.38
1	1	1917	PSU	C6-C5	-3.02	1.34	1.38
2	2	516	PSU	C5-C1'	-2.98	1.49	1.52
1	1	2504	PSU	C6-C5	-2.89	1.34	1.38
1	1	2580	PSU	C6-C5	-2.89	1.34	1.38
2	2	516	PSU	C6-C5	-2.87	1.34	1.38
2	2	1402	4OC	C2-N3	-2.84	1.32	1.38
2	2	1498	UR3	C2'-C1'	-2.74	1.49	1.53
1	1	1911	PSU	C2'-C1'	-2.67	1.51	1.53
2	2	1498	UR3	O4-C4	-2.62	1.18	1.24
2	2	1402	4OC	C6-N1	-2.62	1.32	1.35
1	1	2498	OMC	C2'-C1'	-2.50	1.46	1.53
49	q	89	0TD	CSB-SB	-2.47	1.74	1.79
1	1	1618	6MZ	C2'-C1'	-2.45	1.49	1.53
1	1	2503	2MA	C2'-C3'	-2.45	1.46	1.53
5	5	55	PSU	C6-C5	-2.44	1.35	1.38
5	5	55	PSU	C5-C1'	-2.40	1.50	1.52
1	1	2580	PSU	C5-C1'	-2.37	1.50	1.52
2	2	1498	UR3	C6-N1	-2.29	1.32	1.35
1	1	955	PSU	C3'-C2'	-2.28	1.47	1.53
1	1	1915	3TD	C6-C5	-2.14	1.35	1.38
1	1	1911	PSU	C2-N3	-2.09	1.33	1.38
1	1	1915	3TD	C4-N3	-2.09	1.35	1.38
1	1	1911	PSU	C2-N1	-2.08	1.33	1.38
1	1	2503	2MA	C6-N1	2.16	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2580	PSU	C4-N3	2.43	1.37	1.33
1	1	955	PSU	C4-N3	2.52	1.37	1.33
1	1	2457	PSU	C4-N3	2.67	1.37	1.33
1	1	2605	PSU	C4-N3	2.68	1.37	1.33
2	2	516	PSU	C4-N3	2.72	1.37	1.33
1	1	2504	PSU	C4-N3	2.74	1.38	1.33
1	1	1917	PSU	C4-N3	2.76	1.38	1.33
2	2	527	7MG	C5-C4	2.84	1.46	1.39
1	1	746	PSU	C4-N3	2.86	1.38	1.33
1	1	2552	OMU	C4-N3	2.89	1.38	1.33
1	1	1939	5MU	C4-N3	2.95	1.38	1.33
5	5	55	PSU	C4-N3	3.01	1.38	1.33
1	1	747	5MU	C4-N3	3.02	1.38	1.33
5	5	54	5MU	C4-N3	3.24	1.38	1.33
1	1	2069	G7M	C6-N1	3.24	1.38	1.33
1	1	2503	2MA	C2-N1	3.71	1.40	1.34
2	2	527	7MG	C6-C5	3.75	1.46	1.41
1	1	2445	2MG	C6-N1	4.14	1.40	1.33
1	1	1835	2MG	C6-N1	4.48	1.41	1.33
2	2	1516	2MG	C6-N1	4.75	1.41	1.33
2	2	966	2MG	C6-N1	4.87	1.41	1.33
1	1	2251	OMG	C6-N1	4.95	1.42	1.33
2	2	1207	2MG	C6-N1	5.30	1.42	1.33

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1915	3TD	C5-C1'-C2'	-11.05	96.67	115.44
1	1	1939	5MU	C5-C4-N3	-10.77	116.31	125.35
1	1	747	5MU	C5-C4-N3	-10.76	116.31	125.35
5	5	54	5MU	C5-C4-N3	-10.74	116.33	125.35
1	1	2069	G7M	C4'-O4'-C1'	-9.30	99.79	109.64
1	1	2503	2MA	C4'-O4'-C1'	-9.24	99.85	109.64
2	2	1516	2MG	C5-C6-N1	-9.05	111.69	123.52
1	1	2445	2MG	C5-C6-N1	-9.04	111.70	123.52
1	1	1835	2MG	C5-C6-N1	-9.02	111.72	123.52
2	2	527	7MG	C5-C4-N3	-8.95	117.62	126.74
2	2	966	2MG	C5-C6-N1	-8.92	111.86	123.52
1	1	2251	OMG	C5-C6-N1	-8.82	111.99	123.52
2	2	1207	2MG	C5-C6-N1	-8.56	112.33	123.52
49	q	89	0TD	CB-CA-N	-8.37	93.08	109.83
