wwPDB EM Map/Model Validation Report (i)

Sep 20, 2016 – 09:13 PM EDT

PDB ID	:	5IQR
EMDB ID:	:	EMD-8107
Title	:	Structure of RelA bound to the 70S ribosome
Authors	:	Brown, A.; Fernandez, I.S.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on	:	2016-03-11
Resolution	:	3.00 Å(reported)
Based on PDB ID	:	4YBB

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

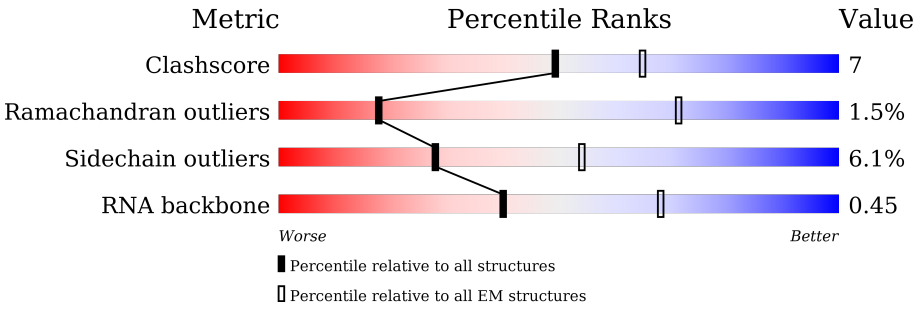
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.00 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	B	273	85% 14% ••
2	C	209	86% 14%
3	D	201	88% 11%
4	E	179	84% 13% ••
5	F	177	89% 11% •
6	G	149	95% • •
7	H	165	72% 7% • 21%
8	I	142	92% 8% •

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Mol	Chain	Length	Quality of chain
9	J	142	91% 8%
10	K	123	90% 10%
11	L	144	90% 10%
12	M	136	92% 8%
13	N	127	67% 24% 6%
14	O	117	80% 17%
15	P	115	93% 5%
16	Q	118	80% 18%
17	R	103	87% 12%
18	S	110	85% 14%
19	T	100	85% 8% 7%
20	U	104	89% 8%
21	V	94	87% 13%
22	W	85	85% 6% 9%
23	X	78	91% 8%
24	Y	63	87% 10%
25	Z	59	85% 14%
26	a	70	91% 6%
27	b	57	95%
28	c	55	89% 9%
29	d	46	87% 13%
30	e	65	89% 9%
31	f	38	89% 11%
32	g	241	88% 5% 7%
33	h	233	84% 5% 11%

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Mol	Chain	Length	Quality of chain
34	i	206	97%
35	j	167	86% 8% 6%
36	k	135	70% 26%
37	l	179	78% 6% 16%
38	m	130	92% 7%
39	n	130	90% 8%
40	o	103	84% 11% 5%
41	p	129	84% 6% 9%
42	q	124	94% 5%
43	r	118	90% 7%
44	s	101	95%
45	t	89	91% 8%
46	u	82	88% 12%
47	v	84	85% 11% 5%
48	w	75	84% 13%
49	x	92	84% 5% 11%
50	y	87	92% 7%
51	z	71	72% 7% 21%
52	1	2904	52% 42% 7%
53	2	1533	52% 43% 5%
54	3	118	58% 38%
55	4	76	55% 36% 9%
56	5	78	26% 44% 29%
57	6	76	21% 51% 25%
58	7	10	60% 40%

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Mol	Chain	Length	Quality of chain
59	8	744	62% 16% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	H2U	6	16	X	-	-	-
57	H2U	6	20	X	-	-	-
57	PSU	6	32	X	-	-	-
57	6IA	6	37	X	-	-	-
57	PSU	6	55	X	-	-	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 154519 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

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

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

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

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	176	1323	832	243	246	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L9.

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

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

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

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

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

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

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

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	77	Total	C	N	O	S	0	0
			588	363	118	106	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 26 is a protein called 50S ribosomal protein L31.

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

- Molecule 27 is a protein called 50S ribosomal protein L32.

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

- Molecule 28 is a protein called 50S ribosomal protein L33.

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

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a protein called 50S ribosomal protein L36.

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

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	207	Total	C	N	O	S	0	0
			1628	1030	306	289	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	207	LEU	ILE	conflict	UNP P0A7V3
h	208	GLY	LEU	conflict	UNP P0A7V3

- Molecule 34 is a protein called 30S ribosomal protein S4.

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

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 36 is a protein called 30S ribosomal protein S6.

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

- Molecule 37 is a protein called 30S ribosomal protein S7.

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

- Molecule 38 is a protein called 30S ribosomal protein S8.

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

- Molecule 39 is a protein called 30S ribosomal protein S9.

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

- Molecule 40 is a protein called 30S ribosomal protein S10.

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

- Molecule 41 is a protein called 30S ribosomal protein S11.

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

- Molecule 42 is a protein called 30S ribosomal protein S12.

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

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

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

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

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

- Molecule 45 is a protein called 30S ribosomal protein S15.

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

- Molecule 46 is a protein called 30S ribosomal protein S16.

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

- Molecule 47 is a protein called 30S ribosomal protein S17.

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

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	65	Total	C	N	O	S	0	0
			539	341	100	97	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	15	GLU	ALA	conflict	UNP P0A7T7

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 52 is a RNA chain called LSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	2904	Total	C	N	O	P	0	0
			62356	27825	11472	20155	2904		

- Molecule 53 is a RNA chain called SSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	1533	Total	C	N	O	P	0	0
			32907	14683	6036	10655	1533		

- Molecule 54 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 55 is a RNA chain called E-site tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 56 is a RNA chain called P-site fMet-tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
56	5	77	Total	C	N	O	P	S	0	0
			1639	734	294	534	76	1		

- Molecule 57 is a RNA chain called A/T tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
57	6	76	Total	C	N	O	P	S	0	0
			1637	734	290	536	76	1		

- Molecule 58 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	7	10	Total	C	N	O	P	0	0
			211	95	36	70	10		

- Molecule 59 is a protein called GTP pyrophosphokinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	8	615	Total	C	N	O	S	0	0
			4792	3010	875	885	22		

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	2	64	Total	Mg	0
			64	64	
60	1	220	Total	Mg	0
			220	220	
60	B	1	Total	Mg	0
			1	1	

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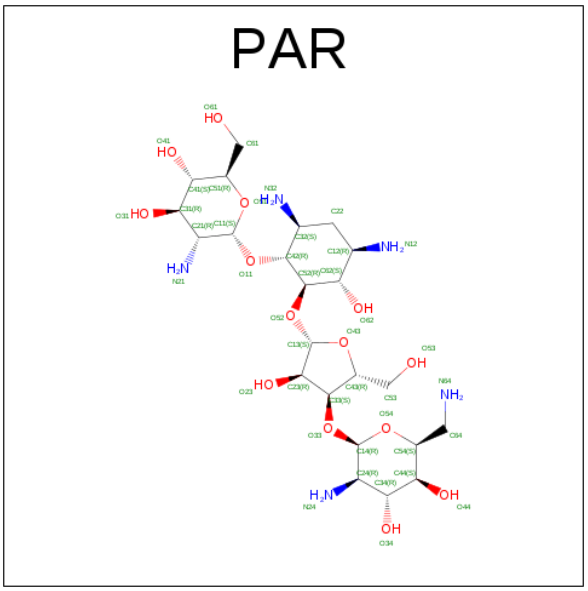
Mol	Chain	Residues	Atoms	AltConf
60	C	1	Total Mg 1 1	0
60	3	6	Total Mg 6 6	0
60	N	1	Total Mg 1 1	0
60	U	1	Total Mg 1 1	0
60	8	1	Total Mg 1 1	0
60	r	1	Total Mg 1 1	0
60	L	2	Total Mg 2 2	0
60	s	1	Total Mg 1 1	0

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

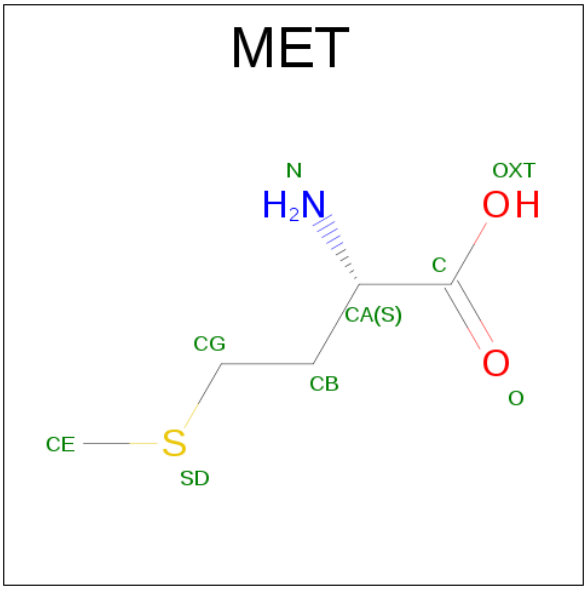
Mol	Chain	Residues	Atoms	AltConf
61	8	1	Total Zn 1 1	0
61	a	1	Total Zn 1 1	0
61	f	1	Total Zn 1 1	0

- Molecule 62 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
62	2	1	42	23	5	14	0

- Molecule 63 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
63	5	1	8	5	1	1	1	0

- Molecule 64 is water.

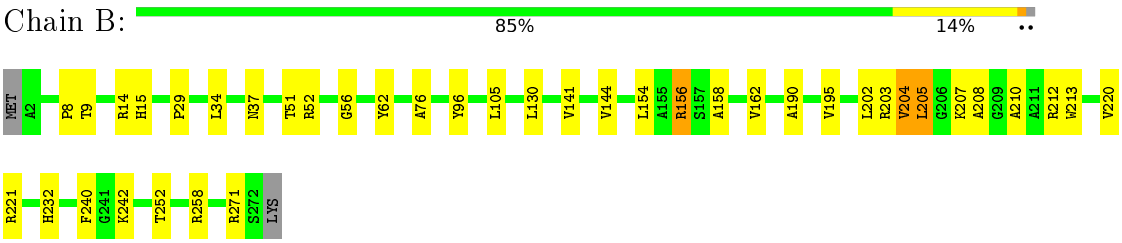
Mol	Chain	Residues	Atoms	AltConf
64	B	2	Total O 2 2	0

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.

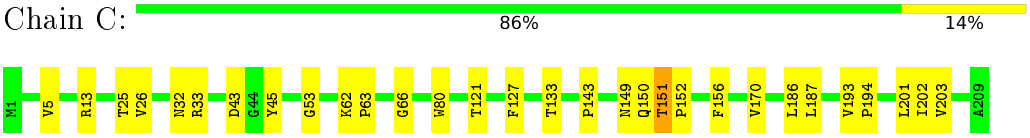
- Molecule 1: 50S ribosomal protein L2

Chain B:



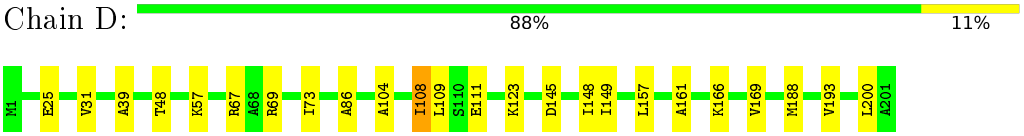
- Molecule 2: 50S ribosomal protein L3

Chain C:



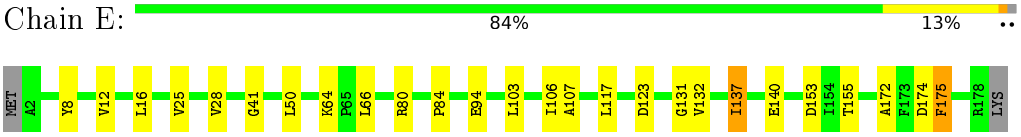
- Molecule 3: 50S ribosomal protein L4

Chain D:



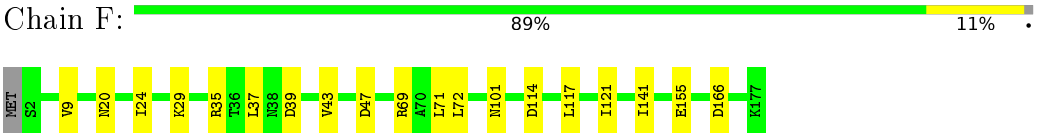
- Molecule 4: 50S ribosomal protein L5

Chain E:



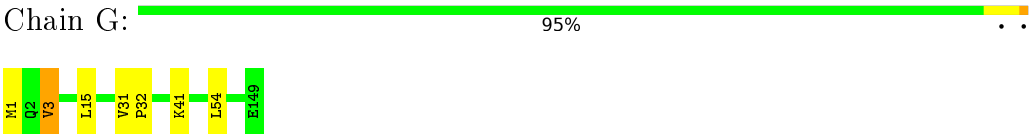
- Molecule 5: 50S ribosomal protein L6

Chain F:



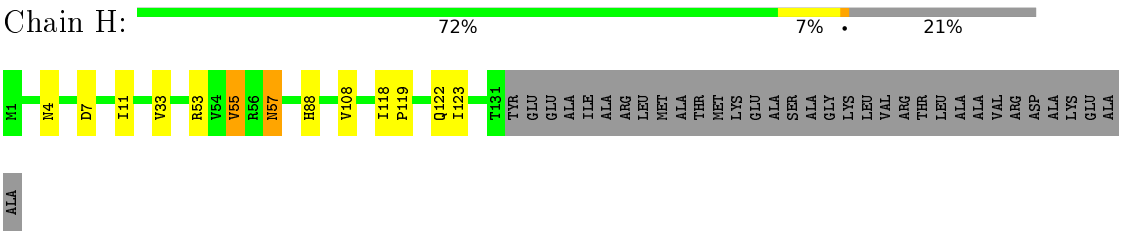
- Molecule 6: 50S ribosomal protein L9

Chain G:



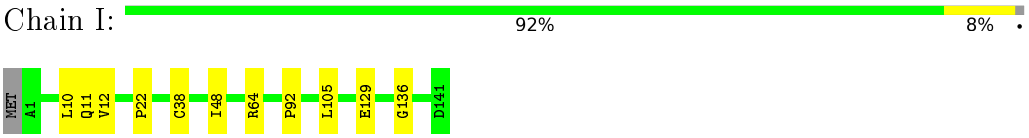
• Molecule 7: 50S ribosomal protein L10

Chain H:



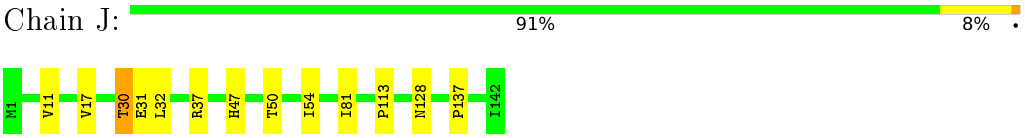
• Molecule 8: 50S ribosomal protein L11

Chain I:



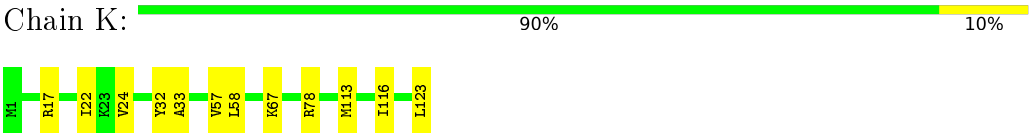
• Molecule 9: 50S ribosomal protein L13

Chain J:



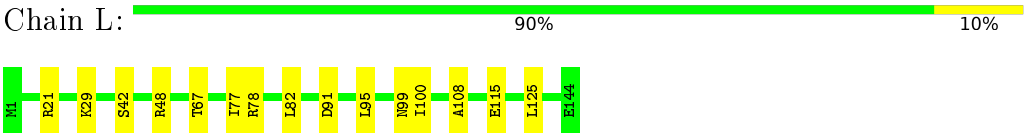
• Molecule 10: 50S ribosomal protein L14

Chain K:



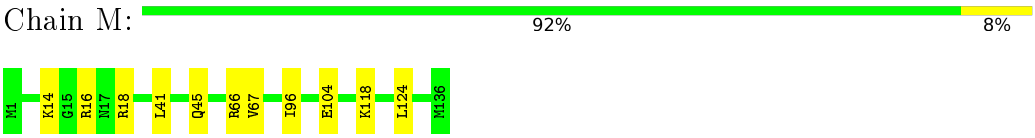
• Molecule 11: 50S ribosomal protein L15

Chain L:



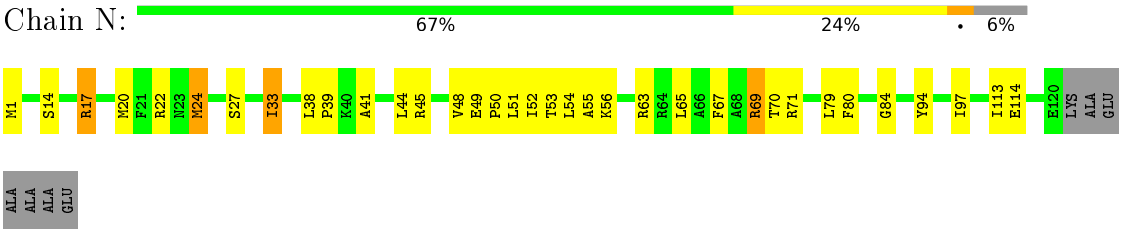
• Molecule 12: 50S ribosomal protein L16

Chain M:



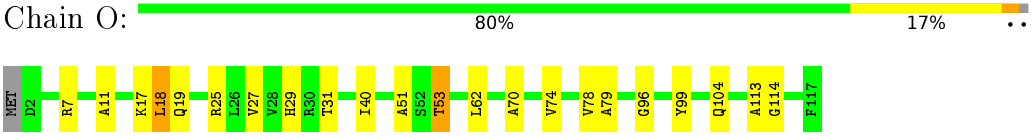
• Molecule 13: 50S ribosomal protein L17

Chain N:



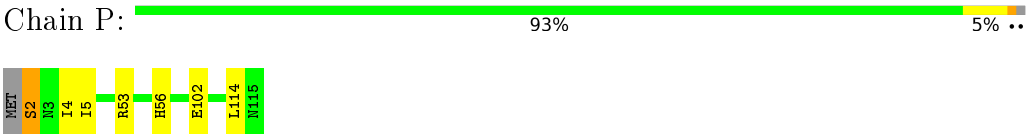
- Molecule 14: 50S ribosomal protein L18

Chain O:



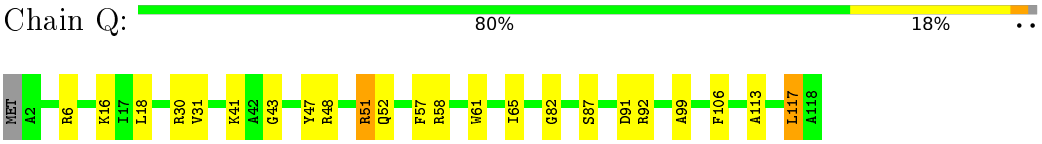
- Molecule 15: 50S ribosomal protein L19

Chain P:



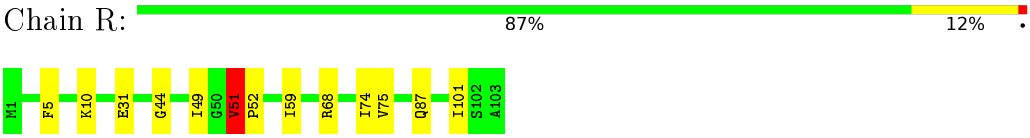
- Molecule 16: 50S ribosomal protein L20

Chain Q:



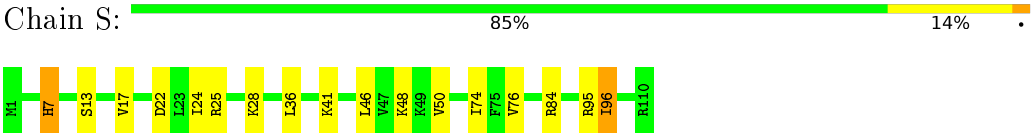
- Molecule 17: 50S ribosomal protein L21

Chain R:



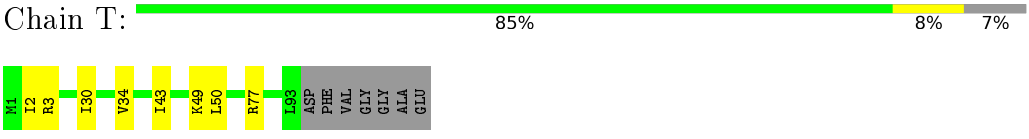
- Molecule 18: 50S ribosomal protein L22

Chain S:



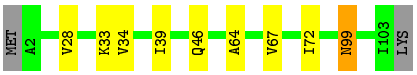
- Molecule 19: 50S ribosomal protein L23

Chain T:



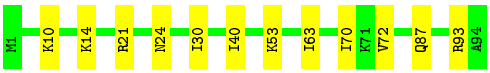
- Molecule 20: 50S ribosomal protein L24

Chain U:



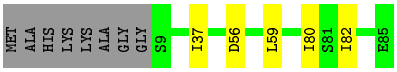
- Molecule 21: 50S ribosomal protein L25

Chain V:



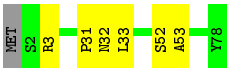
- Molecule 22: 50S ribosomal protein L27

Chain W:



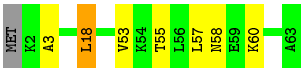
- Molecule 23: 50S ribosomal protein L28

Chain X:



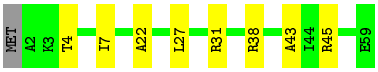
- Molecule 24: 50S ribosomal protein L29

Chain Y:



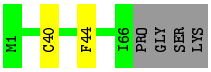
- Molecule 25: 50S ribosomal protein L30

Chain Z:



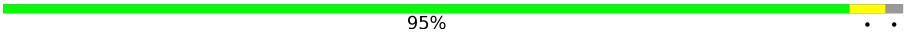
- Molecule 26: 50S ribosomal protein L31

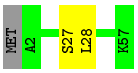
Chain a:



- Molecule 27: 50S ribosomal protein L32

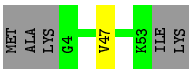
Chain b:





• Molecule 28: 50S ribosomal protein L33

Chain c:



• Molecule 29: 50S ribosomal protein L34

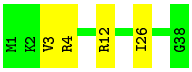
Chain d:

• Molecule 30: 50S ribosomal protein L35

Chain e:

• Molecule 31: 50S ribosomal protein L36

Chain f:



• Molecule 32: 30S ribosomal protein S2

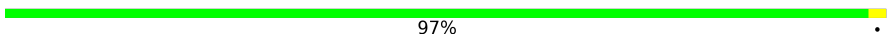
Chain g:

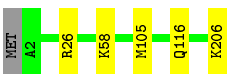
• Molecule 33: 30S ribosomal protein S3

Chain h:

• Molecule 34: 30S ribosomal protein S4

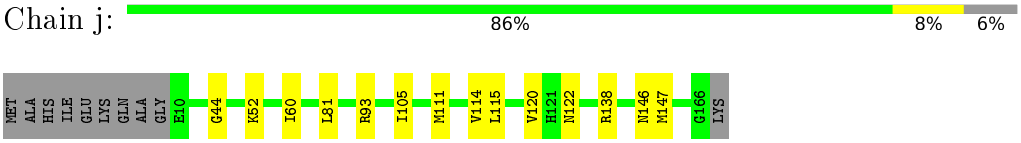
Chain i:





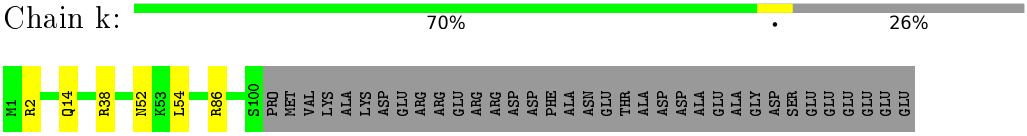
- Molecule 35: 30S ribosomal protein S5

Chain j:



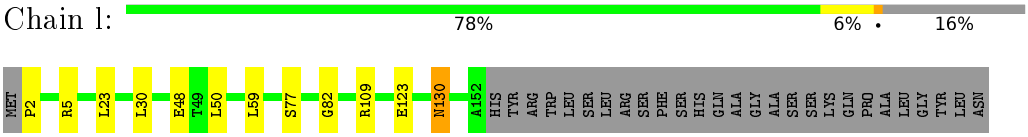
- Molecule 36: 30S ribosomal protein S6

Chain k:



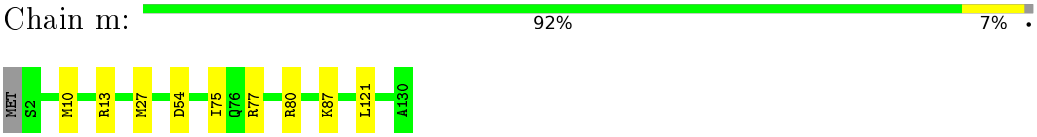
- Molecule 37: 30S ribosomal protein S7

Chain l:



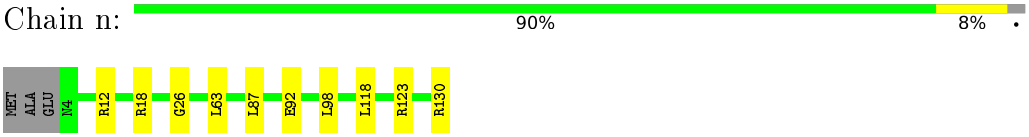
- Molecule 38: 30S ribosomal protein S8

Chain m:



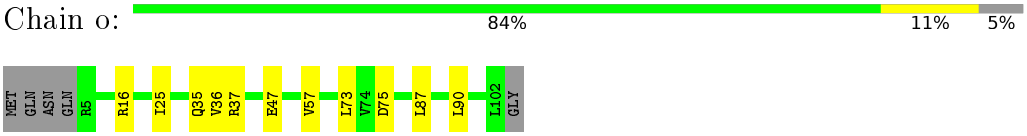
- Molecule 39: 30S ribosomal protein S9

Chain n:



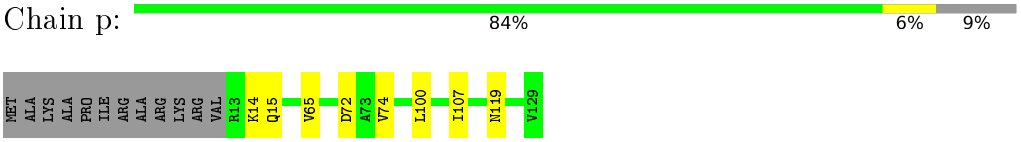
- Molecule 40: 30S ribosomal protein S10