1	1	2069	G7M	C5-C6-N1	-7.81	113.32	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	8	4SU	C4'-O4'-C1'	-5.46	103.86	109.64
2	2	527	7MG	C5-C6-N1	-5.15	115.72	123.39
1	1	1917	PSU	C5-C1'-C2'	-5.11	106.76	115.44
1	1	1911	PSU	C5-C1'-C2'	-5.01	106.92	115.44
1	1	2030	6MZ	C4'-O4'-C1'	-4.99	104.35	109.64
1	1	955	PSU	C4'-O4'-C1'	-4.53	104.88	109.54
2	2	1207	2MG	C1'-N9-C4	-4.18	122.14	126.81
1	1	1915	3TD	C5'-C4'-C3'	-4.12	99.26	115.20
1	1	2605	PSU	C4'-O4'-C1'	-4.02	105.40	109.54
1	1	2503	2MA	O4'-C1'-N9	-3.82	100.89	108.11
1	1	1911	PSU	C5-C6-N1	-3.79	119.10	124.38
2	2	1402	4OC	CM4-N4-C4	-3.75	119.71	122.87
1	1	2251	OMG	N3-C2-N1	-3.52	122.77	127.56
2	2	527	7MG	O4'-C4'-C3'	-3.38	98.30	105.16
1	1	1915	3TD	C5-C6-N1	-3.31	119.76	124.38
1	1	745	1MG	C5-C6-N1	-3.20	114.16	118.35
2	2	966	2MG	C4'-O4'-C1'	-3.03	106.43	109.64
1	1	2504	PSU	C4'-O4'-C1'	-3.01	106.44	109.54
2	2	966	2MG	C2'-C3'-C4'	-2.98	96.54	102.64
2	2	1207	2MG	O2'-C2'-C1'	-2.91	102.52	111.61
1	1	2069	G7M	N3-C2-N1	-2.90	123.61	127.56
1	1	2457	PSU	C4'-O4'-C1'	-2.84	106.61	109.54
1	1	2580	PSU	C4-C5-C1'	-2.84	116.44	121.22
1	1	955	PSU	C2'-C3'-C4'	-2.83	96.85	102.64
1	1	2552	OMU	C5-C4-N3	-2.79	116.42	123.28
2	2	1519	MA6	C4'-O4'-C1'	-2.79	106.68	109.64
2	2	1518	MA6	C1'-N9-C4	-2.75	123.73	126.81
2	2	527	7MG	C8-N9-C1'	-2.65	114.46	122.43
1	1	2605	PSU	C2'-C3'-C4'	-2.65	97.21	102.64
1	1	2457	PSU	C2'-C3'-C4'	-2.62	97.27	102.64
2	2	1402	4OC	O4'-C4'-C3'	-2.54	100.00	105.16
1	1	2069	G7M	C2'-C3'-C4'	-2.51	97.50	102.64
1	1	1915	3TD	C4'-O4'-C1'	-2.45	107.02	109.54
2	2	527	7MG	C3'-C2'-C1'	-2.31	96.80	101.44
2	2	1516	2MG	C1'-N9-C4	-2.29	124.25	126.81
1	1	2504	PSU	C2'-C3'-C4'	-2.27	97.98	102.64
2	2	1519	MA6	C2'-C3'-C4'	-2.24	98.05	102.64
5	5	54	5MU	C4'-O4'-C1'	-2.16	107.36	109.64
1	1	2580	PSU	C5-C6-N1	-2.14	121.40	124.38
1	1	2605	PSU	C5-C6-N1	-2.14	121.40	124.38
1	1	1917	PSU	C5-C6-N1	-2.11	121.44	124.38
2	2	1516	2MG	N3-C2-N1	-2.10	123.05	126.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	8	4SU	C5-C4-N3	-2.10	121.34	123.56
1	1	746	PSU	C5-C6-N1	-2.09	121.46	124.38
49	q	89	0TD	O-C-CA	-2.09	119.97	125.69
1	1	2504	PSU	C5-C6-N1	-2.09	121.47	124.38
1	1	1835	2MG	N3-C2-N1	-2.09	123.07	126.19
1	1	2457	PSU	C5-C6-N1	-2.08	121.48	124.38
5	5	55	PSU	C5-C6-N1	-2.07	121.49	124.38
1	1	955	PSU	C5-C6-N1	-2.07	121.50	124.38
2	2	516	PSU	C5-C6-N1	-2.07	121.50	124.38
1	1	2445	2MG	N3-C2-N1	-2.07	123.10	126.19
2	2	966	2MG	N3-C2-N1	-2.05	123.12	126.19
1	1	745	1MG	C1'-N9-C4	-2.02	124.55	126.81
2	2	1207	2MG	O4'-C1'-N9	2.01	111.90	108.11
2	2	1498	UR3	C4'-O4'-C1'	2.01	111.78	109.64
1	1	1915	3TD	C3'-C2'-C1'	2.02	104.11	101.71
2	2	966	2MG	CM2-N2-C2	2.06	125.35	123.03
2	2	967	5MC	C2'-C1'-N1	2.06	119.00	113.46
2	2	967	5MC	O3'-C3'-C2'	2.09	118.61	111.86
2	2	1407	5MC	O3'-C3'-C4'	2.10	117.28	111.01
1	1	1939	5MU	C5M-C5-C6	2.13	122.95	118.63
1	1	2457	PSU	C3'-C2'-C1'	2.13	104.24	101.71
2	2	1402	4OC	C4'-O4'-C1'	2.14	111.92	109.64
5	5	54	5MU	C5M-C5-C6	2.16	123.02	118.63
1	1	2498	OMC	C3'-C2'-C1'	2.20	106.84	102.63
1	1	747	5MU	C5M-C5-C6	2.20	123.10	118.63
2	2	516	PSU	O4'-C1'-C2'	2.20	107.07	104.69
2	2	1516	2MG	N2-C2-N3	2.25	119.55	116.94
5	5	55	PSU	C3'-C2'-C1'	2.29	104.43	101.71
1	1	746	PSU	O4'-C1'-C2'	2.30	107.18	104.69
1	1	1618	6MZ	C2'-C1'-N9	2.34	119.74	113.47
1	1	1915	3TD	O4'-C1'-C2'	2.36	107.25	104.69
1	1	2498	OMC	O3'-C3'-C4'	2.37	118.07	111.01
1	1	2605	PSU	O4'-C1'-C2'	2.41	107.30	104.69
1	1	2251	OMG	C5'-C4'-C3'	2.46	124.71	115.20
2	2	1207	2MG	N2-C2-N3	2.47	119.80	116.94
1	1	1939	5MU	C2'-C1'-N1	2.55	120.32	113.46
1	1	2445	2MG	N2-C2-N3	2.57	119.92	116.94
1	1	2504	PSU	C5-C1'-C2'	2.62	119.88	115.44
1	1	747	5MU	C2'-C1'-N1	2.63	120.52	113.46
5	5	54	5MU	C2'-C1'-N1	2.63	120.54	113.46
1	1	2069	G7M	O4'-C1'-N9	2.64	113.10	108.11
2	2	527	7MG	O3'-C3'-C4'	2.70	119.09	111.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2445	2MG	O3'-C3'-C4'	2.71	119.09	111.01
1	1	2503	2MA	O2'-C2'-C3'	2.71	120.62	111.86
1	1	745	1MG	O2'-C2'-C3'	2.72	120.63	111.86
1	1	1962	5MC	C2'-C1'-N1	2.72	120.76	113.46
1	1	1835	2MG	N2-C2-N3	2.73	120.11	116.94
1	1	955	PSU	C5-C1'-C2'	2.80	120.19	115.44
2	2	966	2MG	N2-C2-N3	2.84	120.24	116.94
2	2	1516	2MG	O3'-C3'-C4'	2.85	119.53	111.01
1	1	2069	G7M	O3'-C3'-C2'	2.87	121.12	111.86
1	1	1915	3TD	C4-C5-C1'	2.88	126.11	121.24
5	5	32	4OC	O3'-C3'-C4'	2.90	119.68	111.01
1	1	746	PSU	O2'-C2'-C1'	2.91	118.25	111.93
1	1	1962	5MC	O3'-C3'-C2'	2.91	121.27	111.86
5	5	32	4OC	C6-C5-C4	2.92	118.57	117.42
49	q	89	0TD	C-CA-N	2.97	116.50	109.95
5	5	8	4SU	O4'-C1'-N1	2.97	113.74	108.10
1	1	2503	2MA	C1'-N9-C4	2.98	130.13	126.81
1	1	1917	PSU	C3'-C2'-C1'	3.07	105.35	101.71
1	1	2030	6MZ	O3'-C3'-C2'	3.16	122.06	111.86