Chain o:



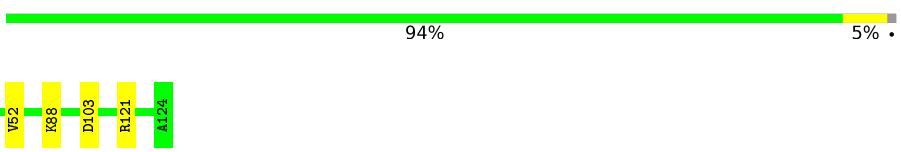
- Molecule 41: 30S ribosomal protein S11

Chain p:



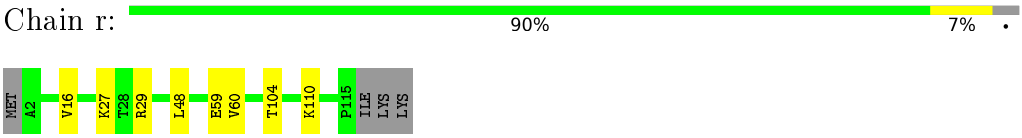
- Molecule 42: 30S ribosomal protein S12

Chain q:



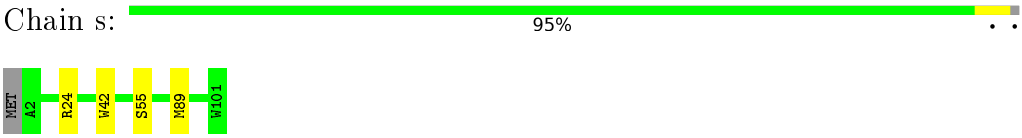
• Molecule 43: 30S ribosomal protein S13

Chain r:



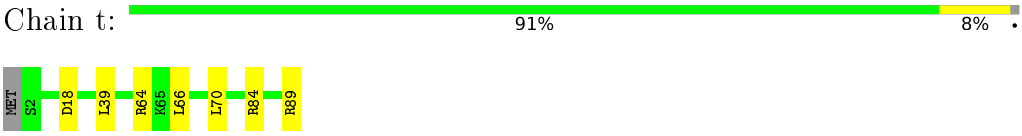
• Molecule 44: 30S ribosomal protein S14

Chain s:



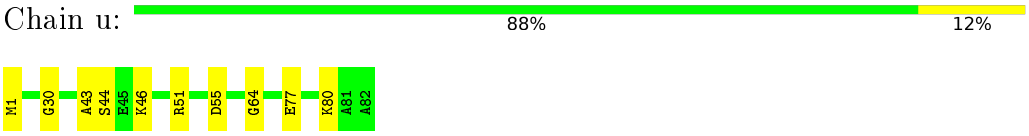
• Molecule 45: 30S ribosomal protein S15

Chain t:



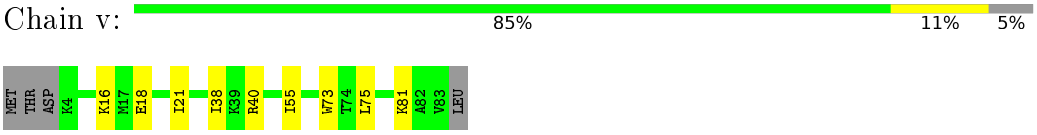
• Molecule 46: 30S ribosomal protein S16

Chain u:



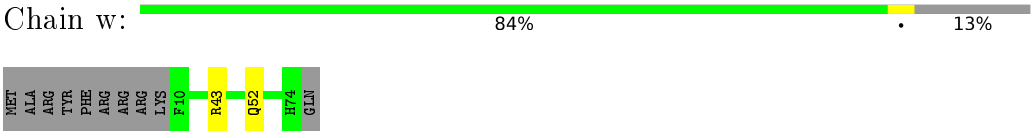
• Molecule 47: 30S ribosomal protein S17

Chain v:



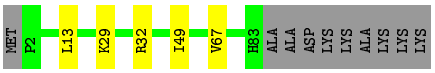
• Molecule 48: 30S ribosomal protein S18

Chain w:



• Molecule 49: 30S ribosomal protein S19

Chain x:

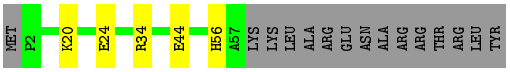


• Molecule 50: 30S ribosomal protein S20

Chain y:

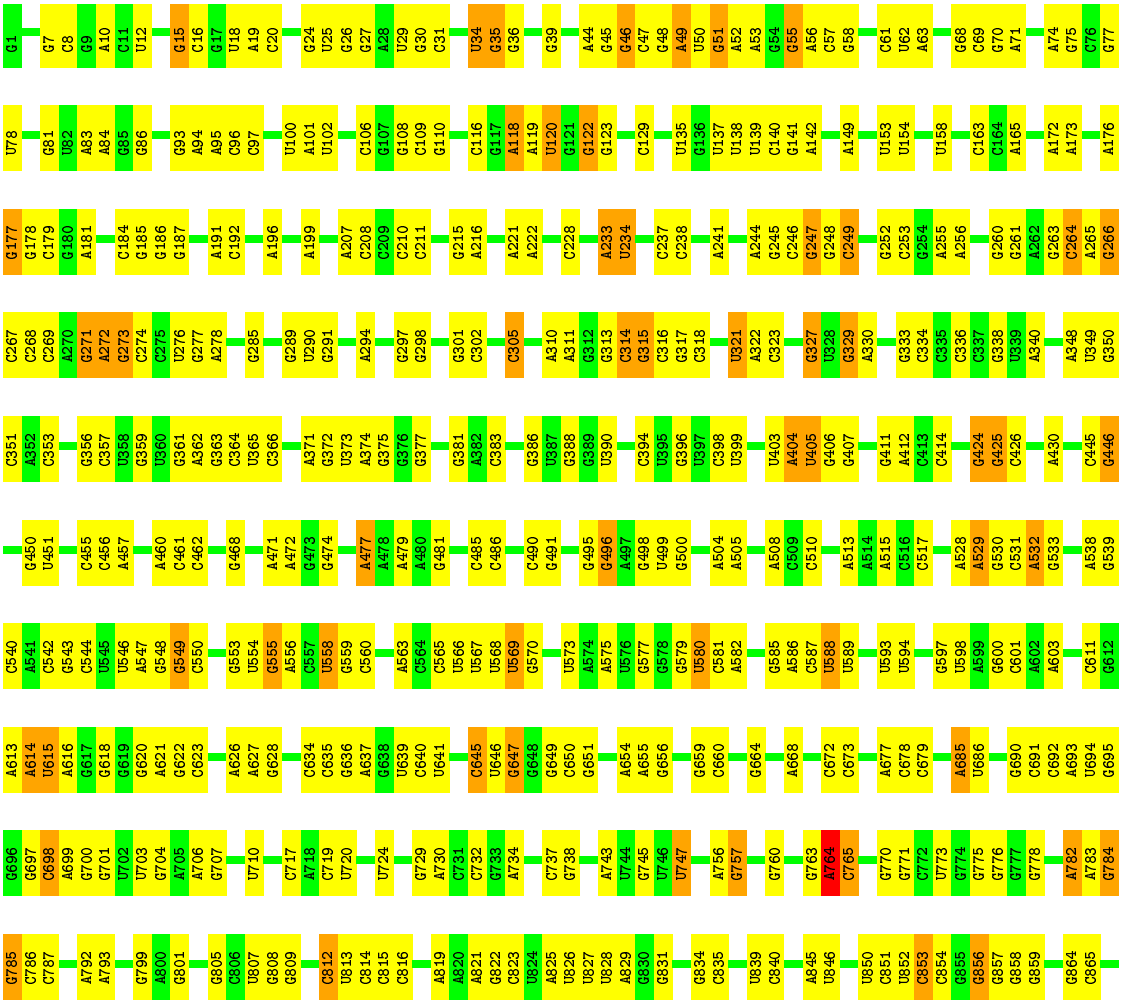
• Molecule 51: 30S ribosomal protein S21

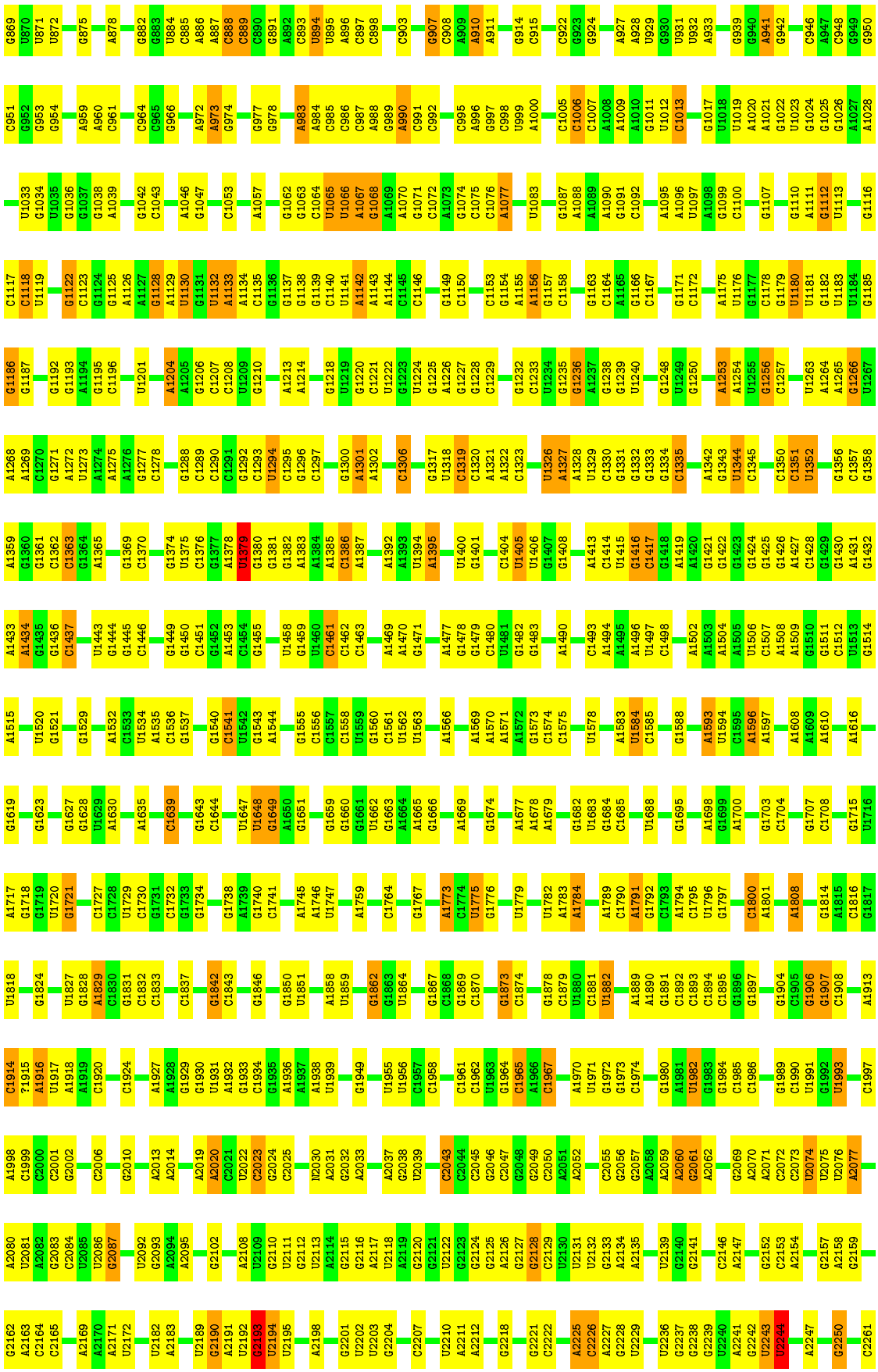
Chain z:

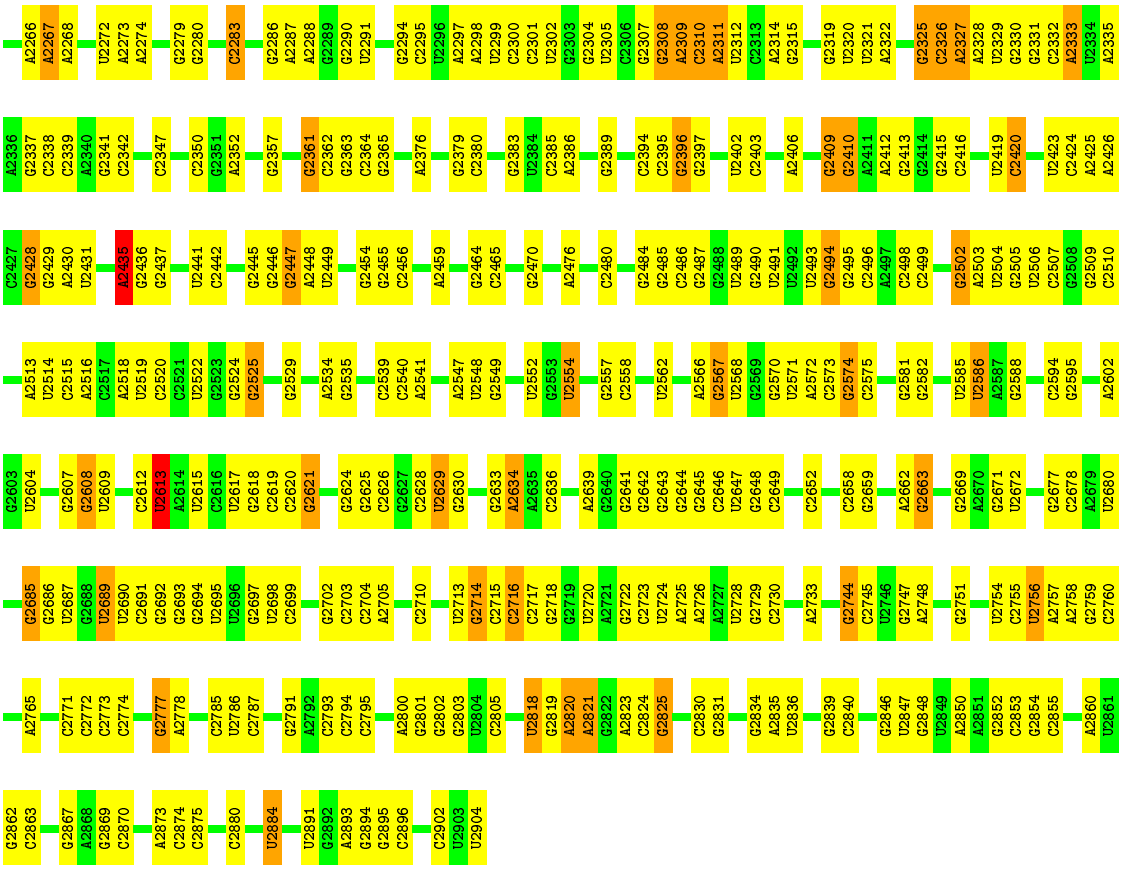


• Molecule 52: LSU rRNA

Chain 1:

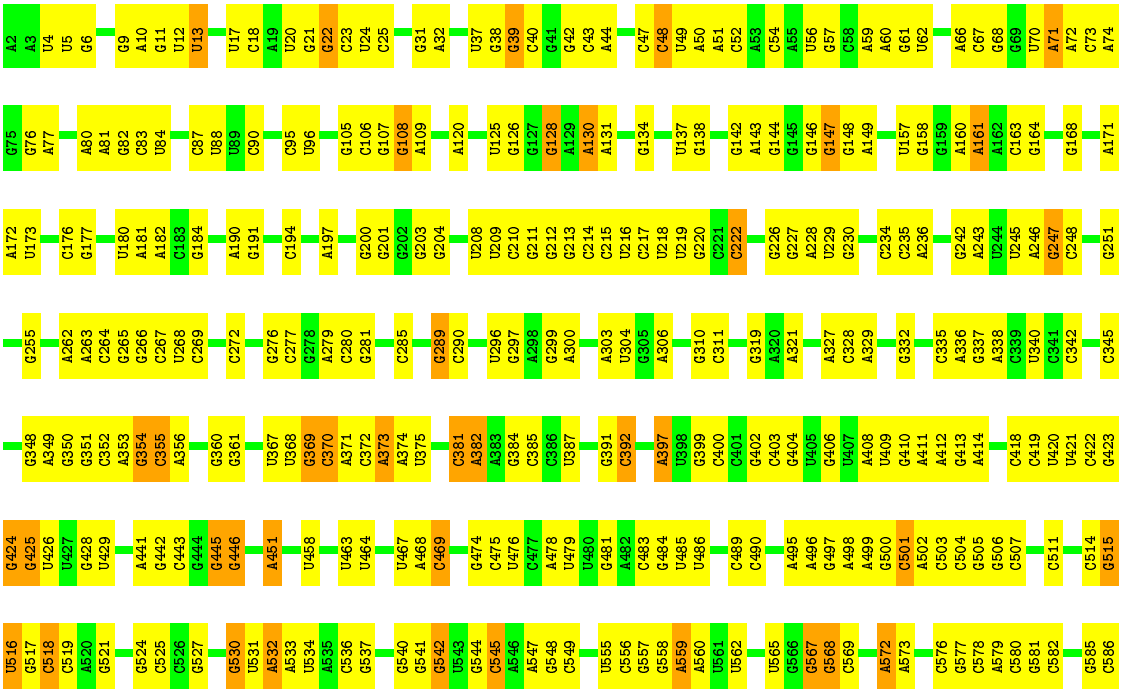


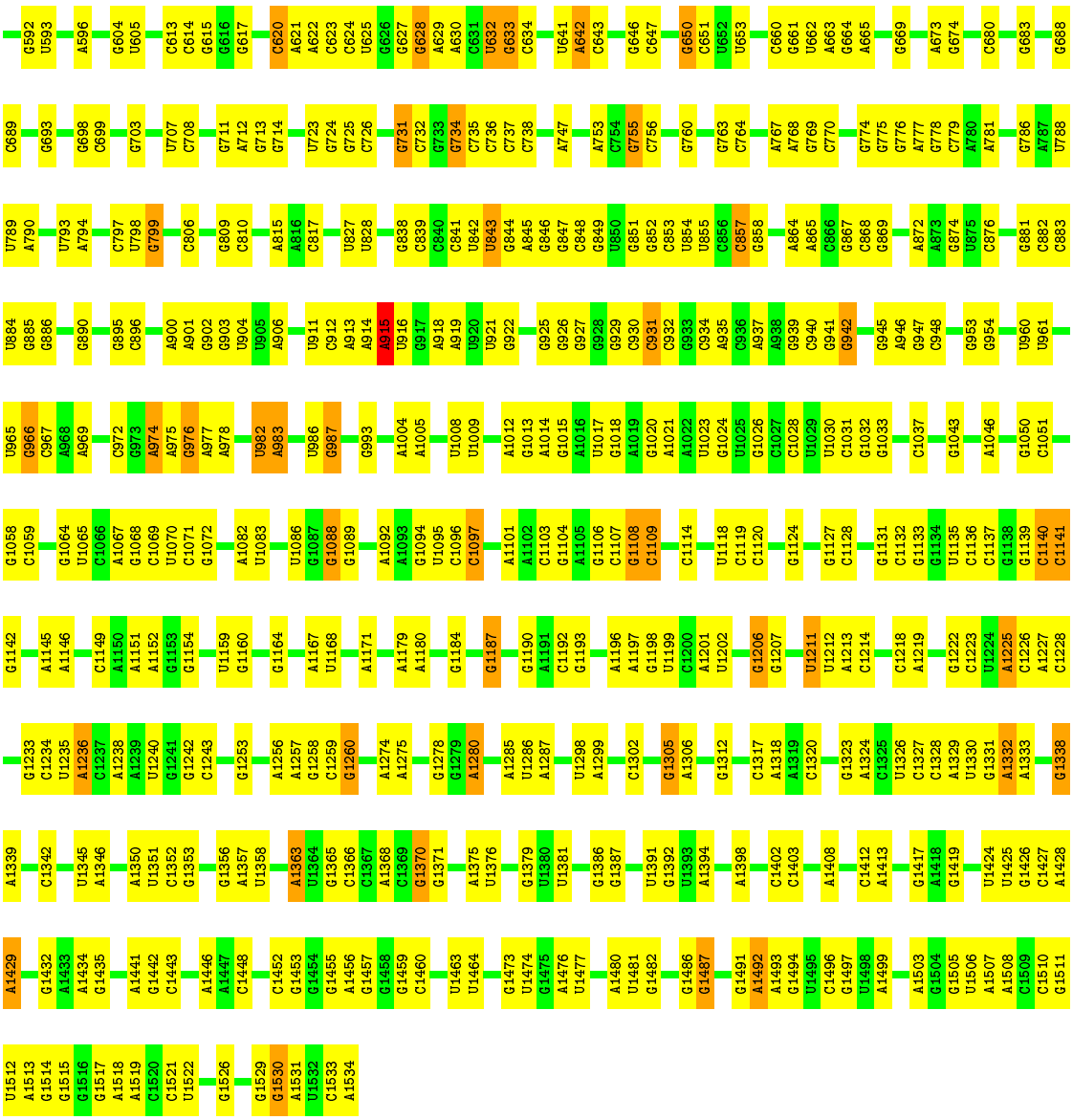




- Molecule 53: SSU rRNA

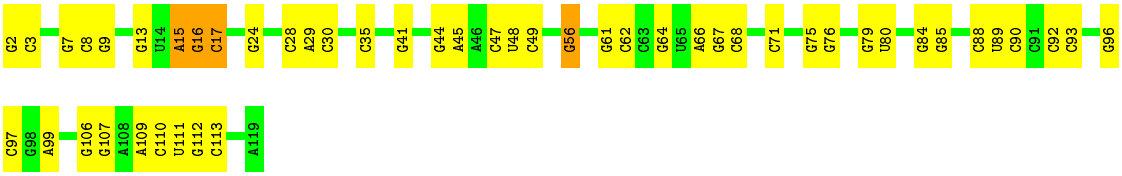
Chain 2:





• Molecule 54: 5S rRNA

Chain 3:

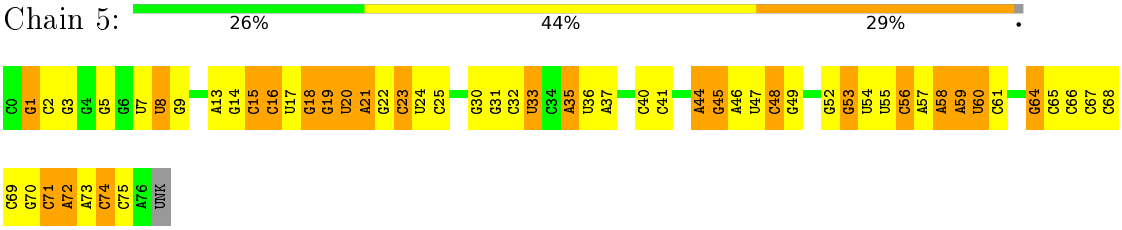


• Molecule 55: E-site tRNA(Phe)

Chain 4:

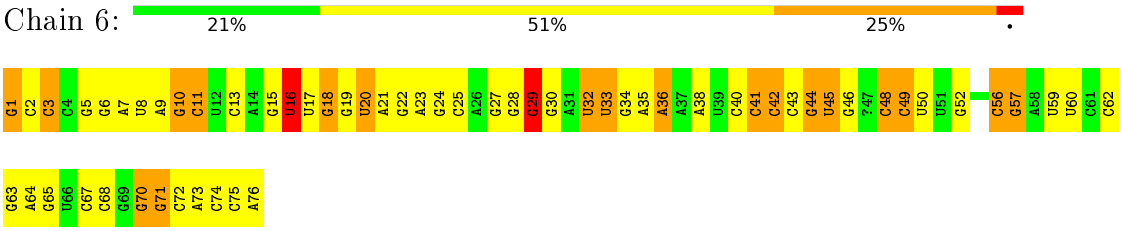
- Molecule 56: P-site fMet-tRNA(fMet)

Chain 5:



- Molecule 57: A/T tRNA(Phe)

Chain 6:

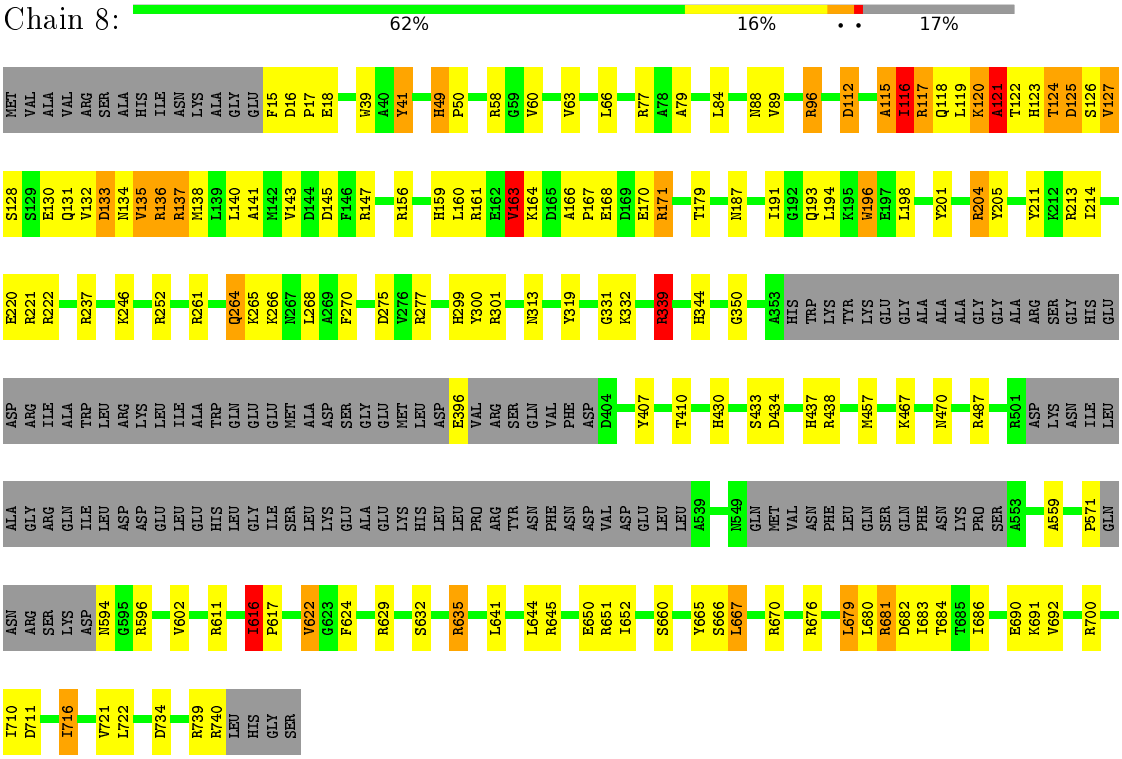


- Molecule 58: mRNA

Chain 7:

- Molecule 59: GTP pyrophosphokinase

Chain 8:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	98498	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	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: PAR, MA6, 2MA, 2MG, 1MG, 3TD, G7M, D2T, 3AU, UR3, 7MG, 5MU, ZN, 6IA, 5MC, 6MZ, OMC, MG, OMG, H2U, OMU, 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	B	0.35	0/2121	0.70	0/2852
10	K	0.35	0/955	0.72	0/1279
11	L	0.38	0/1062	0.74	0/1413
12	M	0.41	0/1093	0.72	0/1460
13	N	0.49	0/973	0.82	0/1301
14	O	0.47	0/902	0.81	0/1209
15	P	0.36	0/929	0.69	0/1242
16	Q	0.55	0/960	0.93	0/1278
17	R	0.33	0/829	0.66	0/1107
18	S	0.42	0/864	0.78	0/1156
19	T	0.41	0/744	0.68	0/994
2	C	0.35	0/1586	0.65	0/2134
20	U	0.35	0/787	0.61	0/1051
21	V	0.39	0/766	0.64	0/1025
22	W	0.34	0/595	0.64	0/787
23	X	0.42	0/635	0.75	0/848
24	Y	0.53	0/502	0.83	0/667
25	Z	0.44	0/453	0.71	0/605
26	a	0.43	0/531	0.66	0/709
27	b	0.41	0/450	0.73	0/599
28	c	0.34	0/416	0.62	0/554
29	d	0.52	0/380	0.95	0/498
3	D	0.43	0/1571	0.74	1/2113 (0.0%)
30	e	0.42	0/513	0.81	0/676
31	f	0.34	0/303	0.71	0/397
32	g	0.47	0/1784	0.71	0/2403
33	h	0.43	0/1655	0.72	0/2230
34	i	0.45	0/1665	0.72	0/2227
35	j	0.43	0/1169	0.76	0/1573
36	k	0.42	0/835	0.72	0/1128
37	l	0.48	0/1195	0.78	0/1602

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
38	m	0.41	0/989	0.71	0/1326
39	n	0.43	0/1034	0.77	0/1375
4	E	0.45	0/1434	0.73	0/1926
40	o	0.42	0/796	0.74	0/1077
41	p	0.40	0/893	0.71	0/1205
42	q	0.35	0/960	0.72	0/1286
43	r	0.46	0/892	0.86	0/1193
44	s	0.47	0/817	0.78	0/1088
45	t	0.54	0/722	0.85	0/964
46	u	0.44	0/659	0.75	0/884
47	v	0.35	0/657	0.64	0/881
48	w	0.45	0/548	0.73	0/736
49	x	0.41	0/675	0.70	0/908
5	F	0.39	0/1343	0.65	0/1816
50	y	0.58	0/676	0.88	0/895
51	z	0.51	0/472	0.89	0/627
52	1	0.34	11/69300 (0.0%)	0.74	21/108089 (0.0%)
53	2	0.27	2/36561 (0.0%)	0.72	2/57019 (0.0%)
54	3	0.24	0/2828	0.70	0/4410
55	4	0.25	0/1808	0.70	0/2815
56	5	0.35	0/1716	0.83	0/2672
57	6	0.42	1/1606 (0.1%)	0.80	1/2497 (0.0%)
58	7	0.31	0/235	0.71	0/363
59	8	0.62	0/4878	1.14	30/6606 (0.5%)
6	G	0.42	0/1122	0.63	0/1515
7	H	0.46	0/1001	0.66	0/1350
8	I	0.42	0/1046	0.62	0/1410
9	J	0.44	0/1152	0.72	0/1551
All	All	0.36	14/166043 (0.0%)	0.75	55/247601 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
52	1	0	9
53	2	0	2
57	6	8	3
59	8	0	19
All	All	8	33

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	1	2244	U	C2-N3	19.23	1.51	1.37
52	1	2244	U	N3-C4	17.42	1.54	1.38
52	1	2435	A	C6-N1	-15.77	1.24	1.35
52	1	2244	U	N1-C2	13.64	1.50	1.38
52	1	1775	U	C2-N3	12.29	1.46	1.37
57	6	1	G	OP3-P	-10.15	1.49	1.61
52	1	1775	U	N3-C4	8.99	1.46	1.38
52	1	1596	A	N1-C2	7.23	1.40	1.34
52	1	1405	U	C2-N3	7.15	1.42	1.37
52	1	2435	A	N1-C2	6.21	1.40	1.34
53	2	13	U	C2-N3	6.08	1.42	1.37
53	2	915	A	C6-N1	-5.73	1.31	1.35
52	1	2244	U	O4'-C1'	5.49	1.48	1.41
52	1	764	A	C6-N1	-5.39	1.31	1.35

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	1	2244	U	C2-N3-C4	-18.02	116.19	127.00
52	1	2435	A	N1-C6-N6	-14.25	110.05	118.60
52	1	2244	U	C2-N1-C1'	13.09	133.41	117.70
52	1	2244	U	C6-N1-C1'	-11.39	105.26	121.20
52	1	2244	U	C5-C4-O4	-10.87	119.38	125.90
59	8	171	ARG	NE-CZ-NH2	10.07	125.34	120.30
52	1	1775	U	C2-N3-C4	-10.05	120.97	127.00
59	8	213	ARG	NE-CZ-NH2	9.31	124.95	120.30
52	1	2435	A	C5-C6-N6	8.63	130.60	123.70
59	8	277	ARG	NE-CZ-NH2	8.37	124.48	120.30
59	8	204	ARG	NE-CZ-NH2	7.82	124.21	120.30
59	8	221	ARG	NE-CZ-NH1	-7.66	116.47	120.30
52	1	2244	U	C4-C5-C6	7.55	124.23	119.70
59	8	58	ARG	NE-CZ-NH2	7.29	123.94	120.30
59	8	130	GLU	CB-CA-C	7.20	124.80	110.40
52	1	1596	A	C6-N1-C2	-7.03	114.38	118.60
59	8	221	ARG	NE-CZ-NH2	6.93	123.76	120.30
59	8	196	TRP	CA-CB-CG	6.84	126.69	113.70
59	8	161	ARG	NE-CZ-NH2	6.80	123.70	120.30
59	8	121	ALA	CB-CA-C	6.74	120.22	110.10
52	1	1405	U	C2-N3-C4	-6.73	122.96	127.00
52	1	1775	U	N1-C1'-C2'	6.49	122.44	114.00
52	1	2193	G	C2'-C3'-O3'	6.46	124.03	113.70
59	8	339	ARG	NE-CZ-NH2	6.35	123.47	120.30
53	2	1211	U	C2'-C3'-O3'	6.33	123.83	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	8	261	ARG	NE-CZ-NH2	6.17	123.38	120.30
57	6	70	G	C2'-C3'-O3'	6.02	123.33	113.70
59	8	222	ARG	NE-CZ-NH2	5.99	123.29	120.30
59	8	319	TYR	CB-CG-CD2	-5.74	117.56	121.00
59	8	163	VAL	CA-CB-CG1	5.72	119.48	110.90
59	8	96	ARG	NE-CZ-NH2	5.67	123.13	120.30
52	1	2244	U	C5'-C4'-O4'	5.60	115.82	109.10
52	1	2244	U	C3'-C2'-C1'	5.55	105.94	101.50
59	8	117	ARG	NE-CZ-NH2	5.53	123.06	120.30
52	1	1379	U	C2'-C3'-O3'	5.47	122.45	113.70
52	1	2244	U	N3-C4-O4	5.45	123.22	119.40
59	8	156	ARG	NE-CZ-NH2	5.41	123.00	120.30
59	8	571	PRO	N-CA-CB	5.40	109.78	103.30
59	8	41	TYR	CB-CG-CD2	-5.39	117.77	121.00
59	8	124	THR	C-N-CA	5.39	135.17	121.70
53	2	632	U	N1-C1'-C2'	5.38	120.99	114.00
59	8	132	VAL	CG1-CB-CG2	-5.37	102.31	110.90
59	8	120	LYS	CB-CA-C	5.24	120.89	110.40
59	8	147	ARG	NE-CZ-NH2	5.20	122.90	120.30
59	8	261	ARG	N-CA-CB	-5.18	101.28	110.60
52	1	2447	G	C2'-C3'-O3'	-5.14	98.18	109.50
52	1	2613	U	O4'-C1'-N1	5.13	112.30	108.20
59	8	201	TYR	CB-CG-CD2	-5.12	117.93	121.00
59	8	222	ARG	CD-NE-CZ	5.10	130.74	123.60
59	8	237	ARG	NE-CZ-NH2	5.08	122.84	120.30
52	1	2074	U	N1-C1'-C2'	5.05	120.56	114.00
59	8	301	ARG	NE-CZ-NH2	5.04	122.82	120.30
3	D	67	ARG	NE-CZ-NH1	5.04	122.82	120.30
52	1	2244	U	N1-C2-O2	-5.00	119.30	122.80
52	1	2613	U	N1-C1'-C2'	5.00	120.50	114.00

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
57	6	16	H2U	C2',C3',C1'
57	6	20	H2U	C2',C1'
57	6	32	PSU	C1'
57	6	37	6IA	C3'
57	6	55	PSU	C1'

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	1	1319	C	Sidechain
52	1	1335	C	Sidechain
52	1	1351	C	Sidechain
52	1	1363	C	Sidechain
52	1	2244	U	Sidechain
52	1	2435	A	Sidechain
52	1	305	C	Sidechain
52	1	314	C	Sidechain
52	1	764	A	Sidechain
53	2	915	A	Sidechain
53	2	931	C	Sidechain
57	6	29	G	Sidechain
57	6	3	C	Sidechain
57	6	42	C	Sidechain
59	8	116	ILE	Peptide
59	8	121	ALA	Peptide
59	8	123	HIS	Peptide
59	8	127	VAL	Peptide
59	8	133	ASP	Peptide
59	8	135	VAL	Peptide
59	8	136	ARG	Peptide
59	8	138	MET	Peptide
59	8	163	VAL	Peptide
59	8	166	ALA	Peptide
59	8	170	GLU	Peptide
59	8	171	ARG	Sidechain
59	8	211	TYR	Sidechain
59	8	252	ARG	Sidechain
59	8	264	GLN	Peptide
59	8	300	TYR	Sidechain
59	8	332	LYS	Peptide
59	8	77	ARG	Sidechain
59	8	96	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2082	0	2154	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1565	0	1616	25	0
3	D	1552	0	1619	9	0
4	E	1410	0	1444	11	0
5	F	1323	0	1371	6	0
6	G	1111	0	1148	2	0
7	H	988	0	1025	2	0
8	I	1032	0	1088	1	0
9	J	1129	0	1162	9	0
10	K	946	0	1023	4	0
11	L	1053	0	1129	6	0
12	M	1074	0	1157	6	0
13	N	960	0	1000	21	0
14	O	892	0	923	10	0
15	P	917	0	962	5	0
16	Q	947	0	1019	13	0
17	R	816	0	839	6	0
18	S	857	0	922	9	0
19	T	738	0	807	1	0
20	U	779	0	831	3	0
21	V	753	0	780	5	0
22	W	588	0	604	4	0
23	X	625	0	652	4	0
24	Y	501	0	531	2	0
25	Z	449	0	488	4	0
26	a	522	0	521	0	0
27	b	444	0	458	0	0
28	c	409	0	440	0	0
29	d	377	0	418	0	0
30	e	504	0	572	0	0
31	f	302	0	342	0	0
32	g	1753	0	1780	0	0
33	h	1628	0	1699	0	0
34	i	1643	0	1707	0	0
35	j	1156	0	1199	0	0
36	k	817	0	808	0	0
37	l	1181	0	1238	0	0
38	m	979	0	1031	0	0
39	n	1022	0	1070	0	0
40	o	786	0	828	0	0
41	p	877	0	887	0	0
42	q	957	0	1017	0	0
43	r	883	0	941	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	s	805	0	844	0	0
45	t	714	0	734	0	0
46	u	649	0	666	0	0
47	v	648	0	691	0	0
48	w	539	0	553	0	0
49	x	658	0	683	0	0
50	y	670	0	719	0	0
51	z	465	0	491	0	0
52	1	62356	0	31391	952	0
53	2	32907	0	16580	469	0
54	3	2529	0	1281	37	0
55	4	1619	0	823	31	0
56	5	1639	0	843	42	0
57	6	1637	0	840	43	0
58	7	211	0	107	14	0
59	8	4792	0	4726	40	0
60	1	220	0	0	0	0
60	2	64	0	0	0	0
60	3	6	0	0	0	0
60	8	1	0	0	0	0
60	B	1	0	0	0	0
60	C	1	0	0	0	0
60	L	2	0	0	0	0
60	N	1	0	0	0	0
60	U	1	0	0	0	0
60	r	1	0	0	0	0
60	s	1	0	0	0	0
61	8	1	0	0	0	0
61	a	1	0	0	0	0
61	f	1	0	0	0	0
62	2	42	0	45	1	0
63	5	8	0	8	1	0
64	B	2	0	0	0	0
All	All	154519	0	105275	1739	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 7.