1	1	2457	PSU	C5-C1'-C2'	3.17	120.82	115.44
5	5	20	H2U	O2'-C2'-C1'	3.27	121.34	109.98
2	2	527	7MG	O3'-C3'-C2'	3.28	122.45	111.86
1	1	2580	PSU	C3'-C2'-C1'	3.29	105.61	101.71
1	1	2605	PSU	C5-C1'-C2'	3.32	121.07	115.44
1	1	1835	2MG	O3'-C3'-C2'	3.40	122.86	111.86
1	1	2498	OMC	C6-C5-C4	3.44	118.78	117.44
1	1	2457	PSU	O2'-C2'-C1'	3.47	119.46	111.93
2	2	1519	MA6	C2-N1-C6	3.54	119.98	111.64
2	2	516	PSU	O2'-C2'-C1'	3.56	119.66	111.93
1	1	2580	PSU	O2'-C2'-C1'	3.63	119.82	111.93
5	5	32	4OC	C2-N3-C4	3.66	120.08	115.43
2	2	1518	MA6	C2-N1-C6	3.71	120.39	111.64
1	1	2251	OMG	O3'-C3'-C2'	3.74	121.93	111.13
1	1	1618	6MZ	C2-N1-C6	3.80	119.20	116.47
1	1	2030	6MZ	C2-N1-C6	3.87	119.26	116.47
1	1	955	PSU	O2'-C2'-C1'	3.90	120.40	111.93
5	5	20	H2U	O3'-C3'-C4'	3.93	122.76	111.01
1	1	1835	2MG	O3'-C3'-C4'	3.94	122.76	111.01
1	1	745	1MG	O3'-C3'-C4'	3.98	122.89	111.01
5	5	55	PSU	C5-C1'-C2'	4.00	122.22	115.44
2	2	1402	4OC	C2-N3-C4	4.00	120.52	115.43
1	1	745	1MG	O3'-C3'-C2'	4.02	124.85	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	55	PSU	O2'-C2'-C1'	4.08	120.80	111.93
1	1	2251	OMG	O3'-C3'-C4'	4.15	123.39	111.01
1	1	2503	2MA	O3'-C3'-C2'	4.19	125.40	111.86
1	1	2069	G7M	O2'-C2'-C1'	4.21	124.78	111.61
1	1	2503	2MA	O3'-C3'-C4'	4.23	123.66	111.01
5	5	32	4OC	O3'-C3'-C2'	4.25	123.40	111.13
1	1	2445	2MG	O3'-C3'-C2'	4.32	125.82	111.86
1	1	746	PSU	O2'-C2'-C3'	4.36	125.94	111.86
1	1	2457	PSU	O2'-C2'-C3'	4.53	126.49	111.86
5	5	20	H2U	O3'-C3'-C2'	4.53	126.50	111.86
1	1	2030	6MZ	O3'-C3'-C4'	4.55	124.60	111.01
1	1	2605	PSU	O2'-C2'-C3'	4.61	126.74	111.86
2	2	1516	2MG	O3'-C3'-C2'	4.64	126.85	111.86
1	1	2580	PSU	C5-C1'-C2'	4.65	123.33	115.44
1	1	955	PSU	O2'-C2'-C3'	4.66	126.93	111.86
2	2	1402	4OC	C6-C5-C4	4.70	119.27	117.42
1	1	2605	PSU	O2'-C2'-C1'	4.72	122.19	111.93
2	2	1407	5MC	O3'-C3'-C2'	4.79	127.34	111.86
1	1	2504	PSU	O2'-C2'-C1'	4.87	122.52	111.93
5	5	20	H2U	O2'-C2'-C3'	4.89	127.66	111.86
1	1	2504	PSU	O2'-C2'-C3'	4.91	127.73	111.86
1	1	2580	PSU	O2'-C2'-C3'	4.97	127.93	111.86
1	1	1618	6MZ	O3'-C3'-C4'	4.99	125.90	111.01
1	1	2498	OMC	O3'-C3'-C2'	5.04	125.69	111.13
1	1	2503	2MA	O2'-C2'-C1'	5.05	127.40	111.61
1	1	2069	G7M	C2'-C1'-N9	5.05	126.98	113.47
1	1	1962	5MC	O3'-C3'-C4'	5.06	126.12	111.01
5	5	55	PSU	O2'-C2'-C3'	5.10	128.34	111.86
2	2	516	PSU	C5-C1'-C2'	5.16	124.20	115.44