All (1739) 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)
52:1:2244:U:N3	52:1:2435:A:C6	1.94	1.32
53:2:13:U:N3	53:2:915:A:N6	1.76	1.31
52:1:2244:U:N3	52:1:2435:A:N6	1.79	1.29
52:1:1067:A:N3	57:6:56:C:N3	1.85	1.23
55:4:31:A:N1	55:4:39:U:O4	1.75	1.19
52:1:2297:A:N1	52:1:2321:U:C4	2.16	1.13
53:2:13:U:N3	53:2:915:A:C6	2.17	1.13
53:2:1358:U:O4	53:2:1363:A:N1	1.82	1.11
55:4:36:A:N1	58:7:13:A:N6	2.00	1.10
52:1:2244:U:H3	52:1:2435:A:N6	1.42	1.08
52:1:2297:A:N1	52:1:2321:U:O4	1.88	1.06
52:1:764:A:N6	52:1:1775:U:N3	2.04	1.05
52:1:49:A:N6	52:1:120:U:N3	2.05	1.04
53:2:13:U:O2	53:2:915:A:N7	1.92	1.01
55:4:31:A:N1	55:4:39:U:C4	2.28	1.00
53:2:827:U:O4	53:2:872:A:N1	1.94	1.00
53:2:13:U:C4	53:2:915:A:N6	2.29	1.00
53:2:13:U:O4	53:2:20:U:O4	1.83	0.97
52:1:234:U:H3	52:1:430:A:N6	1.65	0.95
52:1:2297:A:C2	52:1:2321:U:C4	2.56	0.94
52:1:764:A:C6	52:1:1775:U:N3	2.36	0.94
53:2:37:U:H3	53:2:397:A:H61	1.17	0.93
53:2:37:U:H3	53:2:397:A:N6	1.67	0.92
52:1:234:U:H3	52:1:430:A:H61	0.99	0.90
52:1:568:U:H1'	52:1:2030:6MZ:H9C1	1.52	0.90
53:2:13:U:C2	53:2:915:A:N6	2.41	0.89
59:8:141:ALA:HB2	59:8:407:TYR:OH	1.74	0.88
52:1:2013:A:N6	52:1:2613:U:H3	1.72	0.86
53:2:13:U:C4	53:2:20:U:O4	2.29	0.86
52:1:1067:A:C2	57:6:56:C:N3	2.45	0.85
52:1:2297:A:C6	52:1:2321:U:O4	2.30	0.84
52:1:2297:A:C2	52:1:2321:U:C5	2.65	0.83
52:1:2244:U:N3	52:1:2435:A:C5	2.37	0.83
52:1:1405:U:H2'	52:1:1406:U:C6	2.15	0.82
52:1:1019:U:O4	52:1:1142:A:N1	2.14	0.81
52:1:49:A:C6	52:1:120:U:N3	2.49	0.80
52:1:1596:A:H2'	52:1:1597:A:C8	2.16	0.80
56:5:59:A:O2'	56:5:60:U:O4'	1.97	0.80
52:1:2013:A:H61	52:1:2613:U:H3	1.28	0.79
52:1:764:A:H62	52:1:1776:G:H1'	1.48	0.78
52:1:1326:U:O2'	52:1:2010:G:O2'	1.99	0.77
52:1:118:A:H2'	52:1:120:U:O4	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:1999:C:H4'	52:1:2723:C:O2	1.85	0.76
55:4:36:A:C2	58:7:14:A:C2	2.73	0.76
1:B:208:ALA:HB1	52:1:764:A:C2	2.21	0.76
52:1:2244:U:C4	52:1:2435:A:N6	2.54	0.76
52:1:49:A:N6	52:1:120:U:C4	2.54	0.75
55:4:36:A:C6	58:7:13:A:N6	2.54	0.75
52:1:1067:A:N3	57:6:56:C:C2	2.55	0.75
52:1:1141:U:H4'	52:1:1142:A:O4'	1.87	0.74
59:8:716:ILE:HD12	59:8:721:VAL:HG11	1.70	0.74
53:2:24:U:O4	53:2:559:A:N1	2.21	0.73
53:2:769:G:H4'	53:2:1513:A:H4'	1.71	0.73
55:4:31:A:C2	55:4:39:U:O4	2.41	0.73
14:O:11:ALA:HB2	14:O:96:GLY:N	2.03	0.72
53:2:13:U:O4	53:2:21:G:C2	2.42	0.72
52:1:2297:A:C2	52:1:2321:U:O4	2.41	0.71
52:1:764:A:N6	52:1:1775:U:C4	2.58	0.71
53:2:673:A:H2'	53:2:674:G:C8	2.25	0.71
59:8:681:ARG:O	59:8:684:THR:OG1	2.05	0.70
52:1:1065:U:O2'	52:1:1066:U:O4'	2.10	0.70
52:1:1779:U:H5	52:1:1784:A:N7	1.90	0.70
52:1:2043:C:N4	52:1:2777:G:C6	2.61	0.69
53:2:768:A:N3	53:2:1512:U:O2'	2.24	0.69
18:S:36:LEU:HD13	18:S:48:LYS:HA	1.75	0.69
52:1:1980:G:O2'	52:1:1982:U:OP2	2.11	0.69
53:2:1352:C:O2	53:2:1371:G:C2	2.46	0.68
52:1:1450:G:N2	52:1:1462:C:C2	2.62	0.68
55:4:31:A:C6	55:4:39:U:O4	2.45	0.68
52:1:1964:G:N2	52:1:1967:C:C2	2.62	0.68
52:1:927:A:H2'	52:1:928:A:C8	2.29	0.67
55:4:36:A:C2	58:7:13:A:N6	2.63	0.67
52:1:1021:A:N6	52:1:1141:U:H3	1.93	0.67
52:1:2006:C:O2'	52:1:2823:A:N3	2.27	0.67
56:5:71:C:H2'	56:5:72:A:C8	2.29	0.67
52:1:1450:G:C2	52:1:1462:C:C2	2.83	0.67
59:8:559:ALA:HB2	59:8:681:ARG:CB	2.25	0.66
53:2:1235:U:H2'	53:2:1236:A:O4'	1.94	0.66
53:2:961:U:O4	53:2:974:A:N1	2.28	0.66
52:1:1350:C:C2	52:1:1382:G:C2	2.83	0.66
53:2:13:U:O4	53:2:21:G:C4	2.49	0.66
53:2:1356:G:H2'	53:2:1357:A:C8	2.31	0.66
52:1:743:A:O2'	52:1:1659:G:OP1	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:THR:CG2	52:1:2020:A:H5'	85.13	0.66
59:8:116:ILE:HA	59:8:119:LEU:HB3	1.78	0.65
53:2:384:G:H2'	53:2:385:C:C6	2.31	0.65
53:2:514:C:N4	53:2:537:G:C6	2.65	0.65
57:6:32:PSU:H2'	57:6:33:U:C6	2.31	0.65
52:1:2038:G:H2'	52:1:2039:U:O4'	1.96	0.65
55:4:36:A:N1	58:7:13:A:C6	2.65	0.65
52:1:1400:U:H2'	52:1:1401:G:O4'	1.97	0.64
52:1:1436:G:H2'	52:1:1437:C:O4'	1.98	0.64
53:2:786:G:C2	53:2:797:C:C2	2.86	0.64
52:1:1019:U:C4	52:1:1142:A:N1	2.66	0.64
53:2:354:G:N2	53:2:355:C:C2	2.66	0.64
2:C:63:PRO:O	52:1:2786:U:O2'	2.16	0.64
53:2:37:U:N3	53:2:397:A:N6	2.37	0.63
53:2:384:G:C6	53:2:385:C:N4	2.66	0.63
53:2:864:A:C2	53:2:865:A:C2	2.86	0.63
13:N:17:ARG:O	13:N:20:MET:HG3	1.98	0.63
52:1:118:A:H2'	52:1:120:U:C4	2.32	0.63
52:1:2077:A:C6	52:1:2435:A:N6	2.67	0.63
52:1:234:U:N3	52:1:430:A:N6	2.33	0.63
53:2:1358:U:C4	53:2:1363:A:N1	2.67	0.63
57:6:56:C:H2'	57:6:56:C:O2	1.98	0.63
52:1:2261:C:C2	52:1:2280:G:C2	2.87	0.63
52:1:528:A:C2	52:1:2043:C:H4'	2.34	0.62
52:1:1405:U:C2	52:1:1406:U:C4	2.86	0.62
53:2:13:U:O4	53:2:21:G:N3	2.32	0.62
2:C:45:TYR:HH	52:1:2636:C:HO2'	1.46	0.62
52:1:554:U:O4	52:1:555:G:C6	2.52	0.62
52:1:44:A:H2'	52:1:45:G:O4'	2.00	0.62
53:2:1358:U:O4	53:2:1363:A:C2	2.51	0.62
53:2:264:C:H2'	53:2:265:G:O4'	1.98	0.62
53:2:524:G:C6	53:2:525:C:N4	2.68	0.62
53:2:966:2MG:HM23	53:2:967:5MC:H1'	1.81	0.62
56:5:19:G:H3'	56:5:20:H2U:H5"	1.80	0.62
16:Q:31:VAL:HG13	52:1:580:U:O3'	1.98	0.62
18:S:25:ARG:NH1	18:S:74:ILE:O	2.33	0.62
52:1:1038:G:H2'	52:1:1039:A:C8	2.35	0.61
52:1:2337:G:N2	52:1:2338:C:C2	2.67	0.61
53:2:13:U:C4	53:2:21:G:C2	2.88	0.61
52:1:1361:G:H2'	52:1:1362:C:C6	2.35	0.61
52:1:1932:A:H2'	52:1:1933:G:O4'	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:8:559:ALA:HB2	59:8:681:ARG:HB3	1.82	0.61
52:1:172:A:H2'	52:1:173:A:C8	2.36	0.61
53:2:712:A:H2'	53:2:713:G:O4'	2.00	0.61
52:1:587:C:H4'	52:1:588:U:C6	2.35	0.61
16:Q:48:ARG:NH1	52:1:560:C:O2	2.34	0.61
52:1:1562:U:H2'	52:1:1563:U:O4'	2.01	0.61
52:1:2074:U:H2'	52:1:2075:U:C6	2.36	0.61
56:5:22:G:N2	56:5:23:C:C2	2.69	0.61
52:1:1006:C:C2	52:1:1138:G:N2	2.69	0.60
52:1:815:C:C2	52:1:1193:G:C2	2.89	0.60
53:2:1352:C:C2	53:2:1371:G:C2	2.89	0.60
52:1:569:U:O2'	52:1:983:A:N1	2.31	0.60
24:Y:18:LEU:HB2	24:Y:53:VAL:HG11	1.82	0.60
52:1:764:A:N6	52:1:1776:G:H1'	2.15	0.60
3:D:104:ALA:O	3:D:108:ILE:HG23	2.01	0.60
52:1:1846:G:N2	52:1:1895:C:C2	2.70	0.60
1:B:221:ARG:NH1	52:1:1789:A:OP2	2.35	0.60
55:4:31:A:C2	55:4:39:U:C4	2.89	0.60
12:M:41:LEU:HD22	12:M:124:LEU:HD22	1.84	0.60
53:2:24:U:C4	53:2:559:A:N1	2.70	0.60
13:N:67:PHE:O	13:N:71:ARG:N	2.33	0.60
52:1:692:C:C2	52:1:771:G:C2	2.90	0.59
53:2:369:G:N2	53:2:370:C:C2	2.71	0.59
2:C:25:THR:HG21	2:C:193:VAL:HG22	1.84	0.59
15:P:53:ARG:NH2	52:1:2720:U:OP1	2.36	0.59
52:1:1063:G:H2'	52:1:1064:C:O4'	2.03	0.59
16:Q:92:ARG:NH1	52:1:1153:C:OP1	2.35	0.59
16:Q:6:ARG:NH1	52:1:585:G:N7	2.48	0.59
53:2:371:A:O2'	53:2:373:A:N7	2.36	0.59
52:1:807:U:O2'	52:1:2060:A:N1	2.26	0.59
53:2:613:C:C2	53:2:628:G:N2	2.71	0.59
52:1:1063:G:C6	52:1:1064:C:C4	2.91	0.59
52:1:1779:U:C5	52:1:1784:A:N7	2.69	0.59
52:1:1878:G:C2	52:1:1879:C:C2	2.91	0.59
52:1:2073:C:C2	52:1:2437:G:C2	2.90	0.59
52:1:1074:G:N2	52:1:1075:C:C2	2.70	0.59
53:2:13:U:C2	53:2:915:A:C6	2.88	0.59
52:1:1122:G:N2	52:1:1123:C:C2	2.70	0.59
52:1:1432:G:H2'	52:1:1433:A:C8	2.38	0.59
52:1:784:G:H5'	52:1:785:G:OP1	2.03	0.59
52:1:269:C:C2	52:1:424:G:C2	2.91	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:21:G:H2'	53:2:22:G:C8	2.38	0.58
52:1:2290:G:H2'	52:1:2291:U:O4'	2.03	0.58
53:2:514:C:C4	53:2:537:G:N1	2.71	0.58
52:1:2043:C:N3	52:1:2777:G:C2	2.72	0.58
57:6:41:C:N4	57:6:42:C:N4	2.51	0.58
1:B:210:ALA:HA	1:B:213:TRP:CE3	2.39	0.58
53:2:1442:G:N2	53:2:1443:C:C2	2.72	0.58
52:1:1208:C:C2	52:1:1239:G:C2	2.92	0.58
53:2:128:G:C2	53:2:234:C:C2	2.92	0.58
52:1:207:A:H2'	52:1:208:C:O4'	2.04	0.58
52:1:2320:U:O2	52:1:2333:A:N6	2.37	0.58
52:1:1006:C:C2	52:1:1138:G:C2	2.91	0.57
53:2:1114:C:C2	53:2:1187:G:C2	2.92	0.57
53:2:201:G:HO2'	53:2:469:C:HO2'	1.50	0.57
53:2:532:A:N6	53:2:1206:G:O2'	2.38	0.57
52:1:2070:A:H2'	52:1:2071:A:O4'	2.04	0.57
52:1:2694:G:H2'	52:1:2695:U:O4'	2.05	0.57
52:1:86:G:N2	52:1:97:C:C2	2.72	0.57
53:2:945:G:C2	53:2:946:A:C8	2.92	0.57
52:1:2043:C:C5	52:1:2777:G:C4	2.92	0.57
53:2:235:C:H2'	53:2:236:A:C8	2.39	0.57
53:2:568:G:C2	53:2:883:C:C2	2.92	0.57
52:1:639:U:H2'	52:1:640:C:C6	2.40	0.57
53:2:1510:C:C2	53:2:1526:G:N2	2.72	0.57
53:2:24:U:C4	53:2:559:A:C6	2.93	0.57
52:1:1129:A:O2'	52:1:2515:C:O2	2.21	0.57
52:1:764:A:N7	52:1:1775:U:O2	2.38	0.57
53:2:502:A:H2'	53:2:503:C:O4'	2.05	0.57
2:C:186:LEU:HD21	15:P:4:ILE:HG21	1.87	0.57
52:1:1555:G:N2	52:1:1556:C:C2	2.73	0.57
53:2:50:A:O2'	53:2:360:G:N2	2.36	0.57
53:2:404:G:N2	53:2:498:A:O2'	2.37	0.57
53:2:500:G:C6	53:2:501:C:N4	2.72	0.57
52:1:1195:G:N2	52:1:1196:C:C2	2.73	0.57
53:2:24:U:C5	53:2:559:A:N6	2.72	0.57
52:1:1021:A:N6	52:1:1141:U:N3	2.53	0.57
52:1:2298:A:C4	52:1:2321:U:C4	2.92	0.57
53:2:126:G:H5'	53:2:633:G:N2	2.20	0.57
53:2:184:G:N2	53:2:194:C:C2	2.73	0.57
53:2:22:G:C6	53:2:23:C:C4	2.93	0.57
52:1:2839:G:C6	52:1:2840:C:C4	2.92	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:921:U:H2'	53:2:922:G:O4'	2.05	0.56
53:2:986:U:H2'	53:2:987:G:O4'	2.04	0.56
57:6:24:G:C6	57:6:25:C:C4	2.93	0.56
11:L:95:LEU:HD11	11:L:125:LEU:HD21	1.87	0.56
52:1:764:A:N7	52:1:1776:G:H1'	2.21	0.56
53:2:942:G:C2	53:2:1342:C:C2	2.93	0.56
53:2:798:U:H2'	53:2:799:G:O4'	2.05	0.56
52:1:1099:G:N2	52:1:1100:C:C2	2.74	0.56
52:1:1038:G:C2	52:1:1118:C:O2	2.58	0.56
53:2:514:C:C4	53:2:537:G:C6	2.93	0.56
52:1:2328:A:H2'	52:1:2329:U:C6	2.40	0.56
52:1:2693:G:N2	52:1:2717:C:C2	2.74	0.56
52:1:875:G:C2	52:1:903:C:C2	2.94	0.56
18:S:24:ILE:HD13	18:S:36:LEU:HD11	1.87	0.56
52:1:1350:C:C2	52:1:1382:G:N2	2.73	0.56
53:2:37:U:H2'	53:2:37:U:O2	2.04	0.56
53:2:911:U:H2'	53:2:912:C:C6	2.40	0.56
53:2:481:G:O2'	53:2:483:C:N4	2.38	0.56
52:1:1891:G:C6	52:1:1892:C:C4	2.94	0.56
52:1:1846:G:C2	52:1:1895:C:C2	2.94	0.56
52:1:1837:C:C2	52:1:1904:G:C2	2.94	0.56
52:1:1878:G:C6	52:1:1879:C:C4	2.94	0.56
52:1:2297:A:H2	52:1:2321:U:C5	2.24	0.56
52:1:1297:C:OP1	52:1:2710:C:H4'	2.05	0.56
52:1:404:A:O2'	52:1:405:U:OP2	2.19	0.56
52:1:948:C:H1'	52:1:984:A:C8	2.41	0.56
52:1:94:A:H2'	52:1:95:A:C8	2.41	0.56
52:1:1459:G:C2	52:1:1461:C:C2	2.94	0.55
52:1:2261:C:C2	52:1:2280:G:N2	2.74	0.55
52:1:2697:G:H2'	52:1:2698:U:O4'	2.06	0.55
52:1:301:G:C2	52:1:302:C:C2	2.94	0.55
53:2:1365:G:C6	53:2:1366:C:C4	2.94	0.55
53:2:1510:C:C2	53:2:1526:G:C2	2.94	0.55
53:2:620:C:H2'	53:2:621:A:O4'	2.05	0.55
57:6:24:G:H2'	57:6:25:C:O4'	2.06	0.55
1:B:252:THR:HG21	52:1:1824:G:O2'	2.06	0.55
53:2:568:G:N2	53:2:883:C:C2	2.74	0.55
52:1:1074:G:C6	52:1:1075:C:N4	2.75	0.55
52:1:1327:A:H2'	52:1:1328:A:O4'	2.06	0.55
52:1:1794:A:H2'	52:1:1795:C:C6	2.42	0.55
52:1:2525:G:C2	52:1:2539:C:C2	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:126:G:H5'	53:2:633:G:H21	1.71	0.55
52:1:1011:G:C2	52:1:1013:C:C2	2.94	0.55
53:2:937:A:N6	53:2:1345:U:O4	2.34	0.55
53:2:774:G:C2	53:2:806:C:C2	2.94	0.55
52:1:1405:U:N3	52:1:1406:U:C4	2.75	0.55
52:1:1989:G:H2'	52:1:1990:C:O4'	2.06	0.55
52:1:2031:A:O2'	52:1:2454:G:N2	2.40	0.55
52:1:2415:G:C6	52:1:2416:C:C4	2.94	0.55
52:1:580:U:H2'	52:1:581:C:C6	2.42	0.55
52:1:978:G:C2	52:1:986:C:C2	2.93	0.55
53:2:391:G:H2'	53:2:392:C:O4'	2.07	0.55
54:3:16:G:N2	54:3:17:C:C2	2.75	0.55
55:4:44:G:H2'	55:4:44:G:N3	2.22	0.55
52:1:1351:C:C2	52:1:1381:G:C2	2.95	0.55
52:1:2852:G:C6	52:1:2853:C:C4	2.95	0.55
53:2:1242:G:C6	53:2:1243:C:C4	2.95	0.55
53:2:1352:C:N3	53:2:1371:G:C6	2.74	0.55
53:2:446:G:N2	53:2:489:C:C2	2.74	0.55
52:1:2273:A:H2'	52:1:2274:A:C8	2.41	0.55
52:1:36:G:N3	52:1:450:G:O2'	2.39	0.55
52:1:992:C:C2	52:1:1163:G:C2	2.95	0.55
52:1:2643:G:C2	52:1:2772:C:C2	2.95	0.55
53:2:585:G:C6	53:2:586:C:C4	2.95	0.55
56:5:31:G:N2	56:5:40:C:C2	2.75	0.55
52:1:1416:G:C4	52:1:1417:C:C5	2.95	0.55
52:1:2283:C:C2	52:1:2389:G:C2	2.95	0.55
52:1:68:G:C6	52:1:69:C:C4	2.95	0.55
53:2:1476:A:H2'	53:2:1477:U:O4'	2.06	0.55
54:3:71:C:C2	54:3:106:G:C2	2.95	0.55
55:4:36:A:N1	58:7:14:A:C6	2.75	0.55
55:4:36:A:C2	58:7:14:A:N1	2.75	0.55
52:1:49:A:N7	52:1:120:U:O2	2.40	0.55
52:1:1956:U:O2	52:1:1985:C:H4'	2.07	0.55
53:2:506:G:C6	53:2:507:C:N3	2.75	0.55
53:2:544:G:H2'	53:2:545:C:O4'	2.07	0.55
53:2:13:U:C2	53:2:915:A:N7	2.74	0.55
56:5:59:A:O2'	56:5:60:U:O5'	2.23	0.54
52:1:1914:C:O2	52:1:1914:C:O4'	2.26	0.54
52:1:2074:U:H3	52:1:2435:A:H2	1.52	0.54
52:1:2514:U:H2'	52:1:2515:C:C6	2.42	0.54
52:1:2620:C:H2'	52:1:2621:G:O4'	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:49:A:N6	52:1:120:U:C2	2.73	0.54
53:2:651:C:N4	53:2:753:A:OP2	2.40	0.54
5:F:24:ILE:HD13	5:F:72:LEU:HD21	1.89	0.54
17:R:51:VAL:HG12	17:R:52:PRO:HD3	1.88	0.54
52:1:1767:G:C2	52:1:1986:C:C2	2.95	0.54
52:1:2515:C:C2	52:1:2570:G:C2	2.95	0.54
52:1:588:U:H2'	52:1:589:U:C6	2.42	0.54
52:1:840:C:O2	52:1:939:G:C2	2.61	0.54
53:2:1424:U:H2'	53:2:1425:U:O4'	2.07	0.54
53:2:180:U:C4	53:2:181:A:N7	2.75	0.54
53:2:767:A:H2'	53:2:768:A:O4'	2.06	0.54
52:1:1186:G:H2'	52:1:1187:G:O4'	2.08	0.54
5:F:9:VAL:HG23	5:F:69:ARG:HD2	1.89	0.54
52:1:2221:G:C6	52:1:2222:C:C4	2.95	0.54
16:Q:57:PHE:HB3	16:Q:61:TRP:CZ2	2.42	0.54
22:W:37:ILE:HG21	22:W:80:ILE:HG21	1.90	0.54
52:1:2415:G:C2	52:1:2416:C:C2	2.96	0.54
53:2:203:G:N2	53:2:215:C:C2	2.76	0.54
53:2:408:A:H2'	53:2:409:U:O4'	2.08	0.54
53:2:827:U:O4	53:2:872:A:C2	2.59	0.54
18:S:13:SER:HB3	52:1:1266:G:O6	2.07	0.54
52:1:1949:G:C2	52:1:1958:C:C2	2.96	0.54
52:1:233:A:O5'	52:1:233:A:H8	1.91	0.54
52:1:559:G:C6	52:1:560:C:C4	2.96	0.54
53:2:215:C:H2'	53:2:216:U:O4'	2.08	0.54
1:B:221:ARG:NE	52:1:1827:U:OP2	2.41	0.54
52:1:1139:G:N2	52:1:1140:C:C2	2.76	0.54
52:1:1232:G:C6	52:1:1233:C:C4	2.96	0.54
52:1:1665:A:H2'	52:1:1666:G:O4'	2.08	0.54
52:1:2013:A:N6	52:1:2613:U:N3	2.41	0.54
53:2:130:A:N3	53:2:263:A:O2'	2.34	0.54
55:4:10:G:N2	55:4:11:C:C2	2.76	0.54
52:1:2714:G:C6	52:1:2715:C:C4	2.96	0.54
52:1:2839:G:C2	52:1:2840:C:C2	2.95	0.54
53:2:391:G:C6	53:2:392:C:N3	2.76	0.54
57:6:71:G:C6	57:6:72:C:C4	2.95	0.54
52:1:875:G:N2	52:1:903:C:C2	2.77	0.53
53:2:827:U:C4	53:2:872:A:N1	2.74	0.53
52:1:55:G:C2	52:1:116:C:C2	2.96	0.53
52:1:1891:G:C2	52:1:1892:C:C2	2.97	0.53
52:1:266:G:C6	52:1:267:C:C4	2.96	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:2445:2MG:HM23	52:1:2446:G:H1'	1.89	0.53
52:1:2498:OMC:HM22	52:1:2499:C:O4'	2.09	0.53
53:2:23:C:C4	53:2:24:U:C5	2.96	0.53
53:2:381:C:H2'	53:2:382:A:O4'	2.08	0.53
53:2:881:G:C6	53:2:882:C:C4	2.96	0.53
10:K:113:MET:O	10:K:116:ILE:HG13	2.09	0.53
52:1:1195:G:N1	52:1:1196:C:C4	2.77	0.53
52:1:153:U:C2	52:1:173:A:N1	2.77	0.53
52:1:954:G:C2	52:1:964:C:C2	2.97	0.53
53:2:442:G:N2	53:2:443:C:C2	2.76	0.53
53:2:548:G:C6	53:2:549:C:C4	2.97	0.53
53:2:585:G:H2'	53:2:586:C:O4'	2.09	0.53
52:1:1775:U:H2'	52:1:1776:G:O4'	2.09	0.53
52:1:978:G:N2	52:1:986:C:C2	2.76	0.53
53:2:976:G:C8	53:2:1358:U:O2	2.61	0.53
52:1:1011:G:C6	52:1:1013:C:C4	2.96	0.53
52:1:1021:A:H3'	52:1:1021:A:N3	2.23	0.53
52:1:1416:G:C6	52:1:1417:C:N4	2.76	0.53
52:1:1964:G:N1	52:1:1967:C:C4	2.77	0.53
52:1:2043:C:N4	52:1:2777:G:C5	2.77	0.53
52:1:2648:G:C6	52:1:2649:C:C4	2.97	0.53
53:2:646:G:C6	53:2:647:C:C4	2.97	0.53
55:4:37:A:C5	58:7:13:A:N6	2.77	0.53
56:5:22:G:C6	56:5:23:C:N4	2.76	0.53
57:6:24:G:C2	57:6:25:C:C2	2.97	0.53
52:1:659:G:C6	52:1:660:C:C4	2.97	0.53
53:2:213:G:C8	53:2:214:C:C5	2.97	0.53
59:8:116:ILE:HA	59:8:119:LEU:CB	2.38	0.53
52:1:1421:G:C2	52:1:1422:G:C8	2.97	0.53
52:1:305:C:C2	52:1:313:G:C2	2.97	0.53
53:2:61:G:H2'	53:2:62:U:O4'	2.09	0.53
53:2:778:G:C6	53:2:779:C:C4	2.97	0.53
53:2:915:A:N6	53:2:916:U:C4	2.77	0.53
52:1:1707:G:C6	52:1:1708:C:C4	2.97	0.53
52:1:2300:C:H2'	52:1:2301:C:C6	2.43	0.53
52:1:649:G:C6	52:1:650:C:C4	2.97	0.53
52:1:763:G:C2	52:1:765:C:C2	2.96	0.53
53:2:1332:A:H2'	53:2:1333:A:O4'	2.09	0.53
52:1:1028:A:N3	52:1:2486:C:O2'	2.35	0.53
52:1:2190:G:H2'	52:1:2191:A:O4'	2.09	0.53
52:1:2331:G:C2	52:1:2332:C:C2	2.97	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:84:ARG:HB2	18:S:96:ILE:HD13	1.91	0.53
21:V:72:VAL:HG12	21:V:93:ARG:HA	1.91	0.53
52:1:1425:G:H2'	52:1:1426:G:C8	2.45	0.52
52:1:1436:G:C6	52:1:1437:C:C4	2.97	0.52
53:2:946:A:O2'	53:2:1333:A:N3	2.32	0.52
53:2:1434:A:H2'	53:2:1435:G:O4'	2.09	0.52
53:2:604:G:H2'	53:2:605:U:O4'	2.09	0.52
52:1:1907:G:C6	52:1:1908:C:C4	2.98	0.52
52:1:187:G:C2	52:1:210:C:C2	2.96	0.52
52:1:2557:G:H2'	52:1:2558:C:C6	2.44	0.52
52:1:2607:G:H2'	52:1:2608:G:O4'	2.10	0.52
52:1:697:G:H2'	52:1:698:C:O4'	2.09	0.52
54:3:16:G:C6	54:3:17:C:C5	2.98	0.52
54:3:16:G:N1	54:3:17:C:C4	2.78	0.52
57:6:1:G:C6	57:6:2:C:C4	2.97	0.52
52:1:1319:C:C2	52:1:1334:G:C2	2.97	0.52
53:2:337:G:H2'	53:2:338:A:C8	2.44	0.52
52:1:2547:A:H2'	52:1:2548:U:C6	2.44	0.52
52:1:2689:U:O2	52:1:2713:U:H5"	2.09	0.52
52:1:2715:C:C4	52:1:2716:C:C5	2.97	0.52
52:1:289:G:H2'	52:1:290:U:O4'	2.09	0.52
53:2:1426:G:C2	53:2:1427:C:C2	2.98	0.52
53:2:24:U:O4	53:2:559:A:C6	2.63	0.52
53:2:734:G:C6	53:2:735:C:C4	2.98	0.52
52:1:1099:G:N1	52:1:1100:C:C4	2.77	0.52
52:1:2852:G:C2	52:1:2853:C:C2	2.98	0.52
52:1:68:G:C2	52:1:69:C:C2	2.97	0.52
52:1:816:C:C2	52:1:1192:G:N2	2.78	0.52
52:1:1405:U:O2	52:1:1406:U:C2	2.63	0.52
52:1:2692:G:H4'	52:1:2870:C:O2	2.09	0.52
53:2:622:A:C8	53:2:623:C:C5	2.97	0.52
53:2:650:G:C6	53:2:651:C:C4	2.98	0.52
53:2:786:G:N2	53:2:797:C:C2	2.78	0.52
52:1:2207:C:C2	52:1:2218:G:C2	2.97	0.52
52:1:2331:G:C6	52:1:2332:C:N3	2.78	0.52
53:2:1225:A:H2'	53:2:1226:C:C5	2.44	0.52
52:1:1071:G:C2	52:1:1072:C:N3	2.78	0.52
52:1:1268:A:H2'	52:1:1269:A:O4'	2.09	0.52
52:1:178:G:C6	52:1:179:C:C4	2.98	0.52
52:1:350:G:C6	52:1:351:C:C4	2.97	0.52
52:1:659:G:C2	52:1:660:C:C2	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:17:U:H2'	53:2:18:C:C6	2.45	0.52
53:2:354:G:N1	53:2:355:C:C4	2.77	0.52
53:2:613:C:H2'	53:2:614:C:C6	2.45	0.52
53:2:633:G:C2	53:2:634:C:C2	2.97	0.52
55:4:40:C:H2'	55:4:41:C:C6	2.45	0.52
59:8:266:LYS:HE3	59:8:270:PHE:HA	1.91	0.52
18:S:46:LEU:O	18:S:50:VAL:HG23	2.10	0.52
52:1:108:G:C6	52:1:109:C:C4	2.98	0.52
52:1:2574:G:C6	52:1:2575:C:C4	2.97	0.52
53:2:1426:G:C6	53:2:1427:C:C4	2.98	0.52
53:2:22:G:C2	53:2:23:C:C2	2.98	0.52
52:1:1477:A:N6	52:1:1514:G:O2'	2.42	0.52
52:1:2049:G:C6	52:1:2050:C:C4	2.98	0.52
52:1:2520:C:C6	52:1:2567:G:H1'	2.45	0.52
52:1:807:U:H2'	52:1:808:G:O4'	2.10	0.52
53:2:1365:G:C2	53:2:1366:C:C2	2.98	0.52
53:2:518:C:H2'	53:2:530:G:C8	2.44	0.52
53:2:827:U:H3	53:2:872:A:H61	1.57	0.52
53:2:895:G:C6	53:2:896:C:C4	2.98	0.52
1:B:208:ALA:CB	52:1:764:A:C2	2.93	0.52
11:L:67:THR:HG21	52:1:244:A:H5"	1.92	0.52
52:1:1351:C:O2	52:1:1381:G:C2	2.64	0.51
52:1:313:G:C6	52:1:314:C:C4	2.98	0.51
53:2:1106:G:C6	53:2:1107:C:C4	2.98	0.51
53:2:582:C:N3	53:2:760:G:C6	2.78	0.51
54:3:61:G:C6	54:3:62:C:C4	2.98	0.51
52:1:1149:G:H2'	52:1:1150:C:C6	2.46	0.51
52:1:1660:G:N2	52:1:2001:C:C2	2.77	0.51
52:1:2412:A:H2'	52:1:2413:G:O4'	2.09	0.51
52:1:2648:G:C2	52:1:2649:C:C2	2.98	0.51
52:1:2705:A:O2'	52:1:2852:G:OP1	2.17	0.51
53:2:555:U:H2'	53:2:556:C:C6	2.45	0.51
57:6:71:G:C2	57:6:72:C:C2	2.97	0.51
59:8:433:SER:O	59:8:437:HIS:ND1	2.44	0.51
59:8:616:ILE:HG22	59:8:617:PRO:HD3	1.91	0.51
52:1:122:G:H2'	52:1:123:G:O4'	2.10	0.51
52:1:2618:G:C6	52:1:2619:C:C4	2.98	0.51
53:2:1050:G:N2	53:2:1051:C:C2	2.78	0.51
53:2:827:U:H3	53:2:872:A:N6	2.08	0.51
52:1:1153:C:H2'	52:1:1154:G:O4'	2.10	0.51
52:1:1520:U:O4	52:1:1521:G:C6	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:2397:G:C2	52:1:2420:C:C2	2.98	0.51
52:1:539:G:C6	52:1:540:C:C4	2.99	0.51
52:1:829:A:N7	52:1:2247:A:O2'	2.43	0.51
52:1:856:G:N2	52:1:922:C:C2	2.79	0.51
53:2:1298:U:O4'	53:2:1298:U:O2	2.27	0.51
53:2:504:C:C2	53:2:542:G:N2	2.78	0.51
20:U:28:VAL:HB	20:U:34:VAL:HG12	1.92	0.51
52:1:2509:G:C6	52:1:2510:C:C4	2.99	0.51
52:1:2525:G:N2	52:1:2539:C:C2	2.79	0.51
53:2:500:G:C2	53:2:501:C:N3	2.79	0.51
53:2:585:G:C2	53:2:586:C:C2	2.99	0.51
53:2:734:G:C2	53:2:735:C:C2	2.99	0.51
52:1:991:C:C4	52:1:1185:G:C6	2.99	0.51
52:1:15:G:C6	52:1:16:C:C4	2.98	0.51
52:1:26:G:C6	52:1:27:G:N1	2.78	0.51
52:1:297:G:H2'	52:1:298:G:O4'	2.11	0.51
52:1:49:A:C6	52:1:177:G:C5	2.99	0.51
53:2:548:G:H2'	53:2:549:C:O4'	2.11	0.51
56:5:31:G:C2	56:5:40:C:C2	2.99	0.51
52:1:1449:G:N2	52:1:1463:C:C2	2.79	0.51
52:1:2024:G:C6	52:1:2025:C:C4	2.99	0.51
52:1:2454:G:C2	52:1:2499:C:C2	2.99	0.51
52:1:2831:G:OP1	52:1:2834:G:H4'	2.11	0.51
52:1:586:A:N1	52:1:809:G:O2'	2.39	0.51
52:1:611:C:C2	52:1:618:G:N2	2.79	0.51
53:2:613:C:C2	53:2:628:G:C2	2.99	0.51
1:B:205:LEU:HB3	1:B:210:ALA:HB3	1.91	0.51
52:1:1277:G:H2'	52:1:1278:C:O4'	2.11	0.51
52:1:565:C:H2'	52:1:566:U:O4'	2.10	0.51
53:2:1242:G:C2	53:2:1243:C:C2	2.99	0.51
53:2:778:G:H2'	53:2:779:C:O4'	2.11	0.51
57:6:30:G:N1	57:6:41:C:C2	2.79	0.51
52:1:1361:G:C6	52:1:1362:C:N4	2.79	0.51
52:1:1424:G:C2	52:1:1575:C:C2	2.98	0.51
52:1:178:G:H2'	52:1:179:C:O4'	2.10	0.51
52:1:381:G:N2	52:1:394:C:C2	2.79	0.51
52:1:649:G:H2'	52:1:650:C:O4'	2.10	0.51
53:2:1064:G:O2'	53:2:1190:G:N2	2.44	0.51
53:2:399:G:H2'	53:2:400:C:C6	2.46	0.51
53:2:663:A:H2'	53:2:664:G:O4'	2.11	0.51
52:1:1067:A:H1'	57:6:56:C:C2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:103:LEU:HA	4:E:107:ALA:HB3	1.92	0.51
11:L:21:ARG:NH1	52:1:587:C:OP2	2.44	0.51
52:1:1063:G:C2	52:1:1064:C:C2	2.99	0.51
52:1:1375:U:N3	52:1:1376:C:C5	2.79	0.51
52:1:1352:U:O2'	52:1:1570:A:N3	2.35	0.51
52:1:81:G:C2	52:1:106:C:C2	2.99	0.51
53:2:1352:C:C2	53:2:1371:G:N1	2.78	0.51
53:2:13:U:C2	53:2:915:A:C5	2.98	0.51
53:2:21:G:C2	53:2:22:G:C5	2.99	0.51
53:2:349:A:H2'	53:2:350:G:O4'	2.11	0.51
10:K:78:ARG:NH2	52:1:2685:G:OP1	2.44	0.51
53:2:1305:G:HO2'	53:2:1306:A:H8	1.57	0.50
53:2:13:U:O2	53:2:915:A:C5	2.62	0.50
56:5:56:C:H2'	56:5:57:A:C8	2.46	0.50
52:1:2698:U:H2'	52:1:2699:C:C6	2.47	0.50
52:1:622:G:N2	52:1:623:C:C2	2.80	0.50
53:2:384:G:C2	53:2:385:C:C4	2.99	0.50
57:6:30:G:C2	57:6:41:C:O2	2.64	0.50
25:Z:7:ILE:HD13	25:Z:27:LEU:HD22	1.93	0.50
52:1:1416:G:C2	52:1:1417:C:C2	3.00	0.50
1:B:156:ARG:NH1	52:1:1818:U:OP2	2.44	0.50
52:1:2464:G:C6	52:1:2465:C:C4	2.99	0.50
52:1:56:A:H2'	52:1:57:C:O4'	2.12	0.50
52:1:692:C:C2	52:1:771:G:N2	2.80	0.50
53:2:56:U:H2'	53:2:57:G:C8	2.46	0.50
54:3:61:G:C2	54:3:62:C:C2	2.99	0.50
57:6:1:G:C2	57:6:2:C:C2	2.99	0.50
2:C:121:THR:HB	2:C:127:PHE:CD2	2.46	0.50
52:1:1074:G:C2	52:1:1075:C:C4	2.99	0.50
53:2:384:G:N2	53:2:385:C:C2	2.79	0.50
53:2:736:C:H2'	53:2:737:C:C6	2.47	0.50
52:1:1206:G:C6	52:1:1207:C:C4	3.00	0.50
52:1:1560:G:C6	52:1:1561:C:C4	3.00	0.50
52:1:1707:G:C2	52:1:1708:C:C2	3.00	0.50
52:1:2628:C:H3'	52:1:2629:U:H5'	1.92	0.50
52:1:2862:G:C6	52:1:2863:C:C4	2.99	0.50
52:1:36:G:C2	52:1:445:C:C2	3.00	0.50
52:1:997:G:N2	52:1:998:C:C2	2.78	0.50
53:2:778:G:C2	53:2:779:C:C2	3.00	0.50
52:1:2702:G:C6	52:1:2703:C:C4	3.00	0.50
52:1:406:G:H2'	52:1:407:G:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:68:G:H2'	52:1:69:C:O4'	2.12	0.50
52:1:701:G:C2	52:1:732:C:C2	3.00	0.50
52:1:763:G:C6	52:1:765:C:C4	3.00	0.50
53:2:235:C:H2'	53:2:236:A:H8	1.75	0.50
53:2:384:G:C4	53:2:385:C:C5	3.00	0.50
53:2:39:G:H2'	53:2:40:C:O4'	2.11	0.50
53:2:646:G:C2	53:2:647:C:C2	3.00	0.50
53:2:669:G:N2	53:2:738:C:C2	2.79	0.50
4:E:12:VAL:HG13	4:E:172:ALA:HB1	1.93	0.50
52:1:1076:C:O2'	52:1:1077:A:O4'	2.29	0.50
52:1:1459:G:C6	52:1:1461:C:C4	3.00	0.50
52:1:1660:G:C2	52:1:2001:C:C2	2.99	0.50
53:2:39:G:C6	53:2:40:C:C4	2.99	0.50
53:2:544:G:C6	53:2:545:C:C4	3.00	0.50
54:3:85:G:C2	54:3:92:C:C2	3.00	0.50
5:F:24:ILE:HD11	5:F:43:VAL:HG11	1.94	0.50
52:1:118:A:C8	52:1:120:U:N3	2.80	0.50
52:1:2309:A:H2'	52:1:2310:C:H5'	1.93	0.50
52:1:543:G:C6	52:1:544:C:C4	2.99	0.50
52:1:1356:G:C2	52:1:1376:C:O2	2.65	0.50
52:1:1356:G:C6	52:1:1357:C:C4	3.00	0.50
52:1:2128:G:C6	52:1:2129:C:C4	3.00	0.50
52:1:2221:G:C2	52:1:2222:C:C2	3.00	0.50
52:1:954:G:O2'	52:1:2274:A:N1	2.41	0.50
52:1:2704:C:H2'	52:1:2705:A:O4'	2.12	0.50
52:1:2846:G:H2'	52:1:2847:U:O4'	2.12	0.50
53:2:1127:G:C6	53:2:1128:C:C4	3.00	0.50
53:2:1459:G:C6	53:2:1460:C:C4	2.99	0.50
53:2:310:G:C6	53:2:311:C:C4	3.00	0.50
57:6:10:G:C6	57:6:11:C:N4	2.80	0.50
52:1:1842:G:C6	52:1:1843:C:C4	3.00	0.49
52:1:252:G:C6	52:1:253:C:C4	3.00	0.49
52:1:2646:C:C6	52:1:2646:C:O5'	2.65	0.49
52:1:2693:G:C2	52:1:2717:C:C2	3.01	0.49
52:1:313:G:C2	52:1:314:C:C2	3.00	0.49
53:2:37:U:C4	53:2:38:G:C8	3.00	0.49
52:1:2283:C:C4	52:1:2389:G:C6	3.00	0.49
52:1:237:C:C2	52:1:261:G:N2	2.81	0.49
52:1:856:G:H2'	52:1:857:G:C8	2.48	0.49
53:2:1233:G:N2	53:2:1234:C:C2	2.79	0.49
53:2:781:A:O2'	53:2:1522:U:O2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:544:G:C2	53:2:545:C:C2	3.01	0.49
53:2:633:G:C6	53:2:634:C:C4	3.00	0.49
53:2:693:G:C5	58:7:13:A:H1'	2.48	0.49
53:2:809:G:C6	53:2:810:C:C4	3.00	0.49
53:2:966:2MG:HM23	53:2:967:5MC:C1'	2.42	0.49
54:3:24:G:N7	54:3:56:G:H2'	2.28	0.49
57:6:35:A:H2'	57:6:36:A:O4'	2.11	0.49
57:6:71:G:H2'	57:6:72:C:H6	1.77	0.49
3:D:145:ASP:HA	3:D:166:LYS:HB3	1.92	0.49
20:U:33:LYS:HB3	20:U:64:ALA:HB1	1.93	0.49
52:1:1125:G:C6	52:1:1126:A:N6	2.80	0.49
52:1:1973:G:C6	52:1:1974:C:C4	3.00	0.49
52:1:747:5MU:O2	52:1:2014:A:H1'	2.11	0.49
52:1:2046:G:C6	52:1:2047:C:C4	2.99	0.49
52:1:301:G:C4	52:1:302:C:C5	3.00	0.49
52:1:348:A:H2'	52:1:349:U:O4'	2.12	0.49
56:5:64:G:C6	56:5:65:C:C4	3.00	0.49
52:1:815:C:C2	52:1:1193:G:N2	2.80	0.49
52:1:2337:G:N1	52:1:2338:C:C4	2.80	0.49
52:1:2522:U:O2'	52:1:2647:U:OP1	2.25	0.49
52:1:273:G:C6	52:1:274:C:C4	2.99	0.49
53:2:369:G:C6	53:2:370:C:N4	2.81	0.49
53:2:514:C:N3	53:2:537:G:C2	2.81	0.49
52:1:1091:G:C6	52:1:1092:C:C4	3.01	0.49
52:1:1369:G:C6	52:1:1370:C:C4	3.00	0.49
52:1:1555:G:N1	52:1:1556:C:C4	2.81	0.49
52:1:46:G:C6	52:1:47:C:N4	2.80	0.49
52:1:649:G:C2	52:1:650:C:C2	3.00	0.49
53:2:1058:G:C2	53:2:1059:C:C2	3.01	0.49
53:2:827:U:C2	53:2:874:G:N2	2.80	0.49
53:2:895:G:C2	53:2:896:C:C2	3.01	0.49
2:C:62:LYS:N	2:C:63:PRO:CD	2.74	0.49
52:1:1540:G:C2	52:1:1541:C:C2	3.00	0.49
52:1:1570:A:H2'	52:1:1571:A:C8	2.47	0.49
52:1:2714:G:C2	52:1:2715:C:C2	3.01	0.49
52:1:191:A:H1'	52:1:679:C:H1'	1.94	0.49
18:S:17:VAL:HB	18:S:76:VAL:HG11	1.95	0.49
52:1:1163:G:C6	52:1:1164:C:C4	3.01	0.49
52:1:812:C:C4	52:1:1250:G:C6	3.00	0.49
52:1:2049:G:C2	52:1:2620:C:C2	3.01	0.49
52:1:764:A:H62	52:1:1776:G:C1'	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:514:C:C2	53:2:537:G:N2	2.80	0.49
54:3:84:G:C2	54:3:93:C:C2	3.01	0.49
13:N:55:ALA:O	13:N:56:LYS:C	2.50	0.49
52:1:1483:G:N1	52:1:1507:C:C2	2.81	0.49
52:1:1727:C:C2	52:1:1734:G:C2	3.01	0.49
52:1:19:A:H2'	52:1:20:C:C6	2.47	0.49
52:1:2043:C:C4	52:1:2777:G:C2	3.00	0.49
52:1:2128:G:C2	52:1:2129:C:C2	3.00	0.49
52:1:2331:G:C6	52:1:2332:C:C4	3.01	0.49
52:1:2435:A:C2	52:1:2436:G:C5	3.01	0.49
52:1:685:A:C2'	52:1:773:U:O4	2.61	0.49
52:1:893:C:H2'	52:1:894:U:O4'	2.13	0.49
53:2:128:G:N2	53:2:234:C:C2	2.81	0.49
52:1:1166:G:C6	52:1:1167:C:C4	3.01	0.49
52:1:1643:G:C6	52:1:1644:C:C4	3.01	0.49
52:1:1831:G:C6	52:1:1832:C:N4	2.81	0.49
52:1:1939:5MU:OP1	52:1:2604:U:O2'	2.30	0.49
52:1:2854:G:C6	52:1:2855:C:C4	3.01	0.49
52:1:885:C:C5	52:1:886:A:N7	2.81	0.49
53:2:1338:G:H2'	53:2:1339:A:C8	2.47	0.49
53:2:142:G:C2	53:2:222:C:C2	3.01	0.49
56:5:71:C:O2'	56:5:72:A:O4'	2.22	0.49
57:6:40:C:H2'	57:6:41:C:O4'	2.12	0.49
52:1:1009:A:N3	52:1:1153:C:O2'	2.32	0.49
52:1:1740:G:C6	52:1:1741:C:C4	3.01	0.49
52:1:1842:G:C2	52:1:1843:C:C2	3.01	0.49
52:1:2024:G:C2	52:1:2025:C:C2	3.01	0.49
52:1:2464:G:C2	52:1:2465:C:C2	3.01	0.49
52:1:622:G:C6	52:1:623:C:N4	2.81	0.49
52:1:693:A:H2'	52:1:694:U:O4'	2.13	0.49
53:2:1131:G:C2	53:2:1132:C:C2	3.01	0.49
53:2:1350:A:H2'	53:2:1351:U:O4'	2.13	0.49
53:2:39:G:C2	53:2:40:C:C2	3.01	0.49
56:5:20:H2U:H3'	56:5:21:A:H5"	1.95	0.49
9:J:113:PRO:HD3	52:1:529:A:OP2	2.12	0.49
52:1:184:C:H2'	52:1:185:G:C8	2.48	0.48
52:1:1907:G:C2	52:1:1908:C:C2	3.01	0.48
52:1:2083:G:C6	52:1:2084:C:C4	3.00	0.48
52:1:2294:G:C6	52:1:2295:C:C4	3.01	0.48
52:1:245:G:C6	52:1:246:C:C4	3.01	0.48
52:1:549:G:N2	52:1:550:C:C2	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:1014:A:H2'	53:2:1015:G:C8	2.48	0.48
53:2:402:G:C6	53:2:403:C:C4	3.00	0.48
53:2:713:G:H2'	53:2:714:G:C8	2.48	0.48
53:2:693:G:C4	58:7:13:A:H1'	2.48	0.48
59:8:141:ALA:HB2	59:8:407:TYR:CZ	2.48	0.48
4:E:12:VAL:HG13	4:E:172:ALA:CB	2.43	0.48
52:1:1511:G:C2	52:1:1512:C:C2	3.01	0.48
52:1:2379:G:C2	52:1:2380:C:C2	3.01	0.48
52:1:593:U:H2'	52:1:594:U:C6	2.48	0.48
53:2:373:A:O2'	53:2:451:A:N7	2.46	0.48
53:2:42:G:C6	53:2:43:C:C4	3.01	0.48
53:2:524:G:C2	53:2:525:C:N3	2.82	0.48
53:2:946:A:H2'	53:2:947:G:C8	2.49	0.48
52:1:1071:G:C6	52:1:1072:C:N4	2.81	0.48
52:1:1470:A:H2'	52:1:1471:G:O4'	2.13	0.48
52:1:1496:A:H2'	52:1:1498:C:C5	2.48	0.48
52:1:2702:G:C2	52:1:2703:C:C2	3.02	0.48
52:1:381:G:C2	52:1:394:C:C2	3.02	0.48
52:1:7:G:C6	52:1:8:C:C4	3.01	0.48
53:2:548:G:C2	53:2:549:C:C2	3.01	0.48
53:2:688:G:C6	53:2:689:C:C4	3.01	0.48
55:4:39:U:O2	55:4:39:U:O4'	2.31	0.48
13:N:45:ARG:O	13:N:48:VAL:HG22	6.39	0.48
52:1:1139:G:C6	52:1:1140:C:C4	3.01	0.48
52:1:1256:G:N2	52:1:1257:C:C2	2.81	0.48
52:1:1416:G:N2	52:1:1417:C:C2	2.82	0.48
52:1:2057:G:C2	52:1:2612:C:C2	3.02	0.48
52:1:2298:A:C4	52:1:2321:U:C5	3.02	0.48
52:1:2363:G:N2	52:1:2364:C:C2	2.81	0.48
52:1:2895:G:C2	52:1:2896:C:C2	3.01	0.48
52:1:425:G:C6	52:1:426:C:C4	3.01	0.48
52:1:907:G:C6	52:1:908:C:C4	3.01	0.48
53:2:1496:C:H2'	53:2:1497:G:O4'	2.12	0.48
53:2:303:A:H2'	53:2:304:U:O4'	2.14	0.48
53:2:335:C:H2'	53:2:336:A:C8	2.49	0.48
54:3:112:G:C2	54:3:113:C:C2	3.01	0.48
54:3:48:U:H2'	54:3:49:C:C6	2.49	0.48
56:5:15:C:H3'	56:5:16:C:O4'	2.14	0.48
57:6:30:G:C2	57:6:41:C:C2	3.00	0.48
52:1:1292:G:C6	52:1:1293:C:C4	3.01	0.48
52:1:1433:A:H2'	52:1:1434:A:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:1933:G:C6	52:1:1934:C:C4	3.01	0.48
52:1:622:G:C2	52:1:623:C:C2	3.01	0.48
52:1:1703:G:O3'	53:2:1429:A:O2'	2.31	0.48
53:2:247:G:C6	53:2:248:C:C4	3.02	0.48
53:2:881:G:C2	53:2:882:C:C2	3.01	0.48
54:3:2:G:N2	54:3:3:C:C2	2.81	0.48
55:4:30:G:N2	55:4:41:C:C2	2.82	0.48
59:8:683:ILE:O	59:8:686:ILE:HG22	2.14	0.48
1:B:212:ARG:HG3	52:1:764:A:H1'	1.96	0.48
1:B:14:ARG:NH2	52:1:1695:G:N7	2.59	0.48
52:1:317:G:C2	52:1:318:C:C2	3.02	0.48
52:1:365:U:H2'	52:1:366:C:C6	2.49	0.48
52:1:543:G:C2	52:1:544:C:C2	3.01	0.48
52:1:834:G:C2	52:1:835:C:C2	3.02	0.48
53:2:1218:C:H2'	53:2:1219:A:C8	2.49	0.48
53:2:1326:U:H2'	53:2:1327:C:C6	2.49	0.48
53:2:342:C:C2	53:2:348:G:C2	3.01	0.48
53:2:613:C:N3	53:2:628:G:C2	2.82	0.48
54:3:96:G:C6	54:3:97:C:C4	3.01	0.48
55:4:40:C:H2'	55:4:41:C:H6	1.77	0.48
59:8:622:VAL:HG13	59:8:652:ILE:HG23	1.95	0.48
3:D:161:ALA:CB	3:D:169:VAL:HG23	2.43	0.48
52:1:1301:A:N3	52:1:1301:A:H2'	2.28	0.48
52:1:1915:3TD:H2'	52:1:1916:A:O4'	2.13	0.48
52:1:2641:G:N2	52:1:2774:C:C2	2.82	0.48
52:1:2043:C:C2	52:1:2777:G:C2	3.01	0.48
2:C:66:GLY:HA3	52:1:2787:C:H5'	1.94	0.48
52:1:317:G:C6	52:1:318:C:C4	3.02	0.48
52:1:51:G:N2	52:1:120:U:O2	2.47	0.48
53:2:1131:G:C6	53:2:1132:C:C4	3.01	0.48
53:2:915:A:H2'	53:2:916:U:O4'	2.14	0.48
52:1:1643:G:C2	52:1:1644:C:C2	3.02	0.48
52:1:2043:C:C4	52:1:2777:G:C4	3.01	0.48
52:1:2524:G:C2	52:1:2540:C:C2	3.01	0.48
52:1:2795:C:C2	52:1:2802:G:N2	2.82	0.48
52:1:499:U:O4	52:1:500:G:C6	2.67	0.48
53:2:504:C:N3	53:2:542:G:C2	2.82	0.48
53:2:867:G:N2	53:2:868:C:C2	2.81	0.48
54:3:79:G:H2'	54:3:80:U:O4'	2.13	0.48
52:1:15:G:C2	52:1:16:C:C2	3.02	0.48
52:1:2618:G:C2	52:1:2619:C:C2	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:2686:G:H2'	52:1:2687:U:O4'	2.14	0.48
52:1:350:G:C2	52:1:351:C:C2	3.02	0.48
52:1:634:C:H2'	52:1:635:C:C6	2.49	0.48
52:1:928:A:H2'	52:1:929:U:O4'	2.14	0.48
53:2:24:U:H2'	53:2:25:C:C6	2.49	0.48
53:2:474:G:C6	53:2:475:C:N3	2.82	0.48
56:5:53:G:H2'	56:5:54:5MU:C6	2.48	0.48
57:6:28:G:C2	57:6:43:C:C2	3.02	0.48
23:X:32:ASN:O	23:X:52:SER:HA	2.13	0.48
53:2:1068:G:C6	53:2:1069:C:C4	3.02	0.48
53:2:774:G:N2	53:2:806:C:C2	2.82	0.48
53:2:838:G:C6	53:2:839:C:C4	3.01	0.48
54:3:112:G:C6	54:3:113:C:C4	3.02	0.48
13:N:24:MET:HG2	13:N:44:LEU:HD22	1.95	0.48
52:1:1042:G:C6	52:1:1043:C:C4	3.02	0.47
52:1:2818:U:HO2'	52:1:2836:U:HO2'	1.57	0.47
52:1:327:G:C2	52:1:336:C:C2	3.02	0.47
52:1:539:G:C2	52:1:540:C:C2	3.02	0.47
52:1:559:G:C2	52:1:560:C:C2	3.02	0.47
52:1:989:G:OP1	52:1:1157:G:O2'	2.28	0.47
53:2:504:C:C2	53:2:542:G:C2	3.01	0.47
59:8:66:LEU:HD12	59:8:79:ALA:HB2	1.96	0.47
52:1:1074:G:C4	52:1:1075:C:C5	3.03	0.47
52:1:238:C:C2	52:1:260:G:C2	3.02	0.47
52:1:374:A:C2	52:1:375:G:H1'	2.50	0.47
52:1:55:G:N2	52:1:116:C:C2	2.82	0.47
53:2:1106:G:C2	53:2:1107:C:C2	3.02	0.47
53:2:1222:G:C6	53:2:1223:C:C4	3.02	0.47
53:2:1412:C:H2'	53:2:1413:A:C8	2.49	0.47
53:2:1459:G:C2	53:2:1460:C:C2	3.02	0.47
53:2:384:G:C2	53:2:385:C:N3	2.83	0.47
53:2:650:G:C2	53:2:651:C:C2	3.03	0.47
53:2:838:G:C2	53:2:839:C:C2	3.02	0.47
53:2:953:G:H2'	53:2:954:G:O4'	2.14	0.47
57:6:10:G:H2'	57:6:11:C:C6	2.49	0.47
59:8:137:ARG:HE	59:8:140:LEU:HD12	1.79	0.47
11:L:77:ILE:HD11	11:L:108:ALA:HB1	1.96	0.47
12:M:66:ARG:NH1	12:M:104:GLU:OE1	2.47	0.47
13:N:38:LEU:N	13:N:39:PRO:CD	2.76	0.47
23:X:32:ASN:HD22	23:X:53:ALA:HB2	1.79	0.47
25:Z:22:ALA:HB1	52:1:850:U:H5'	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:1011:G:C5	52:1:1013:C:C5	3.02	0.47
52:1:1573:G:C8	52:1:1574:C:C5	3.02	0.47
52:1:1662:U:H2'	52:1:1663:G:O4'	2.14	0.47
52:1:1703:G:H2'	52:1:1704:C:C6	2.49	0.47
52:1:2250:G:H8	52:1:2250:G:O5'	1.97	0.47
52:1:24:G:C2	52:1:517:C:C2	3.02	0.47
52:1:2646:C:O5'	52:1:2646:C:H6	1.98	0.47
53:2:1058:G:C6	53:2:1059:C:C4	3.02	0.47
53:2:227:G:H2'	53:2:228:A:O4'	2.14	0.47
53:2:369:G:C2	53:2:370:C:C4	3.03	0.47
53:2:629:A:H2'	53:2:630:A:O4'	2.14	0.47
53:2:884:U:H4'	53:2:885:G:H5"	1.96	0.47
59:8:624:PHE:CZ	59:8:651:ARG:HD3	2.49	0.47
14:O:53:THR:HG23	14:O:74:VAL:CG2	2.44	0.47
16:Q:82:GLY:HA2	16:Q:117:LEU:HD13	1.95	0.47
52:1:1369:G:C2	52:1:1370:C:C2	3.02	0.47
52:1:2242:G:H2'	52:1:2243:U:O4'	2.14	0.47
52:1:2574:G:C2	52:1:2575:C:C2	3.02	0.47
52:1:2854:G:C2	52:1:2855:C:C2	3.02	0.47
53:2:255:G:C2	53:2:272:C:C2	3.02	0.47
53:2:725:G:C6	53:2:726:C:C4	3.03	0.47
1:B:207:LYS:HB2	52:1:729:G:C5	2.50	0.47
52:1:1063:G:C5	52:1:1064:C:C5	3.02	0.47
52:1:1296:G:N2	52:1:1297:C:C2	2.83	0.47
52:1:1405:U:C2	52:1:1406:U:C5	3.02	0.47
52:1:2046:G:C2	52:1:2047:C:C2	3.02	0.47
52:1:2298:A:C5	52:1:2321:U:C4	3.02	0.47
52:1:2557:G:C2	52:1:2558:C:C2	3.02	0.47
52:1:2729:G:C2	52:1:2730:C:C2	3.02	0.47
52:1:273:G:C2	52:1:274:C:C2	3.02	0.47
52:1:2852:G:H2'	52:1:2853:C:O4'	2.15	0.47
52:1:445:C:N4	52:1:446:G:C6	2.82	0.47
53:2:982:U:H4'	53:2:983:A:O4'	2.14	0.47
52:1:1068:G:N2	52:1:1095:A:O2'	2.48	0.47
52:1:1122:G:N1	52:1:1123:C:C4	2.83	0.47
52:1:1511:G:C6	52:1:1512:C:C4	3.02	0.47
52:1:1678:A:H2'	52:1:1679:A:O4'	2.14	0.47
52:1:1873:G:C2	52:1:1874:C:C2	3.03	0.47
52:1:2308:G:O6	52:1:2311:A:N7	2.48	0.47
52:1:2489:U:C4	52:1:2490:G:C6	3.02	0.47
52:1:333:G:C6	52:1:334:C:C4	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:580:U:H2'	52:1:581:C:H6	1.78	0.47
53:2:1120:C:C2	53:2:1154:G:N2	2.83	0.47
53:2:1515:G:N2	53:2:1521:C:C2	2.83	0.47
3:D:31:VAL:HG21	3:D:104:ALA:CB	2.45	0.47
6:G:1:MET:HB3	6:G:3:VAL:HG23	1.96	0.47
52:1:1540:G:C6	52:1:1541:C:C4	3.02	0.47
52:1:178:G:C2	52:1:179:C:C2	3.03	0.47
52:1:1933:G:C2	52:1:1934:C:C2	3.03	0.47
52:1:2455:G:C6	52:1:2456:C:N4	2.83	0.47
52:1:2869:G:C2	52:1:2870:C:C2	3.02	0.47
52:1:784:G:C2	52:1:792:A:O4'	2.68	0.47
55:4:19:G:C6	55:4:56:C:N3	2.83	0.47
16:Q:47:TYR:O	16:Q:51:ARG:NE	2.34	0.47
52:1:108:G:C2	52:1:109:C:C2	3.03	0.47
52:1:1317:G:H2'	52:1:1318:U:O4'	2.14	0.47
52:1:2294:G:C2	52:1:2339:C:C2	3.02	0.47
52:1:2300:C:H2'	52:1:2301:C:H6	1.79	0.47
2:C:194:PRO:HA	52:1:2680:U:H5'	1.96	0.47
52:1:268:C:C2	52:1:425:G:C2	3.03	0.47
52:1:813:U:H2'	52:1:814:C:H6	1.79	0.47
53:2:1473:G:H2'	53:2:1474:U:O4'	2.14	0.47
53:2:976:G:C8	53:2:1358:U:C2	3.02	0.47
59:8:118:GLN:HA	59:8:121:ALA:HB3	1.97	0.47
52:1:1011:G:C4	52:1:1013:C:C6	3.02	0.47
52:1:1479:G:C2	52:1:1480:C:C2	3.03	0.47
52:1:1893:C:C5	52:1:1894:C:C5	3.02	0.47
52:1:1964:G:C2	52:1:1967:C:C4	3.02	0.47
53:2:755:G:C6	53:2:756:C:C4	3.02	0.47
10:K:22:ILE:HD11	10:K:57:VAL:HG13	1.96	0.47
25:Z:27:LEU:O	25:Z:38:ARG:NE	2.47	0.47
52:1:1091:G:C2	52:1:1092:C:C2	3.03	0.47
52:1:1228:G:C2	52:1:1229:C:C2	3.03	0.47
52:1:123:G:C2	52:1:129:C:C2	3.03	0.47
52:1:1873:G:C6	52:1:1874:C:C4	3.03	0.47
52:1:1268:A:H1'	52:1:2613:U:N3	2.30	0.47
52:1:266:G:C2	52:1:267:C:C2	3.02	0.47
52:1:622:G:C6	52:1:623:C:C4	3.03	0.47
53:2:1323:G:H2'	53:2:1324:A:C8	2.50	0.47
53:2:369:G:N1	53:2:370:C:C4	2.83	0.47
53:2:399:G:C2	53:2:400:C:C2	3.02	0.47
52:1:1228:G:C6	52:1:1229:C:C4	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:1232:G:C2	52:1:1233:C:C2	3.03	0.47
52:1:1560:G:C2	52:1:1561:C:C2	3.03	0.47
52:1:1703:G:C6	52:1:1704:C:C4	3.03	0.47
52:1:2201:G:H2'	52:1:2202:U:O4'	2.15	0.47
52:1:2658:C:H2'	52:1:2659:G:O4'	2.15	0.47
52:1:553:G:H2'	52:1:554:U:O4'	2.15	0.47
1:B:220:VAL:HG21	52:1:782:A:N7	2.30	0.47
53:2:1127:G:C2	53:2:1128:C:C2	3.02	0.47
53:2:1513:A:H2'	53:2:1514:G:C8	2.50	0.47
53:2:299:G:H2'	53:2:300:A:C8	2.50	0.47
53:2:299:G:N2	53:2:565:U:O2	2.48	0.47
54:3:84:G:N2	54:3:93:C:C2	2.82	0.47
2:C:150:GLN:HB2	52:1:2572:A:N7	2.30	0.47
52:1:1065:U:O2'	52:1:1066:U:O5'	2.25	0.46
52:1:1017:G:N2	52:1:1146:C:C2	2.83	0.46
52:1:1385:A:H1'	52:1:1386:C:C6	2.50	0.46
52:1:2824:C:C4	52:1:2825:G:C5	3.03	0.46
52:1:2869:G:C6	52:1:2870:C:C4	3.03	0.46
52:1:363:G:C2	52:1:364:C:C2	3.03	0.46
52:1:86:G:C2	52:1:97:C:C2	3.02	0.46
53:2:11:G:H2'	53:2:12:U:O4'	2.14	0.46
53:2:580:C:H2'	53:2:581:G:O4'	2.15	0.46
54:3:48:U:H2'	54:3:49:C:H6	1.80	0.46
56:5:22:G:C2	56:5:23:C:C4	3.03	0.46
52:1:1479:G:C6	52:1:1480:C:C4	3.04	0.46
52:1:2266:A:C2	52:1:2272:U:C5	3.03	0.46
52:1:2795:C:C2	52:1:2802:G:C2	3.03	0.46
52:1:813:U:H2'	52:1:814:C:C6	2.50	0.46
52:1:966:G:O4'	52:1:2267:A:N6	2.48	0.46
54:3:16:G:C6	54:3:17:C:C4	3.04	0.46
56:5:72:A:H2'	56:5:73:A:C8	2.49	0.46
56:5:8:4SU:O2'	56:5:45:G:N2	2.48	0.46
52:1:1042:G:C2	52:1:1043:C:C2	3.04	0.46
52:1:1256:G:C6	52:1:1257:C:N4	2.82	0.46
52:1:2152:G:C2	52:1:2153:C:C2	3.04	0.46
52:1:2722:G:C2	52:1:2723:C:C2	3.03	0.46
52:1:315:G:C2	52:1:316:C:C2	3.04	0.46
52:1:327:G:N2	52:1:336:C:C2	2.83	0.46
52:1:333:G:C2	52:1:334:C:C2	3.04	0.46
53:2:106:C:H2'	53:2:107:G:O4'	2.15	0.46
53:2:399:G:C6	53:2:400:C:C4	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:37:ARG:NH2	52:1:1007:C:OP1	2.49	0.46
10:K:24:VAL:HG13	10:K:33:ALA:HB2	1.97	0.46
52:1:1356:G:C2	52:1:1357:C:C2	3.03	0.46
52:1:1775:U:O4	52:1:1790:C:H1'	2.15	0.46
52:1:2083:G:C2	52:1:2084:C:C2	3.04	0.46
52:1:2152:G:C6	52:1:2153:C:C4	3.03	0.46
52:1:2294:G:C2	52:1:2295:C:C2	3.04	0.46
52:1:2759:G:C2	52:1:2760:C:C2	3.03	0.46
52:1:2759:G:C6	52:1:2760:C:C4	3.03	0.46
52:1:706:A:H2'	52:1:707:G:O4'	2.15	0.46
53:2:201:G:C2	53:2:217:C:O2	2.69	0.46
53:2:725:G:C2	53:2:726:C:C2	3.03	0.46
3:D:188:MET:HE2	3:D:193:VAL:HG22	1.98	0.46
4:E:132:VAL:HG11	4:E:137:ILE:HD11	1.97	0.46
52:1:987:C:O2'	52:1:1000:A:N3	2.42	0.46
52:1:1149:G:C2	52:1:1150:C:C2	3.03	0.46
52:1:1157:G:N2	52:1:1158:C:C2	2.83	0.46
52:1:2671:G:H2'	52:1:2672:U:O4'	2.16	0.46
52:1:301:G:C6	52:1:302:C:N4	2.84	0.46
52:1:363:G:N2	52:1:364:C:C2	2.83	0.46
1:B:220:VAL:HG21	52:1:782:A:C8	2.51	0.46
52:1:785:G:C2	52:1:786:C:C2	3.04	0.46
52:1:984:A:H2'	52:1:984:A:N3	2.31	0.46
53:2:13:U:O4	53:2:20:U:C4	2.65	0.46
53:2:255:G:N2	53:2:272:C:C2	2.83	0.46
55:4:38:A:H2'	55:4:39:U:C4'	2.46	0.46
17:R:5:PHE:HB3	17:R:59:ILE:HD12	1.97	0.46
52:1:1139:G:C2	52:1:1140:C:C2	3.04	0.46
52:1:25:U:H2'	52:1:26:G:O4'	2.16	0.46
52:1:2862:G:C2	52:1:2863:C:C2	3.03	0.46
52:1:425:G:C2	52:1:426:C:C2	3.04	0.46
53:2:1463:U:H2'	53:2:1464:U:C6	2.51	0.46
53:2:577:G:C6	53:2:578:C:C4	3.04	0.46
53:2:698:G:C2	53:2:699:C:C2	3.03	0.46
53:2:763:G:C6	53:2:764:C:C4	3.04	0.46
52:1:1067:A:C4	57:6:56:C:N3	2.74	0.46
5:F:24:ILE:HD12	5:F:37:LEU:HD12	1.98	0.46
52:1:1746:A:H2'	52:1:1747:U:C6	2.51	0.46
52:1:2331:G:C5	52:1:2332:C:C4	3.04	0.46
52:1:2594:C:H2'	52:1:2595:G:O4'	2.16	0.46
52:1:538:A:H2'	52:1:539:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:7:G:C2	52:1:8:C:C2	3.04	0.46
53:2:384:G:H2'	53:2:385:C:H6	1.79	0.46
57:6:10:G:C2	57:6:11:C:C2	3.04	0.46
57:6:16:H2U:O2'	57:6:18:G:OP2	2.32	0.46
13:N:33:ILE:HA	13:N:114:GLU:HA	1.98	0.46
13:N:14:SER:HA	13:N:17:ARG:NH1	2.31	0.46
52:1:1017:G:C2	52:1:1146:C:C2	3.03	0.46
52:1:1206:G:C2	52:1:1207:C:C2	3.04	0.46
52:1:1717:A:H2'	52:1:1718:G:O4'	2.14	0.46
52:1:1934:C:H4'	52:1:1974:C:O3'	2.16	0.46
52:1:2301:C:H2'	52:1:2302:U:C6	2.50	0.46
52:1:2552:OMU:HM23	52:1:2554:U:C6	2.51	0.46
52:1:2895:G:C6	52:1:2896:C:C4	3.03	0.46
52:1:301:G:C5	52:1:302:C:C4	3.04	0.46
52:1:363:G:C6	52:1:364:C:C4	3.04	0.46
52:1:907:G:C2	52:1:908:C:C2	3.04	0.46
53:2:402:G:C2	53:2:403:C:C2	3.04	0.46
53:2:617:G:C2	53:2:624:C:C2	3.04	0.46
53:2:941:G:H2'	53:2:942:G:O4'	2.15	0.46
54:3:2:G:C2	54:3:3:C:C2	3.04	0.46
21:V:63:ILE:HD12	21:V:72:VAL:HG21	1.97	0.46
52:1:52:A:C5	52:1:118:A:C2	3.03	0.46
52:1:1220:G:C2	52:1:1221:C:C2	3.04	0.46
52:1:1462:C:H2'	52:1:1463:C:C6	2.50	0.46
52:1:1682:G:H2'	52:1:1683:U:C6	2.51	0.46
52:1:1964:G:C6	52:1:1967:C:N4	2.83	0.46
52:1:2321:U:H6	52:1:2321:U:H3'	1.81	0.46
52:1:485:C:C2	52:1:496:G:N2	2.84	0.46
53:2:1233:G:C6	53:2:1234:C:N4	2.84	0.46
53:2:698:G:C6	53:2:699:C:C4	3.04	0.46
25:Z:43:ALA:O	52:1:851:C:O2'	2.34	0.46
52:1:1020:A:C2	52:1:1141:U:C2	3.04	0.46
52:1:1157:G:C2	52:1:1158:C:C2	3.04	0.46
52:1:301:G:C6	52:1:302:C:C4	3.03	0.46
52:1:587:C:H4'	52:1:588:U:H6	1.78	0.46
52:1:778:G:C2	52:1:787:C:C2	3.04	0.46
53:2:125:U:H2'	53:2:126:G:O4'	2.16	0.46
53:2:769:G:C6	53:2:770:C:C4	3.04	0.46
54:3:85:G:N2	54:3:92:C:C2	2.83	0.46
52:1:1628:G:C2	52:1:1639:C:O2	2.68	0.45
52:1:2557:G:C6	52:1:2558:C:C4	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:2652:C:C2	52:1:2669:G:C2	3.04	0.45
52:1:2744:G:N2	52:1:2745:C:C2	2.84	0.45
52:1:356:G:C6	52:1:357:C:C4	3.04	0.45
53:2:1258:G:C6	53:2:1259:C:N4	2.84	0.45
53:2:289:G:C6	53:2:290:C:C4	3.04	0.45
53:2:568:G:C6	53:2:569:C:N4	2.84	0.45
9:J:32:LEU:CD2	9:J:54:ILE:HG21	2.46	0.45
13:N:22:ARG:HG3	13:N:70:THR:HA	1.97	0.45
24:Y:55:THR:HG21	52:1:77:G:O4'	2.17	0.45
52:1:186:G:N2	52:1:211:C:C2	2.84	0.45
52:1:1783:A:C2	52:1:2588:G:O4'	2.69	0.45
52:1:237:C:C2	52:1:261:G:C2	3.05	0.45
52:1:356:G:C2	52:1:357:C:C2	3.05	0.45
53:2:1442:G:N1	53:2:1443:C:C4	2.83	0.45
53:2:1486:G:H2'	53:2:1487:G:O4'	2.16	0.45
53:2:688:G:C2	53:2:689:C:C2	3.03	0.45
53:2:731:G:C6	53:2:732:C:C4	3.05	0.45
56:5:72:A:O2'	56:5:73:A:O4'	2.31	0.45
13:N:51:LEU:HD21	13:N:69:ARG:HG2	1.98	0.45
16:Q:65:ILE:CD1	16:Q:92:ARG:HB2	2.46	0.45
52:1:1319:C:O2	52:1:1334:G:C2	2.69	0.45
52:1:770:G:H1'	52:1:1379:U:C4	2.51	0.45
52:1:1385:A:C4	52:1:1386:C:C5	3.03	0.45
52:1:1881:C:H2'	52:1:1882:U:O4'	2.16	0.45
52:1:1949:G:N2	52:1:1958:C:C2	2.84	0.45
52:1:245:G:C2	52:1:246:C:C2	3.04	0.45
52:1:252:G:C2	52:1:253:C:C2	3.04	0.45
52:1:2744:G:C6	52:1:2745:C:C4	3.04	0.45
52:1:756:A:H2'	52:1:757:G:O4'	2.16	0.45
53:2:1370:G:C2	53:2:1371:G:C8	3.04	0.45
53:2:384:G:C2	53:2:385:C:C2	3.04	0.45
53:2:442:G:C2	53:2:443:C:C2	3.05	0.45
53:2:624:C:H2'	53:2:625:U:O4'	2.17	0.45
56:5:64:G:C2	56:5:65:C:C2	3.04	0.45
57:6:49:C:H2'	57:6:50:U:C6	2.51	0.45
57:6:56:C:C2'	57:6:56:C:O2	2.61	0.45
57:6:67:C:H2'	57:6:68:C:C6	2.51	0.45
4:E:8:TYR:HA	4:E:12:VAL:HB	1.97	0.45
23:X:31:PRO:HG2	23:X:33:LEU:HD13	1.98	0.45
52:1:1138:G:H2'	52:1:1139:G:O4'	2.16	0.45
52:1:2037:A:H2'	52:1:2038:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:2509:G:C2	52:1:2510:C:C2	3.05	0.45
52:1:2514:U:H2'	52:1:2515:C:H6	1.81	0.45
52:1:785:G:C6	52:1:786:C:C4	3.04	0.45
52:1:997:G:C6	52:1:998:C:C4	3.05	0.45
53:2:868:C:H2'	53:2:869:G:O4'	2.15	0.45
2:C:80:TRP:CD1	2:C:202:ILE:HD11	2.51	0.45
52:1:816:C:C2	52:1:1192:G:C2	3.04	0.45
52:1:1204:A:O4'	52:1:1206:G:C8	2.70	0.45
52:1:12:U:O2	52:1:12:U:H2'	2.17	0.45
52:1:1374:G:H2'	52:1:1375:U:O4'	2.16	0.45
52:1:1703:G:C2	52:1:1704:C:C2	3.05	0.45
52:1:2415:G:C5	52:1:2416:C:C4	3.04	0.45
52:1:2641:G:C2	52:1:2774:C:C2	3.04	0.45
53:2:1258:G:C2	53:2:1259:C:C2	3.05	0.45
53:2:775:G:H2'	53:2:776:G:O4'	2.17	0.45
53:2:853:C:C4	53:2:854:U:C5	3.04	0.45
57:6:28:G:C2	57:6:43:C:O2	2.70	0.45
59:8:670:ARG:N	59:8:739:ARG:O	2.50	0.45
5:F:35:ARG:HD3	5:F:71:LEU:HD13	1.97	0.45
12:M:67:VAL:HG11	12:M:96:ILE:HD12	1.99	0.45
52:1:1122:G:C2	52:1:1123:C:C6	3.05	0.45
52:1:118:A:C8	52:1:120:U:C4	3.05	0.45
52:1:1506:U:H2'	52:1:1507:C:C6	2.51	0.45
52:1:1560:G:N2	52:1:1561:C:C2	2.85	0.45
52:1:1873:G:N2	52:1:1874:C:C2	2.85	0.45
52:1:2086:U:H2'	52:1:2087:G:C8	2.51	0.45
52:1:2241:A:H2'	52:1:2242:G:C8	2.51	0.45
4:E:155:THR:HG21	52:1:2314:A:H1'	1.98	0.45
52:1:2409:G:H2'	52:1:2410:G:O4'	2.16	0.45
52:1:2722:G:C6	52:1:2723:C:C4	3.04	0.45
52:1:2729:G:C6	52:1:2730:C:C4	3.04	0.45
53:2:105:G:C6	53:2:106:C:C4	3.04	0.45
53:2:731:G:C2	53:2:732:C:C2	3.05	0.45
53:2:947:G:C2	53:2:948:C:C2	3.05	0.45
52:1:2061:G:N2	63:5:101:MET:SD	2.90	0.45
57:6:34:G:O6	58:7:21:C:N3	2.50	0.45
1:B:141:VAL:HG11	1:B:190:ALA:HB1	1.98	0.45
13:N:44:LEU:HD23	13:N:113:ILE:HG21	1.98	0.45
15:P:53:ARG:HB2	15:P:56:HIS:HB2	1.99	0.45
52:1:1166:G:C2	52:1:1167:C:C2	3.05	0.45
1:B:204:VAL:HG23	52:1:1792:G:H5'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:1933:G:C6	52:1:1934:C:N3	2.85	0.45
52:1:2045:C:C2	52:1:2624:G:C2	3.05	0.45
52:1:812:C:C2	52:1:1250:G:C2	3.05	0.45
52:1:825:A:H2'	52:1:826:U:O4'	2.17	0.45
52:1:988:A:H4'	52:1:1155:A:N1	2.32	0.45
53:2:1050:G:C6	53:2:1051:C:C4	3.04	0.45
53:2:1068:G:C2	53:2:1069:C:C2	3.05	0.45
53:2:1222:G:C2	53:2:1223:C:C2	3.05	0.45
53:2:1442:G:C6	53:2:1443:C:N4	2.84	0.45
53:2:506:G:C6	53:2:507:C:C4	3.05	0.45
53:2:633:G:N2	53:2:634:C:C2	2.85	0.45
55:4:35:A:H2'	55:4:36:A:C8	2.52	0.45
1:B:37:ASN:HB2	1:B:62:TYR:HB2	1.98	0.45
9:J:30:THR:HG22	9:J:31:GLU:N	2.31	0.45
13:N:52:ILE:HG21	13:N:94:TYR:CG	2.52	0.45
13:N:27:SER:HB3	52:1:1278:C:O2'	2.16	0.45
52:1:1791:A:C8	52:1:1792:G:C8	3.05	0.45
52:1:1850:G:H2'	52:1:1851:U:O4'	2.17	0.45
52:1:191:A:H2'	52:1:192:C:C6	2.51	0.45
52:1:2046:G:C4	52:1:2047:C:C5	3.04	0.45
52:1:2507:C:O5'	52:1:2507:C:H6	2.00	0.45
52:1:321:U:O2'	52:1:340:A:N3	2.43	0.45
53:2:1120:C:C2	53:2:1154:G:C2	3.04	0.45
53:2:1428:A:H2'	53:2:1429:A:O4'	2.17	0.45
54:3:16:G:C2	54:3:17:C:C2	3.05	0.45
52:1:2194:U:H2'	52:1:2195:U:O4'	2.17	0.45
52:1:2207:C:C2	52:1:2218:G:N2	2.85	0.45
52:1:2820:A:C2'	52:1:2821:A:OP1	2.65	0.45
52:1:977:G:C2	52:1:987:C:C2	3.05	0.45
53:2:1050:G:C6	53:2:1051:C:N4	2.85	0.45
53:2:1330:U:O4	53:2:1331:G:C6	2.70	0.45
53:2:147:G:H2'	53:2:148:G:C8	2.51	0.45
53:2:391:G:C6	53:2:392:C:C4	3.05	0.45
53:2:445:G:N2	53:2:490:C:C2	2.85	0.45
53:2:755:G:C2	53:2:756:C:C2	3.05	0.45
53:2:947:G:C6	53:2:948:C:C4	3.05	0.45
56:5:5:G:C2	56:5:68:C:C2	3.04	0.45
59:8:667:LEU:HD11	59:8:716:ILE:HB	1.98	0.45
1:B:9:THR:HG22	52:1:2020:A:H5'	85.20	0.45
2:C:193:VAL:HG21	2:C:201:LEU:HD11	1.98	0.45
52:1:1099:G:C6	52:1:1100:C:C4	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:1122:G:C6	52:1:1123:C:C4	3.04	0.45
52:1:1128:G:O4'	52:1:2516:A:O2'	2.34	0.45
52:1:1208:C:C2	52:1:1239:G:N2	2.85	0.45
52:1:1277:G:C2	52:1:1278:C:C2	3.05	0.45
52:1:2236:U:H2'	52:1:2237:G:O4'	2.17	0.45
52:1:2395:C:H2'	52:1:2396:G:O4'	2.16	0.45
52:1:2747:G:O6	52:1:2755:C:H5"	2.17	0.45
52:1:793:A:N6	52:1:2073:C:OP1	2.50	0.45
52:1:991:C:C2	52:1:1185:G:C2	3.05	0.45
53:2:247:G:N2	53:2:248:C:C2	2.85	0.45
53:2:680:C:C2	53:2:711:G:C2	3.05	0.45
55:4:35:A:N6	58:7:14:A:H61	2.15	0.45
59:8:679:LEU:HD23	59:8:734:ASP:CB	2.47	0.45
2:C:187:LEU:HD21	2:C:203:VAL:HG11	1.99	0.45
52:1:1074:G:N1	52:1:1075:C:C4	2.84	0.44
52:1:1648:U:H2'	52:1:1649:G:O4'	2.17	0.44
52:1:1907:G:C2	52:1:1924:C:O2	2.70	0.44
52:1:2221:G:H2'	52:1:2222:C:O4'	2.17	0.44
52:1:2379:G:C6	52:1:2380:C:C4	3.04	0.44
52:1:2244:U:C2	52:1:2435:A:C6	2.86	0.44
52:1:29:U:H2'	52:1:30:G:C8	2.51	0.44
52:1:585:G:C2'	52:1:1254:A:H61	2.30	0.44
52:1:622:G:C4	52:1:623:C:C5	3.05	0.44
52:1:628:G:C6	52:1:636:G:C2	3.05	0.44
53:2:582:C:C4	53:2:760:G:O6	2.70	0.44
53:2:852:G:C6	53:2:853:C:C4	3.05	0.44
11:L:78:ARG:HD3	52:1:626:A:C2	2.52	0.44
52:1:1182:G:H2'	52:1:1183:U:O4'	2.17	0.44
52:1:1277:G:C6	52:1:1278:C:C4	3.06	0.44
52:1:1889:A:H2'	52:1:1890:A:O4'	2.18	0.44
52:1:2519:U:C5	52:1:2541:A:C6	3.05	0.44
52:1:2677:G:C6	52:1:2678:C:C4	3.05	0.44
52:1:2694:G:C2	52:1:2716:C:C2	3.05	0.44
52:1:567:U:H2'	52:1:568:U:O4'	2.17	0.44
52:1:834:G:C6	52:1:835:C:C4	3.05	0.44
53:2:1426:G:H2'	53:2:1427:C:O4'	2.16	0.44
53:2:769:G:C2	53:2:770:C:C2	3.05	0.44
14:O:27:VAL:HG21	14:O:40:ILE:HD12	1.99	0.44
52:1:1239:G:H2'	52:1:1240:U:O4'	2.16	0.44
52:1:1296:G:C6	52:1:1297:C:C4	3.06	0.44
52:1:1469:A:H2'	52:1:1470:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:2642:G:C2	52:1:2773:C:C2	3.05	0.44
53:2:335:C:H2'	53:2:336:A:H8	1.82	0.44
53:2:42:G:C2	53:2:43:C:C2	3.05	0.44
53:2:442:G:C6	53:2:443:C:C4	3.05	0.44
53:2:71:A:C2	53:2:72:A:C8	3.05	0.44
53:2:977:A:N3	53:2:977:A:H3'	2.31	0.44
56:5:53:G:H2'	56:5:54:5MU:H6	1.83	0.44
17:R:68:ARG:NH1	52:1:1224:U:OP2	2.50	0.44
52:1:1436:G:C2	52:1:1437:C:C2	3.06	0.44
52:1:1555:G:C6	52:1:1556:C:C4	3.06	0.44
52:1:734:A:O2'	52:1:1635:A:H4'	2.18	0.44
52:1:1984:G:C6	52:1:1985:C:C4	3.05	0.44
52:1:569:U:H5"	52:1:821:A:C2	2.52	0.44
52:1:959:A:C6	52:1:960:A:C6	3.06	0.44
53:2:1114:C:C2	53:2:1187:G:N2	2.85	0.44
53:2:1417:G:C6	53:2:1482:G:C6	3.06	0.44
53:2:160:A:H2'	53:2:161:A:O4'	2.17	0.44
53:2:247:G:C2	53:2:248:C:C2	3.05	0.44
53:2:369:G:H2'	53:2:370:C:C6	2.52	0.44
53:2:59:A:H5"	53:2:387:U:H5"	2.00	0.44
53:2:939:G:C6	53:2:940:C:C4	3.06	0.44
53:2:939:G:C2	53:2:940:C:C2	3.06	0.44
55:4:10:G:C2	55:4:11:C:C2	3.06	0.44
55:4:10:G:C6	55:4:11:C:C4	3.06	0.44
59:8:683:ILE:HG21	59:8:710:ILE:CD1	2.47	0.44
2:C:26:VAL:HG21	15:P:5:ILE:HD13	1.98	0.44
13:N:79:LEU:O	13:N:84:GLY:N	2.49	0.44
52:1:1074:G:C2	52:1:1075:C:C2	3.05	0.44
52:1:1235:G:C6	52:1:1236:G:N1	2.85	0.44
52:1:1394:U:H2'	52:1:1395:A:O4'	2.17	0.44
52:1:172:A:C2	52:1:173:A:C5	3.06	0.44
52:1:645:C:H2'	52:1:647:G:C8	2.52	0.44
53:2:442:G:N1	53:2:443:C:C4	2.85	0.44
53:2:763:G:C2	53:2:764:C:C2	3.05	0.44
59:8:616:ILE:HG12	59:8:667:LEU:HD23	1.99	0.44
52:1:2294:G:N2	52:1:2339:C:C2	2.85	0.44
52:1:2445:2MG:HM21	52:1:2449:U:O4	2.17	0.44
52:1:2744:G:C2	52:1:2745:C:C2	3.05	0.44
52:1:614:A:O2'	52:1:615:U:OP2	2.24	0.44
52:1:701:G:N2	52:1:732:C:C2	2.85	0.44
53:2:1233:G:C2	53:2:1234:C:C2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:399:G:C4	53:2:400:C:C5	3.05	0.44
53:2:577:G:C2	53:2:578:C:C2	3.05	0.44
12:M:45:GLN:HG2	52:1:2485:G:H5'	2.00	0.44
52:1:1322:A:C5	52:1:1323:C:C5	3.06	0.44
52:1:2329:U:H2'	52:1:2330:G:O4'	2.17	0.44
53:2:105:G:C2	53:2:106:C:C2	3.05	0.44
53:2:1071:C:H2'	53:2:1072:G:C8	2.52	0.44
53:2:1233:G:C6	53:2:1234:C:C4	3.06	0.44
53:2:218:U:H2'	53:2:219:U:O4'	2.18	0.44
53:2:402:G:H2'	53:2:403:C:O4'	2.18	0.44
53:2:627:G:H2'	53:2:628:G:O4'	2.18	0.44
53:2:662:U:H2'	53:2:663:A:C8	2.53	0.44
53:2:864:A:H2'	53:2:865:A:N9	2.32	0.44
53:2:867:G:C2	53:2:868:C:C2	3.05	0.44
54:3:28:C:H2'	54:3:29:A:O4'	2.18	0.44
59:8:683:ILE:HD13	59:8:710:ILE:HD11	1.99	0.44