1	1	2069	G7M	C6-N1-C2	5.22	122.00	115.88
1	1	2251	OMG	C3'-C2'-C1'	5.24	112.66	102.63
1	1	746	PSU	C5-C1'-C2'	5.26	124.37	115.44
2	2	1207	2MG	C6-N1-C2	5.26	122.78	115.24
2	2	516	PSU	O2'-C2'-C3'	5.47	129.52	111.86
2	2	967	5MC	O3'-C3'-C4'	5.53	127.52	111.01
2	2	527	7MG	C6-N1-C2	5.57	122.41	115.88
1	1	1911	PSU	C4-N3-C2	5.84	120.03	115.16
2	2	966	2MG	C6-N1-C2	6.11	123.99	115.24
2	2	1516	2MG	C6-N1-C2	6.18	124.08	115.24
1	1	1835	2MG	C6-N1-C2	6.35	124.33	115.24
1	1	2445	2MG	C6-N1-C2	6.38	124.38	115.24
49	q	89	0TD	CSB-SB-CB	6.52	113.63	101.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2069	G7M	O2'-C2'-C3'	6.62	133.26	111.86
2	2	966	2MG	O3'-C3'-C4'	6.77	131.23	111.01
1	1	2251	OMG	C6-N1-C2	6.88	123.95	115.88
1	1	1915	3TD	O5'-C5'-C4'	7.28	135.17	109.09
1	1	746	PSU	C3'-C2'-C1'	7.53	110.64	101.71
2	2	527	7MG	N3-C4-N9	9.20	138.88	126.98
1	1	2552	OMU	C4-N3-C2	9.58	124.31	114.21
1	1	1939	5MU	C4-N3-C2	11.11	124.43	115.16
1	1	746	PSU	C4-N3-C2	11.45	124.71	115.16
5	5	54	5MU	C4-N3-C2	11.47	124.73	115.16
1	1	1917	PSU	C4-N3-C2	11.48	124.74	115.16
1	1	747	5MU	C4-N3-C2	11.51	124.76	115.16
1	1	2605	PSU	C4-N3-C2	11.55	124.80	115.16
5	5	55	PSU	C4-N3-C2	11.61	124.85	115.16
1	1	2504	PSU	C4-N3-C2	11.69	124.91	115.16
2	2	516	PSU	C4-N3-C2	11.69	124.91	115.16
1	1	2457	PSU	C4-N3-C2	11.70	124.92	115.16
1	1	955	PSU	C4-N3-C2	11.72	124.94	115.16
1	1	2580	PSU	C4-N3-C2	11.85	125.04	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1911	PSU	2	0
1	1	1915	3TD	4	0
1	1	1917	PSU	3	0
1	1	1939	5MU	1	0
1	1	1962	5MC	1	0
1	1	2030	6MZ	2	0
1	1	2251	OMG	1	0
1	1	2445	2MG	2	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	1402	4OC	1	0
2	2	1518	MA6	2	0
2	2	1519	MA6	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	516	PSU	6	0
2	2	527	7MG	4	0
2	2	966	2MG	3	0
2	2	967	5MC	2	0
5	5	20	H2U	1	0
5	5	32	4OC	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 441 ligands modelled in this entry, 440 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	$\#\|Z\| > 2$
60	FME	5	101	5	8,9,10	0.48	0	5,9,11	1.51	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
60	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(^{o})	Ideal(^{o})
60	5	101	FME	O-C-CA	-3.37	116.50	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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	2196:C	O3'	2197:U	P	2.55