7:H:53:ARG:HB3	7:H:55:VAL:HG13	2.00	0.44
8:I:105:LEU:HD13	8:I:129:GLU:HG2	1.99	0.44
52:1:1320:C:N4	52:1:1331:G:N7	2.66	0.44
52:1:579:G:O2'	52:1:2019:A:OP1	2.36	0.44
52:1:2221:G:C5	52:1:2222:C:C5	3.06	0.44
52:1:2327:A:H2'	52:1:2328:A:C8	2.52	0.44
52:1:2557:G:C6	52:1:2558:C:N4	2.86	0.44
52:1:2819:G:H2'	52:1:2821:A:N7	2.32	0.44
52:1:315:G:C6	52:1:316:C:C4	3.05	0.44
53:2:1050:G:C2	53:2:1051:C:C2	3.05	0.44
53:2:1071:C:H2'	53:2:1072:G:H8	1.83	0.44
53:2:391:G:C2	53:2:392:C:C2	3.05	0.44
56:5:32:4OC:HM22	56:5:33:U:H5'	2.00	0.44
13:N:63:ARG:HA	13:N:80:PHE:CE1	2.53	0.44
52:1:1063:G:C4	52:1:1064:C:C6	3.06	0.44
52:1:1593:A:H2'	52:1:1594:U:O4'	2.18	0.44
52:1:1973:G:C2	52:1:1974:C:C2	3.05	0.44
52:1:2625:G:C6	52:1:2626:C:C4	3.06	0.44
52:1:822:G:C2	52:1:823:C:C2	3.06	0.44
53:2:1179:A:H2'	53:2:1180:A:O4'	2.17	0.44
53:2:1511:G:H2'	53:2:1512:U:O4'	2.18	0.44
53:2:310:G:C2	53:2:311:C:C2	3.05	0.44
53:2:737:C:H2'	53:2:738:C:C6	2.53	0.44
56:5:30:G:C2	56:5:41:C:C2	3.06	0.44
57:6:71:G:H2'	57:6:72:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:1220:G:C6	52:1:1221:C:C4	3.06	0.43
52:1:1430:G:H2'	52:1:1431:A:O4'	2.18	0.43
52:1:1745:A:H2'	52:1:1746:A:O4'	2.18	0.43
52:1:2049:G:C2	52:1:2050:C:C2	3.06	0.43
52:1:2227:A:H2'	52:1:2228:G:O4'	2.18	0.43
52:1:2057:G:C2	52:1:2612:C:O2	2.71	0.43
53:2:1140:C:HO2'	53:2:1141:C:P	2.41	0.43
53:2:1258:G:C6	53:2:1259:C:C4	3.06	0.43
53:2:1402:4OC:H2'	53:2:1403:C:O4'	2.18	0.43
53:2:354:G:C2	53:2:355:C:C4	3.06	0.43
53:2:49:U:C2	53:2:361:G:N2	2.86	0.43
56:5:35:A:H2'	56:5:36:U:C6	2.53	0.43
1:B:76:ALA:HB2	1:B:96:TYR:CD2	2.53	0.43
19:T:34:VAL:HG21	19:T:43:ILE:HD11	2.00	0.43
52:1:1163:G:C2	52:1:1164:C:C2	3.06	0.43
52:1:1796:U:H2'	52:1:1797:G:C8	2.53	0.43
52:1:1773:A:C8	52:1:1829:A:C8	3.06	0.43
52:1:388:G:N7	52:1:390:U:H2'	2.34	0.43
52:1:460:A:H2'	52:1:461:C:O4'	2.18	0.43
52:1:329:G:O4'	52:1:477:A:H1'	2.18	0.43
52:1:532:A:H4'	52:1:533:G:C8	2.53	0.43
52:1:532:A:N3	52:1:532:A:H2'	2.32	0.43
52:1:825:A:H4'	52:1:2428:G:C5	2.53	0.43
53:2:10:A:N1	53:2:24:U:O2	2.51	0.43
53:2:146:G:H2'	53:2:147:G:O4'	2.18	0.43
53:2:142:G:N2	53:2:222:C:C2	2.86	0.43
56:5:22:G:N1	56:5:23:C:C4	2.86	0.43
52:1:1343:G:H1'	52:1:1597:A:C4	2.53	0.43
52:1:2030:6MZ:C2	52:1:2499:C:H5"	2.49	0.43
52:1:2625:G:C2	52:1:2626:C:C2	3.06	0.43
52:1:2662:A:H2'	52:1:2663:G:O4'	2.18	0.43
52:1:2831:G:O2'	52:1:2884:U:OP1	2.29	0.43
53:2:342:C:C2	53:2:348:G:N2	2.85	0.43
53:2:867:G:C6	53:2:868:C:N4	2.86	0.43
53:2:931:C:C2	53:2:1387:G:C2	3.06	0.43
54:3:2:G:C6	54:3:3:C:C4	3.06	0.43
52:1:1296:G:C2	52:1:1297:C:C2	3.06	0.43
53:2:1442:G:C2	53:2:1443:C:C2	3.07	0.43
53:2:1456:A:H2'	53:2:1457:G:O4'	2.18	0.43
53:2:1518:MA6:N6	53:2:1519:MA6:H93	2.33	0.43
53:2:201:G:N1	53:2:217:C:C2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:424:G:O2'	53:2:425:G:H5'	2.17	0.43
55:4:36:A:N1	58:7:14:A:N1	2.67	0.43
59:8:118:GLN:CB	59:8:127:VAL:HG23	2.49	0.43
2:C:193:VAL:HG21	2:C:201:LEU:CD1	2.48	0.43
14:O:18:LEU:HD23	14:O:25:ARG:HD2	2.01	0.43
14:O:27:VAL:CG2	14:O:40:ILE:HD12	2.49	0.43
52:1:1361:G:C2	52:1:1362:C:C2	3.06	0.43
52:1:2852:G:C5	52:1:2853:C:C5	3.07	0.43
53:2:1198:G:C6	53:2:1199:U:C4	3.06	0.43
53:2:399:G:C6	53:2:400:C:N4	2.87	0.43
53:2:424:G:O2'	53:2:425:G:C8	2.69	0.43
53:2:515:G:H2'	53:2:516:PSU:O4'	2.18	0.43
53:2:592:G:H2'	53:2:593:U:O4'	2.18	0.43
54:3:16:G:C2	54:3:17:C:C6	3.05	0.43
56:5:20:H2U:C3'	56:5:21:A:H5"	2.49	0.43
56:5:44:A:H2'	56:5:45:G:H5'	2.01	0.43
59:8:60:VAL:HA	59:8:63:VAL:HG12	2.01	0.43
9:J:47:HIS:HB3	52:1:558:U:H1'	2.01	0.43
52:1:1225:G:C2	52:1:1226:A:C2	3.07	0.43
52:1:1361:G:C6	52:1:1362:C:C4	3.06	0.43
52:1:1740:G:C2	52:1:1741:C:C2	3.06	0.43
52:1:221:A:C4	52:1:266:G:N7	2.87	0.43
52:1:2283:C:C4	52:1:2389:G:C5	3.07	0.43
52:1:252:G:N2	52:1:253:C:C2	2.87	0.43
13:N:53:THR:HG21	52:1:2840:C:H5"	2.01	0.43
53:2:541:G:H2'	53:2:542:G:O4'	2.19	0.43
53:2:867:G:C6	53:2:868:C:C4	3.07	0.43
57:6:27:G:H2'	57:6:28:G:O4'	2.19	0.43
2:C:151:THR:O	52:1:1130:U:O4	2.36	0.43
16:Q:99:ALA:HB2	16:Q:106:PHE:CE1	2.53	0.43
52:1:1064:C:H2'	52:1:1065:U:C6	2.53	0.43
52:1:1053:C:C2	52:1:1107:G:C2	3.06	0.43
52:1:1180:U:C5	52:1:1181:U:C5	3.07	0.43
52:1:1195:G:C6	52:1:1196:C:C4	3.07	0.43
52:1:1483:G:C6	52:1:1507:C:N3	2.87	0.43
52:1:2485:G:C6	52:1:2486:C:C4	3.07	0.43
53:2:296:U:H2'	53:2:297:G:O4'	2.19	0.43
53:2:683:G:C2	53:2:708:C:C2	3.07	0.43
53:2:755:G:N2	53:2:756:C:C2	2.87	0.43
53:2:827:U:N3	53:2:874:G:C2	2.87	0.43
53:2:915:A:C5	53:2:916:U:C5	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:918:A:H2'	53:2:919:A:O4'	2.18	0.43
55:4:9:A:O2'	55:4:10:G:N7	2.49	0.43
55:4:9:A:C8	55:4:46:G:N2	2.87	0.43
1:B:258:ARG:NH2	52:1:1800:C:OP1	2.51	0.43
52:1:1157:G:C6	52:1:1158:C:C4	3.06	0.43
52:1:1292:G:C2	52:1:1293:C:C2	3.06	0.43
52:1:1416:G:C2	52:1:1417:C:N3	2.87	0.43
52:1:1707:G:C4	52:1:1708:C:C5	3.06	0.43
52:1:255:A:H2'	52:1:256:A:O4'	2.18	0.43
52:1:2642:G:N2	52:1:2773:C:C2	2.86	0.43
52:1:554:U:C4	52:1:555:G:C6	3.07	0.43
52:1:673:C:C2	52:1:808:G:N2	2.87	0.43
52:1:822:G:C6	52:1:823:C:C4	3.07	0.43
52:1:871:U:H2'	52:1:872:U:C6	2.53	0.43
52:1:997:G:C2	52:1:998:C:C2	3.07	0.43
56:5:52:G:C2'	56:5:53:G:H5'	2.48	0.43
59:8:434:ASP:O	59:8:438:ARG:HG3	2.19	0.43
13:N:41:ALA:HB1	13:N:97:ILE:HD12	2.01	0.43
52:1:1195:G:C2	52:1:1196:C:C2	3.07	0.43
52:1:1416:G:C2	52:1:1417:C:C4	3.07	0.43
52:1:1555:G:C2	52:1:1556:C:C2	3.06	0.43
52:1:1688:U:N3	52:1:1698:A:C2	2.87	0.43
52:1:30:G:C2	52:1:31:C:C2	3.07	0.43
52:1:34:U:HO2'	52:1:35:G:C5'	2.32	0.43
52:1:812:C:C5	52:1:1250:G:C6	3.07	0.43
52:1:864:G:C6	52:1:865:C:N4	2.87	0.43
52:1:985:C:C2	52:1:986:C:C5	3.06	0.43
53:2:915:A:H8	53:2:915:A:O5'	2.02	0.43
52:1:1157:G:C6	52:1:1158:C:N4	2.86	0.43
52:1:1268:A:H1'	52:1:2613:U:H3	1.83	0.43
52:1:2493:U:C4	52:1:2494:G:C8	3.07	0.43
52:1:2747:G:C2	52:1:2756:U:C5	3.07	0.43
52:1:634:C:H2'	52:1:635:C:H6	1.84	0.43
52:1:672:C:OP1	52:1:801:G:N2	2.51	0.43
52:1:719:C:H2'	52:1:720:U:O4'	2.19	0.43
53:2:1109:C:C3'	53:2:1109:C:C5'	2.97	0.43
53:2:368:U:O2	53:2:368:U:H2'	2.17	0.43
54:3:75:G:H2'	54:3:76:G:O4'	2.19	0.43
14:O:25:ARG:NH1	54:3:8:C:O3'	2.52	0.43
52:1:1007:C:C2	52:1:1137:G:C2	3.07	0.42
52:1:1149:G:C6	52:1:1150:C:C4	3.06	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:1256:G:C2	52:1:1257:C:C2	3.07	0.42
52:1:1356:G:C2	52:1:1376:C:C2	3.07	0.42
52:1:1416:G:C6	52:1:1417:C:C4	3.07	0.42
52:1:2502:G:H5"	52:1:2503:2MA:H5"	2.01	0.42
52:1:2729:G:H2'	52:1:2730:C:O4'	2.18	0.42
52:1:377:G:C2	52:1:398:C:C2	3.07	0.42
53:2:1206:G:H2'	53:2:1207:2MG:O4'	2.19	0.42
1:B:29:PRO:HG2	1:B:34:LEU:HD11	2.01	0.42
2:C:62:LYS:HB2	2:C:63:PRO:HD3	2.01	0.42
21:V:30:ILE:HG23	21:V:72:VAL:HG11	2.01	0.42
23:X:3:ARG:NH1	52:1:1808:A:O2'	2.52	0.42
52:1:2077:A:N6	52:1:2435:A:N6	2.66	0.42
52:1:2633:G:H2'	52:1:2634:A:O4'	2.19	0.42
52:1:690:G:C2	52:1:691:C:C2	3.07	0.42
52:1:990:A:H1'	52:1:1156:A:N3	2.34	0.42
53:2:24:U:O4	53:2:559:A:C2	2.71	0.42
53:2:557:G:C6	53:2:558:G:C6	3.08	0.42
53:2:632:U:C2'	53:2:632:U:O2	2.66	0.42
56:5:18:G:C4	56:5:58:A:C2	3.07	0.42
13:N:38:LEU:HB3	13:N:39:PRO:HD3	2.01	0.42
1:B:8:PRO:HD2	52:1:1263:U:O2'	77.53	0.42
52:1:1436:G:N1	52:1:1437:C:C2	2.87	0.42
52:1:186:G:C2	52:1:211:C:C2	3.07	0.42
52:1:2436:G:C2	52:1:2437:G:C8	3.08	0.42
52:1:2677:G:C2	52:1:2678:C:C2	3.07	0.42
52:1:323:C:C4	52:1:333:G:C8	3.07	0.42
52:1:1916:A:N6	53:2:1408:A:O2'	2.44	0.42
53:2:1442:G:C2	53:2:1443:C:C4	3.07	0.42
53:2:847:G:N2	53:2:848:C:C2	2.88	0.42
53:2:900:A:H2'	53:2:901:A:C8	2.54	0.42
53:2:903:G:H2'	53:2:904:U:O4'	2.19	0.42
59:8:112:ASP:O	59:8:115:ALA:HB2	2.19	0.42
52:1:1005:C:C2	52:1:1006:C:C5	3.08	0.42
52:1:1296:G:C6	52:1:1297:C:N4	2.87	0.42
52:1:1795:C:H2'	52:1:1796:U:O4'	2.18	0.42
16:Q:30:ARG:NH1	52:1:18:U:OP1	2.52	0.42
52:1:2314:A:N6	52:1:2315:G:O6	2.52	0.42
52:1:2361:G:C6	52:1:2362:C:C4	3.08	0.42
52:1:30:G:C6	52:1:31:C:C4	3.07	0.42
52:1:697:G:C2	52:1:698:C:C2	3.07	0.42
52:1:852:U:C4	52:1:853:C:N4	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:950:G:C6	52:1:951:C:C4	3.07	0.42
9:J:30:THR:CG2	9:J:31:GLU:N	2.82	0.42
52:1:1099:G:C2	52:1:1100:C:C2	3.08	0.42
52:1:565:C:H4'	52:1:1253:A:C6	2.55	0.42
52:1:1831:G:C2	52:1:1832:C:C2	3.07	0.42
52:1:2283:C:C5	52:1:2389:G:C4	3.07	0.42
53:2:809:G:C2	53:2:810:C:C2	3.07	0.42
55:4:34:G:C6	55:4:35:A:C6	3.08	0.42
5:F:121:ILE:HD12	5:F:141:ILE:HG22	2.01	0.42
52:1:123:G:N2	52:1:129:C:C2	2.88	0.42
52:1:2043:C:C2	52:1:2777:G:N2	2.87	0.42
52:1:2485:G:N2	52:1:2486:C:C2	2.88	0.42
52:1:2586:U:C5	52:1:2608:G:N2	2.87	0.42
52:1:424:G:H2'	52:1:425:G:O4'	2.19	0.42
52:1:699:A:H2'	52:1:700:G:O4'	2.18	0.42
52:1:763:G:C5	52:1:765:C:C4	3.08	0.42
52:1:840:C:C2	52:1:939:G:C2	3.07	0.42
52:1:854:C:C2	52:1:924:G:C2	3.07	0.42
53:2:242:G:N2	53:2:285:C:C2	2.87	0.42
54:3:96:G:C2	54:3:97:C:C2	3.07	0.42
56:5:22:G:C6	56:5:23:C:C4	3.08	0.42
59:8:692:VAL:HG12	59:8:716:ILE:HG13	2.02	0.42
13:N:63:ARG:HA	13:N:80:PHE:CZ	2.55	0.42
52:1:48:G:O2'	52:1:118:A:N1	2.53	0.42
52:1:2081:U:C4	52:1:2237:G:C2	3.07	0.42
52:1:2397:G:C2	52:1:2420:C:O2	2.73	0.42
52:1:2771:C:C2	52:1:2772:C:C5	3.07	0.42
52:1:462:C:C2	52:1:468:G:C2	3.07	0.42
52:1:515:A:H1'	52:1:581:C:H1'	2.01	0.42
52:1:840:C:N3	52:1:939:G:C6	2.88	0.42
53:2:1530:G:H2'	53:2:1531:A:C8	2.54	0.42
53:2:660:C:H2'	53:2:661:G:O4'	2.19	0.42
53:2:857:C:H2'	53:2:858:G:O4'	2.20	0.42
1:B:232:HIS:CG	1:B:240:PHE:CE2	3.08	0.42
2:C:121:THR:HG21	2:C:143:PRO:HB3	2.01	0.42
4:E:16:LEU:HD13	4:E:28:VAL:CG2	2.50	0.42
4:E:66:LEU:HD11	54:3:41:G:H8	1.84	0.42
22:W:56:ASP:HA	52:1:2386:A:H4'	2.02	0.42
22:W:59:LEU:HD12	22:W:80:ILE:HD12	2.02	0.42
52:1:1289:C:O2'	52:1:1330:C:H4'	2.20	0.42
52:1:263:G:N1	52:1:264:C:C2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:52:A:H2'	52:1:53:A:C8	2.54	0.42
52:1:672:C:H2'	52:1:673:C:O4'	2.20	0.42
53:2:585:G:C5	53:2:586:C:C5	3.07	0.42
53:2:669:G:C2	53:2:738:C:C2	3.07	0.42
53:2:707:U:N3	53:2:708:C:C5	2.88	0.42
59:8:118:GLN:C	59:8:127:VAL:H	2.22	0.42
59:8:667:LEU:HD13	59:8:722:LEU:HD13	2.01	0.42
2:C:156:PHE:CE1	9:J:81:ILE:HD13	2.55	0.42
52:1:1024:G:H1'	52:1:1144:A:O2'	2.20	0.42
52:1:1356:G:H2'	52:1:1357:C:C6	2.55	0.42
52:1:1862:G:C2	52:1:1881:C:C2	3.08	0.42
52:1:247:G:N7	52:1:249:C:C2	2.88	0.42
52:1:2557:G:C4	52:1:2558:C:C5	3.08	0.42
52:1:2644:G:N7	52:1:2645:G:C6	2.88	0.42
52:1:2895:G:C4	52:1:2896:C:C5	3.08	0.42
52:1:597:G:H2'	52:1:598:U:O4'	2.19	0.42
52:1:640:C:H2'	52:1:641:U:O4'	2.19	0.42
53:2:1103:C:H2'	53:2:1104:G:O4'	2.20	0.42
53:2:1118:U:H2'	53:2:1119:C:C6	2.54	0.42
53:2:147:G:C2	53:2:176:C:C2	3.08	0.42
53:2:1480:A:H2'	53:2:1481:U:O4'	2.20	0.42
53:2:369:G:C2	53:2:370:C:C2	3.08	0.42
53:2:725:G:N2	53:2:726:C:C2	2.88	0.42
53:2:22:G:O2'	53:2:913:A:N1	2.48	0.42
54:3:2:G:C6	54:3:3:C:N4	2.88	0.42
57:6:41:C:C4	57:6:42:C:N4	2.88	0.42
2:C:5:VAL:HG21	2:C:80:TRP:CE3	2.55	0.42
13:N:49:GLU:HB2	13:N:50:PRO:HD3	2.01	0.42
14:O:79:ALA:CB	14:O:113:ALA:HB3	2.50	0.42
52:1:1350:C:N3	52:1:1382:G:C2	2.87	0.42
52:1:176:A:C6	52:1:177:G:N7	2.88	0.42
52:1:2337:G:C6	52:1:2338:C:C4	3.07	0.42
52:1:2059:A:N6	52:1:2503:2MA:H2'	2.35	0.42
52:1:471:A:H2'	52:1:472:A:O4'	2.19	0.42
53:2:1082:A:H2'	53:2:1083:U:O4'	2.20	0.42
53:2:60:A:N1	53:2:107:G:O2'	2.40	0.42
57:6:29:G:N2	57:6:42:C:C2	2.88	0.42
3:D:39:ALA:HB2	52:1:615:U:O4	2.20	0.42
20:U:34:VAL:HG13	20:U:67:VAL:HG22	2.01	0.42
52:1:1720:U:H2'	52:1:1721:G:O4'	2.20	0.41
52:1:1918:A:O2'	52:1:1920:C:N4	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:634:C:H6	52:1:634:C:O5'	2.02	0.41
53:2:1242:G:H2'	53:2:1243:C:O4'	2.20	0.41
53:2:229:U:H2'	53:2:230:G:O4'	2.20	0.41
53:2:446:G:C2	53:2:489:C:C2	3.08	0.41
53:2:890:G:O2'	53:2:906:A:N6	2.53	0.41
53:2:915:A:C6	53:2:916:U:C4	3.08	0.41
56:5:1:G:O6	56:5:71:C:N3	2.53	0.41
56:5:18:G:N2	56:5:57:A:H2'	2.35	0.41
56:5:70:G:H2'	56:5:71:C:H5'	2.02	0.41
57:6:44:G:H1'	57:6:45:U:C6	2.55	0.41
12:M:16:ARG:NH2	52:1:954:G:OP2	2.53	0.41
52:1:1306:C:C2	52:1:1623:G:C2	3.08	0.41
52:1:1540:G:H2'	52:1:1541:C:C6	2.55	0.41
52:1:1684:G:C2	52:1:1685:C:C2	3.08	0.41
52:1:2070:A:C2	52:1:2442:C:C2	3.08	0.41
52:1:2337:G:C2	52:1:2338:C:C2	3.08	0.41
52:1:2485:G:C2	52:1:2486:C:C2	3.07	0.41
52:1:2495:G:C6	52:1:2496:C:C4	3.09	0.41
52:1:2895:G:H2'	52:1:2896:C:C6	2.55	0.41
52:1:690:G:C6	52:1:691:C:C4	3.08	0.41
52:1:697:G:C6	52:1:698:C:C4	3.09	0.41
52:1:954:G:C2	52:1:964:C:O2	2.73	0.41
53:2:1515:G:C2	53:2:1521:C:C2	3.08	0.41
54:3:110:C:C4	54:3:111:U:C5	3.08	0.41
54:3:15:A:HO2'	54:3:16:G:C5'	2.33	0.41
55:4:10:G:N1	55:4:11:C:C4	2.87	0.41
57:6:10:G:C6	57:6:11:C:C4	3.08	0.41
59:8:624:PHE:CD1	59:8:644:LEU:HD13	2.55	0.41
4:E:131:GLY:HA2	4:E:153:ASP:HA	2.01	0.41
52:1:1256:G:C6	52:1:1257:C:C4	3.08	0.41
52:1:1334:G:C6	52:1:1335:C:C4	3.08	0.41
52:1:1445:G:C5	52:1:1446:C:C5	3.08	0.41
52:1:2080:A:H2'	52:1:2081:U:O4'	2.20	0.41
52:1:2618:G:H2'	52:1:2619:C:O4'	2.20	0.41
52:1:273:G:H2'	52:1:274:C:O4'	2.20	0.41
52:1:600:G:C6	52:1:601:C:C4	3.08	0.41
1:B:207:LYS:HB2	52:1:729:G:C6	2.55	0.41
53:2:1258:G:N2	53:2:1259:C:C2	2.88	0.41
53:2:1149:C:O2'	53:2:1280:A:N1	2.45	0.41
53:2:1391:U:H2'	53:2:1392:G:C8	2.55	0.41
53:2:1492:A:N3	58:7:20:U:O2'	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:31:G:O2'	53:2:48:C:N4	2.52	0.41
53:2:24:U:C4	53:2:559:A:N6	2.87	0.41
57:6:48:C:HO2'	57:6:49:C:P	2.42	0.41
59:8:160:LEU:HD12	59:8:198:LEU:HD23	2.02	0.41
7:H:7:ASP:O	7:H:11:ILE:HG12	2.20	0.41
9:J:11:VAL:HG11	9:J:50:THR:HA	2.03	0.41
52:1:1122:G:C2	52:1:1123:C:C2	3.09	0.41
52:1:1684:G:C6	52:1:1685:C:C4	3.09	0.41
52:1:2283:C:C5	52:1:2389:G:C5	3.08	0.41
52:1:2325:G:C6	52:1:2326:C:N4	2.89	0.41
52:1:2515:C:O2	52:1:2570:G:C2	2.74	0.41
52:1:554:U:O4	52:1:555:G:N1	2.54	0.41
52:1:745:1MG:HM11	52:1:745:1MG:HN21	1.74	0.41
53:2:197:A:N1	53:2:220:G:O2'	2.40	0.41
53:2:418:C:H2'	53:2:419:C:C6	2.56	0.41
53:2:567:G:H2'	53:2:568:G:O4'	2.19	0.41
53:2:642:A:H2'	53:2:643:C:O4'	2.20	0.41
53:2:852:G:C2	53:2:853:C:C2	3.08	0.41
54:3:16:G:H2'	54:3:17:C:O4'	2.20	0.41
1:B:144:VAL:HB	1:B:154:LEU:HB2	2.02	0.41
2:C:151:THR:HB	2:C:152:PRO:HD3	2.02	0.41
18:S:7:HIS:HB2	18:S:50:VAL:HG22	2.02	0.41
52:1:1225:G:C6	52:1:1226:A:C6	3.08	0.41
52:1:1443:U:C2	52:1:1444:G:C8	3.09	0.41
52:1:1459:G:C4	52:1:1461:C:C5	3.08	0.41
52:1:1461:C:C2	52:1:1462:C:C5	3.09	0.41
52:1:1483:G:C2	52:1:1507:C:O2	2.74	0.41
52:1:1827:U:O4	52:1:1828:G:C6	2.74	0.41
52:1:1906:G:H2'	52:1:1907:G:O4'	2.20	0.41
52:1:2548:U:C4	52:1:2549:G:N7	2.88	0.41
52:1:2785:C:H2'	52:1:2786:U:O4'	2.20	0.41
52:1:737:C:C2	52:1:760:G:N2	2.89	0.41
53:2:1258:G:H2'	53:2:1259:C:C6	2.55	0.41
53:2:289:G:N2	53:2:290:C:C2	2.89	0.41
59:8:193:GLN:HA	59:8:196:TRP:CE2	2.55	0.41
14:O:62:LEU:HD13	14:O:70:ALA:HB1	2.03	0.41
52:1:1139:G:N1	52:1:1140:C:C4	2.88	0.41
52:1:1759:A:H4'	52:1:2715:C:O4'	2.21	0.41
52:1:414:C:O2'	52:1:1864:U:O2'	2.27	0.41
52:1:2419:U:H2'	52:1:2420:C:C6	2.55	0.41
52:1:2677:G:N2	52:1:2678:C:C2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:109:A:C6	53:2:327:A:C6	3.09	0.41
53:2:1375:A:H2'	53:2:1376:U:O4'	2.20	0.41
53:2:190:A:C5	53:2:191:G:H1'	2.55	0.41
53:2:354:G:C6	53:2:355:C:N4	2.89	0.41
53:2:763:G:N2	53:2:764:C:C2	2.89	0.41
56:5:22:G:C2	56:5:23:C:C2	3.08	0.41
57:6:6:G:C2	57:6:68:C:C2	3.09	0.41
57:6:71:G:C5	57:6:72:C:C5	3.08	0.41
52:1:1149:G:H2'	52:1:1150:C:H6	1.83	0.41
52:1:1221:C:H2'	52:1:1222:U:O4'	2.21	0.41
52:1:1263:U:C4	52:1:1264:A:C6	3.08	0.41
52:1:1342:A:HO2'	52:1:1344:U:P	2.44	0.41
52:1:1964:G:H4'	52:1:1965:C:OP2	2.20	0.41
52:1:2548:U:H2'	52:1:2549:G:O4'	2.20	0.41
52:1:498:G:C6	52:1:499:U:C4	3.08	0.41
52:1:554:U:C4	52:1:555:G:C5	3.09	0.41
52:1:839:U:H2'	52:1:840:C:C6	2.56	0.41
52:1:910:A:H2'	52:1:911:A:C8	2.55	0.41
53:2:242:G:C2	53:2:285:C:C2	3.09	0.41
53:2:633:G:C4	53:2:634:C:C5	3.09	0.41
56:5:44:A:N6	56:5:45:G:C6	2.89	0.41
2:C:33:ARG:NH1	2:C:53:GLY:O	2.54	0.41
2:C:5:VAL:HG21	2:C:80:TRP:CD2	2.55	0.41
3:D:148:ILE:HB	3:D:169:VAL:HG22	2.02	0.41
4:E:155:THR:HG21	52:1:2314:A:C1'	2.50	0.41
6:G:31:VAL:N	6:G:32:PRO:HD2	2.36	0.41
12:M:41:LEU:HG	12:M:96:ILE:HG13	2.03	0.41
16:Q:82:GLY:HA3	16:Q:113:ALA:HB1	2.02	0.41
21:V:70:ILE:HG22	21:V:72:VAL:HG13	2.01	0.41
52:1:1112:G:H2'	52:1:1113:U:O4'	2.21	0.41
18:S:13:SER:CB	52:1:1266:G:O6	2.68	0.41
52:1:1334:G:C2	52:1:1335:C:C2	3.08	0.41
52:1:1386:C:H2'	52:1:1387:A:C8	2.56	0.41
52:1:1511:G:N2	52:1:1512:C:C2	2.89	0.41
52:1:2006:C:H1'	52:1:2823:A:O2'	2.20	0.41
15:P:2:SER:OG	52:1:2875:C:O3'	2.24	0.41
52:1:539:G:H2'	52:1:540:C:O4'	2.21	0.41
53:2:108:G:N2	53:2:109:A:N1	2.68	0.41
53:2:1192:C:H2'	53:2:1193:G:O4'	2.21	0.41
53:2:1365:G:C4	53:2:1366:C:C5	3.09	0.41
53:2:931:C:O2	53:2:1387:G:C2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:289:G:C2	53:2:290:C:C2	3.08	0.41
53:2:886:G:C2	53:2:912:C:C2	3.08	0.41
57:6:32:PSU:H4'	57:6:33:U:OP1	2.21	0.41
59:8:49:HIS:CG	59:8:50:PRO:HD2	2.55	0.41
13:N:54:LEU:HD21	13:N:65:LEU:HB3	2.03	0.41
52:1:1067:A:C2	57:6:57:G:C5	3.08	0.41
52:1:1228:G:H2'	52:1:1229:C:C6	2.56	0.41
52:1:1363:C:O2	52:1:1369:G:C2	2.74	0.41
52:1:2192:U:H2'	52:1:2193:G:O4'	2.21	0.41
52:1:2298:A:H2'	52:1:2299:U:O4'	2.20	0.41
52:1:2363:G:N1	52:1:2364:C:C4	2.89	0.41
52:1:2567:G:H2'	52:1:2568:U:C6	2.56	0.41
52:1:884:U:C4	52:1:885:C:C5	3.09	0.41
53:2:1096:C:H2'	53:2:1097:C:O4'	2.21	0.41
53:2:203:G:C2	53:2:215:C:C2	3.09	0.41
53:2:838:G:H2'	53:2:839:C:O4'	2.21	0.41
53:2:915:A:C6	53:2:916:U:C5	3.08	0.41
56:5:21:A:C6	56:5:48:C:C2	3.09	0.41
59:8:339:ARG:HH21	59:8:339:ARG:HG3	1.86	0.41
1:B:51:THR:HG21	52:1:1814:G:H4'	2.03	0.41
11:L:77:ILE:HG23	11:L:100:ILE:HG21	2.03	0.41
14:O:51:ALA:HB3	14:O:78:VAL:CG2	2.50	0.41
21:V:21:ARG:HE	21:V:87:GLN:HA	1.86	0.41
52:1:1878:G:C5	52:1:1879:C:C5	3.08	0.41
52:1:191:A:H2'	52:1:192:C:O4'	2.20	0.41
52:1:1964:G:C6	52:1:1967:C:C4	3.09	0.41
52:1:2329:U:H2'	52:1:2330:G:C8	2.56	0.41
52:1:271:G:HO2'	52:1:272:A:C5'	2.34	0.41
52:1:2847:U:O4	52:1:2848:G:N1	2.54	0.41
52:1:579:G:H2'	52:1:580:U:C6	2.56	0.41
52:1:679:C:C2	52:1:799:G:C2	3.09	0.41
52:1:888:C:H2'	52:1:889:C:O4'	2.20	0.41
52:1:972:A:N1	52:1:973:A:N6	2.69	0.41
53:2:1330:U:O4	53:2:1331:G:N1	2.54	0.41
53:2:1507:A:H2'	53:2:1508:A:C8	2.56	0.41
53:2:268:U:H2'	53:2:269:C:C6	2.55	0.41
53:2:300:A:H1'	53:2:565:U:O2	2.21	0.41
53:2:842:U:H3'	53:2:843:U:C5'	2.50	0.41
53:2:929:G:C6	53:2:930:C:C4	3.09	0.41
54:3:47:C:C4	54:3:48:U:C5	3.09	0.41
59:8:622:VAL:HG11	59:8:641:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:8:645:ARG:HA	59:8:652:ILE:HD12	2.03	0.41
59:8:680:LEU:O	59:8:684:THR:HG23	2.21	0.41
3:D:157:LEU:HG	3:D:169:VAL:HG21	2.01	0.41
1:B:15:HIS:NE2	52:1:1829:A:N3	2.69	0.41
52:1:1998:A:H2'	52:1:1999:C:O4'	2.20	0.41
52:1:2073:C:O2	52:1:2437:G:C2	2.74	0.41
52:1:486:C:C2	52:1:495:G:C2	3.09	0.41
52:1:568:U:O2'	52:1:570:G:N7	2.52	0.41
52:1:600:G:C2	52:1:601:C:C2	3.09	0.41
53:2:13:U:N3	53:2:915:A:C5	2.81	0.41
53:2:39:G:C5	53:2:40:C:C5	3.08	0.41
53:2:736:C:H2'	53:2:737:C:H6	1.84	0.41
54:3:16:G:C2	54:3:17:C:N1	2.89	0.41
1:B:221:ARG:HG3	52:1:1789:A:OP1	2.20	0.41
52:1:1232:G:C5	52:1:1233:C:C5	3.08	0.40
52:1:1405:U:O2	52:1:1406:U:N3	2.54	0.40
52:1:2023:C:O5'	52:1:2617:U:H4'	2.21	0.40
52:1:2643:G:H2'	52:1:2644:G:O4'	2.21	0.40
52:1:2895:G:N2	52:1:2896:C:C2	2.88	0.40
52:1:36:G:N2	52:1:445:C:C2	2.89	0.40
52:1:703:U:H2'	52:1:704:G:O4'	2.21	0.40
53:2:1050:G:C4	53:2:1051:C:C5	3.09	0.40
53:2:105:G:H2'	53:2:106:C:O4'	2.21	0.40
53:2:1260:G:C2	53:2:1274:A:C2	3.09	0.40
53:2:1442:G:C6	53:2:1443:C:C4	3.09	0.40
53:2:171:A:H2'	53:2:172:A:C8	2.56	0.40
53:2:403:C:H2'	53:2:404:G:O4'	2.21	0.40
53:2:558:G:C8	53:2:559:A:H2'	2.56	0.40
53:2:572:A:N1	53:2:864:A:C5	2.89	0.40
53:2:788:U:H2'	53:2:789:U:O4'	2.20	0.40
56:5:73:A:H5'	56:5:74:C:O4'	2.21	0.40
59:8:17:PRO:HB3	59:8:63:VAL:HG13	2.03	0.40
52:1:1459:G:C5	52:1:1461:C:C4	3.09	0.40
52:1:1831:G:C6	52:1:1832:C:C4	3.09	0.40
52:1:2030:6MZ:H2	52:1:2499:C:H5"	2.03	0.40
52:1:414:C:C2	52:1:2410:G:N2	2.88	0.40
52:1:2728:U:HO2'	52:1:2729:G:H8	1.69	0.40
52:1:941:A:H2'	52:1:942:G:O4'	2.21	0.40
53:2:1494:G:N7	62:2:1665:PAR:N32	2.70	0.40
53:2:22:G:C5	53:2:23:C:C5	3.10	0.40
53:2:925:G:C2	53:2:927:G:C8	3.08	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:3:106:G:H2'	54:3:107:G:O4'	2.21	0.40
14:O:29:HIS:CE1	54:3:7:G:H5'	2.56	0.40
56:5:15:C:H3'	56:5:16:C:H5"	2.03	0.40
56:5:44:A:H2'	56:5:45:G:C5'	2.51	0.40
4:E:25:VAL:O	4:E:28:VAL:HG12	2.21	0.40
17:R:59:ILE:HG23	17:R:101:ILE:HD13	2.03	0.40
17:R:74:ILE:HB	17:R:87:GLN:HB3	2.02	0.40
52:1:1062:G:C2	52:1:1077:A:C2	3.09	0.40
52:1:1139:G:C2	52:1:1140:C:C6	3.09	0.40
16:Q:58:ARG:NH1	52:1:1154:G:OP2	2.54	0.40
52:1:1789:A:H2'	52:1:1790:C:O4'	2.21	0.40
2:C:133:THR:HG22	52:1:1993:U:H4'	2.04	0.40
52:1:2341:G:C6	52:1:2342:C:C4	3.10	0.40
52:1:2352:A:N6	52:1:2365:G:O2'	2.53	0.40
52:1:2643:G:N2	52:1:2772:C:C2	2.89	0.40
53:2:441:A:C2	53:2:497:G:C6	3.09	0.40
53:2:501:C:H2'	53:2:502:A:C8	2.56	0.40
53:2:540:G:C6	53:2:541:G:C5	3.09	0.40
53:2:67:C:H2'	53:2:68:G:C8	2.57	0.40
56:5:24:U:C4	56:5:25:C:C5	3.09	0.40
1:B:141:VAL:O	1:B:162:VAL:N	2.50	0.40
22:W:37:ILE:HD11	22:W:82:ILE:HD11	2.03	0.40
52:1:1132:U:H3'	52:1:1133:A:H5"	2.03	0.40
52:1:1424:G:H2'	52:1:1425:G:O4'	2.21	0.40
52:1:1560:G:C4	52:1:1561:C:C5	3.09	0.40
52:1:2225:A:H4'	52:1:2226:C:O5'	2.21	0.40
52:1:2261:C:N3	52:1:2280:G:C2	2.90	0.40
52:1:2570:G:H2'	52:1:2571:U:O4'	2.22	0.40
53:2:1067:A:N1	53:2:1108:G:O2'	2.52	0.40
53:2:1088:G:H2'	53:2:1089:G:O4'	2.22	0.40
53:2:1328:C:H2'	53:2:1329:A:O4'	2.21	0.40
53:2:932:C:C2	53:2:1386:G:C2	3.09	0.40
53:2:506:G:C2	53:2:507:C:C2	3.10	0.40
53:2:632:U:O2	53:2:632:U:H2'	2.20	0.40
53:2:847:G:C2	53:2:848:C:C2	3.09	0.40
57:6:24:G:C5	57:6:25:C:C5	3.09	0.40
59:8:143:VAL:HG12	59:8:145:ASP:H	1.86	0.40
3:D:48:THR:HG23	3:D:86:ALA:HB3	2.04	0.40
9:J:17:VAL:HG23	9:J:137:PRO:HB2	2.04	0.40
52:1:1074:G:C6	52:1:1075:C:C4	3.09	0.40
52:1:30:G:O2'	52:1:1214:A:N3	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:1289:C:H2'	52:1:1290:C:C6	2.57	0.40
52:1:1294:U:C4	52:1:1295:C:C5	3.10	0.40
52:1:1584:U:O2	52:1:1584:U:H2'	2.22	0.40
52:1:221:A:C8	52:1:266:G:O6	2.75	0.40
52:1:2839:G:C5	52:1:2840:C:C4	3.10	0.40
52:1:600:G:C6	52:1:601:C:N3	2.89	0.40
53:2:201:G:C6	53:2:217:C:N3	2.90	0.40
53:2:276:G:C2	53:2:277:C:C2	3.10	0.40
53:2:945:G:H2'	53:2:945:G:N3	2.36	0.40
54:3:112:G:H2'	54:3:113:C:C6	2.56	0.40
55:4:8:U:O4	55:4:21:A:N1	2.55	0.40
56:5:22:G:C4	56:5:23:C:C5	3.09	0.40
56:5:66:C:N4	56:5:67:C:N4	2.70	0.40
2:C:26:VAL:HG12	2:C:186:LEU:HD22	2.03	0.40
2:C:202:ILE:HD12	2:C:202:ILE:N	2.37	0.40
16:Q:43:GLY:HA3	17:R:75:VAL:HB	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
1	B	269/273 (98%)	249 (93%)	18 (7%)	2 (1%)	26 70
2	C	207/209 (99%)	190 (92%)	16 (8%)	1 (0%)	34 76
3	D	199/201 (99%)	184 (92%)	14 (7%)	1 (0%)	34 76
4	E	175/179 (98%)	158 (90%)	13 (7%)	4 (2%)	8 36
5	F	174/177 (98%)	156 (90%)	17 (10%)	1 (1%)	30 72
6	G	147/149 (99%)	126 (86%)	17 (12%)	4 (3%)	6 32
7	H	129/165 (78%)	103 (80%)	18 (14%)	8 (6%)	2 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	I	139/142 (98%)	113 (81%)	20 (14%)	6 (4%)	3 19
9	J	140/142 (99%)	135 (96%)	5 (4%)	0	100 100
10	K	121/123 (98%)	110 (91%)	11 (9%)	0	100 100
11	L	142/144 (99%)	131 (92%)	9 (6%)	2 (1%)	14 51
12	M	134/136 (98%)	125 (93%)	9 (7%)	0	100 100
13	N	118/127 (93%)	107 (91%)	10 (8%)	1 (1%)	24 66
14	O	114/117 (97%)	103 (90%)	9 (8%)	2 (2%)	11 45
15	P	112/115 (97%)	100 (89%)	12 (11%)	0	100 100
16	Q	115/118 (98%)	111 (96%)	3 (3%)	1 (1%)	21 64
17	R	101/103 (98%)	90 (89%)	9 (9%)	2 (2%)	9 41
18	S	108/110 (98%)	102 (94%)	6 (6%)	0	100 100
19	T	91/100 (91%)	85 (93%)	6 (7%)	0	100 100
20	U	100/104 (96%)	91 (91%)	7 (7%)	2 (2%)	9 41
21	V	92/94 (98%)	89 (97%)	3 (3%)	0	100 100
22	W	75/85 (88%)	74 (99%)	1 (1%)	0	100 100
23	X	75/78 (96%)	69 (92%)	6 (8%)	0	100 100
24	Y	60/63 (95%)	56 (93%)	3 (5%)	1 (2%)	11 46
25	Z	56/59 (95%)	51 (91%)	5 (9%)	0	100 100
26	a	64/70 (91%)	51 (80%)	12 (19%)	1 (2%)	12 48
27	b	54/57 (95%)	51 (94%)	3 (6%)	0	100 100
28	c	48/55 (87%)	41 (85%)	7 (15%)	0	100 100
29	d	44/46 (96%)	43 (98%)	1 (2%)	0	100 100
30	e	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	12 48
31	f	36/38 (95%)	35 (97%)	1 (3%)	0	100 100
32	g	222/241 (92%)	200 (90%)	15 (7%)	7 (3%)	5 27
33	h	205/233 (88%)	185 (90%)	18 (9%)	2 (1%)	19 61
34	i	203/206 (98%)	194 (96%)	9 (4%)	0	100 100
35	j	155/167 (93%)	142 (92%)	10 (6%)	3 (2%)	10 43
36	k	98/135 (73%)	88 (90%)	9 (9%)	1 (1%)	19 61
37	l	149/179 (83%)	140 (94%)	7 (5%)	2 (1%)	15 53
38	m	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	24 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
39	n	125/130 (96%)	113 (90%)	10 (8%)	2 (2%)	12 48
40	o	96/103 (93%)	82 (85%)	11 (12%)	3 (3%)	5 28
41	p	115/129 (89%)	98 (85%)	15 (13%)	2 (2%)	11 46
42	q	120/124 (97%)	109 (91%)	10 (8%)	1 (1%)	24 66
43	r	112/118 (95%)	106 (95%)	6 (5%)	0	100 100
44	s	98/101 (97%)	93 (95%)	5 (5%)	0	100 100
45	t	86/89 (97%)	81 (94%)	5 (6%)	0	100 100
46	u	80/82 (98%)	69 (86%)	7 (9%)	4 (5%)	3 15
47	v	78/84 (93%)	72 (92%)	4 (5%)	2 (3%)	7 33
48	w	63/75 (84%)	60 (95%)	3 (5%)	0	100 100
49	x	80/92 (87%)	73 (91%)	5 (6%)	2 (2%)	7 34
50	y	84/87 (97%)	83 (99%)	1 (1%)	0	100 100
51	z	54/71 (76%)	52 (96%)	1 (2%)	1 (2%)	10 43
59	8	604/744 (81%)	528 (87%)	55 (9%)	21 (4%)	4 24
All	All	6455/6964 (93%)	5874 (91%)	487 (8%)	94 (2%)	18 50

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	175	PHE
7	H	4	ASN
7	H	123	ILE
11	L	99	ASN
17	R	51	VAL
32	g	130	THR
32	g	131	LYS
46	u	43	ALA
59	8	117	ARG
59	8	125	ASP
59	8	136	ARG
59	8	137	ARG
59	8	167	PRO
59	8	596	ARG
59	8	616	ILE
6	G	15	LEU
6	G	41	LYS
11	L	29	LYS

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Mol	Chain	Res	Type
26	a	40	CYS
32	g	127	ASP
37	l	130	ASN
40	o	57	VAL
47	v	18	GLU
59	8	115	ALA
59	8	131	GLN
59	8	168	GLU
59	8	350	GLY
4	E	41	GLY
4	E	174	ASP
5	F	47	ASP
8	I	64	ARG
16	Q	87	SER
20	U	99	ASN
24	Y	3	ALA
32	g	100	MET
33	h	80	LYS
35	j	111	MET
35	j	147	MET
36	k	52	ASN
41	p	14	LYS
42	q	16	VAL
47	v	16	LYS
59	8	120	LYS
59	8	124	THR
59	8	126	SER
59	8	133	ASP
1	B	158	ALA
6	G	54	LEU
7	H	57	ASN
7	H	108	VAL
7	H	118	ILE
7	H	119	PRO
8	I	38	CYS
32	g	126	PHE
32	g	129	LEU
49	x	29	LYS
59	8	666	SER
6	G	3	VAL
7	H	88	HIS
8	I	12	VAL

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Mol	Chain	Res	Type
8	I	92	PRO
13	N	33	ILE
14	O	99	TYR
32	g	165	ASP
38	m	75	ILE
40	o	36	VAL
40	o	75	ASP
46	u	64	GLY
51	z	56	HIS
59	8	268	LEU
59	8	635	ARG
59	8	660	SER
2	C	151	THR
3	D	69	ARG
33	h	101	ILE
39	n	92	GLU
46	u	44	SER
30	e	32	ILE
7	H	55	VAL
49	x	67	VAL
59	8	331	GLY
4	E	84	PRO
17	R	44	GLY
20	U	39	ILE
37	l	82	GLY
39	n	26	GLY
59	8	89	VAL
1	B	56	GLY
8	I	22	PRO
8	I	136	GLY
35	j	44	GLY
14	O	114	GLY
41	p	74	VAL
46	u	30	GLY

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
1	B	216/218 (99%)	205 (95%)	11 (5%)	29 69
2	C	164/164 (100%)	159 (97%)	5 (3%)	48 83
3	D	165/165 (100%)	156 (94%)	9 (6%)	27 65
4	E	148/150 (99%)	138 (93%)	10 (7%)	20 56
5	F	137/138 (99%)	129 (94%)	8 (6%)	25 63
6	G	114/114 (100%)	114 (100%)	0	100 100
7	H	100/123 (81%)	97 (97%)	3 (3%)	48 83
8	I	109/110 (99%)	106 (97%)	3 (3%)	51 84
9	J	116/116 (100%)	114 (98%)	2 (2%)	68 91
10	K	104/104 (100%)	99 (95%)	5 (5%)	31 71
11	L	103/103 (100%)	98 (95%)	5 (5%)	31 71
12	M	109/109 (100%)	106 (97%)	3 (3%)	51 84
13	N	100/103 (97%)	96 (96%)	4 (4%)	38 77
14	O	86/87 (99%)	79 (92%)	7 (8%)	15 47
15	P	99/100 (99%)	96 (97%)	3 (3%)	48 83
16	Q	89/90 (99%)	82 (92%)	7 (8%)	15 48
17	R	84/84 (100%)	80 (95%)	4 (5%)	31 71
18	S	93/93 (100%)	87 (94%)	6 (6%)	21 58
19	T	80/84 (95%)	74 (92%)	6 (8%)	17 51
20	U	83/85 (98%)	80 (96%)	3 (4%)	42 79
21	V	78/78 (100%)	73 (94%)	5 (6%)	22 59
22	W	59/63 (94%)	59 (100%)	0	100 100
23	X	67/68 (98%)	67 (100%)	0	100 100
24	Y	54/55 (98%)	50 (93%)	4 (7%)	17 52
25	Z	48/49 (98%)	45 (94%)	3 (6%)	22 60
26	a	59/62 (95%)	58 (98%)	1 (2%)	68 91
27	b	47/48 (98%)	45 (96%)	2 (4%)	35 75
28	c	45/49 (92%)	44 (98%)	1 (2%)	60 88
29	d	38/38 (100%)	32 (84%)	6 (16%)	3 15
30	e	51/52 (98%)	46 (90%)	5 (10%)	10 36
31	f	34/34 (100%)	30 (88%)	4 (12%)	6 26
32	g	186/199 (94%)	179 (96%)	7 (4%)	40 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
33	h	170/189 (90%)	160 (94%)	10 (6%)	24 63
34	i	172/173 (99%)	167 (97%)	5 (3%)	50 84
35	j	119/126 (94%)	108 (91%)	11 (9%)	11 40
36	k	87/116 (75%)	82 (94%)	5 (6%)	25 64
37	l	124/147 (84%)	113 (91%)	11 (9%)	12 42
38	m	104/105 (99%)	96 (92%)	8 (8%)	16 50
39	n	105/107 (98%)	97 (92%)	8 (8%)	16 51
40	o	86/90 (96%)	78 (91%)	8 (9%)	11 39
41	p	90/99 (91%)	84 (93%)	6 (7%)	20 57
42	q	102/103 (99%)	97 (95%)	5 (5%)	31 71
43	r	92/96 (96%)	84 (91%)	8 (9%)	13 43
44	s	83/84 (99%)	79 (95%)	4 (5%)	31 71
45	t	76/77 (99%)	69 (91%)	7 (9%)	11 40
46	u	65/65 (100%)	59 (91%)	6 (9%)	11 40
47	v	74/78 (95%)	67 (90%)	7 (10%)	11 38
48	w	57/66 (86%)	55 (96%)	2 (4%)	43 80
49	x	72/79 (91%)	69 (96%)	3 (4%)	36 76
50	y	65/66 (98%)	59 (91%)	6 (9%)	11 40
51	z	48/61 (79%)	44 (92%)	4 (8%)	14 46
59	8	500/629 (80%)	438 (88%)	62 (12%)	6 24
All	All	5356/5691 (94%)	5028 (94%)	328 (6%)	28 61

All (328) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	52	ARG
1	B	105	LEU
1	B	130	LEU
1	B	156	ARG
1	B	195	VAL
1	B	202	LEU
1	B	203	ARG
1	B	204	VAL
1	B	205	LEU
1	B	242	LYS

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Mol	Chain	Res	Type
1	B	271	ARG
2	C	13	ARG
2	C	32	ASN
2	C	43	ASP
2	C	149	ASN
2	C	170	VAL
3	D	25	GLU
3	D	57	LYS
3	D	73	ILE
3	D	108	ILE
3	D	109	LEU
3	D	111	GLU
3	D	123	LYS
3	D	149	ILE
3	D	200	LEU
4	E	50	LEU
4	E	64	LYS
4	E	80	ARG
4	E	94	GLU
4	E	106	ILE
4	E	117	LEU
4	E	123	ASP
4	E	137	ILE
4	E	140	GLU
4	E	175	PHE
5	F	20	ASN
5	F	29	LYS
5	F	39	ASP
5	F	101	ASN
5	F	114	ASP
5	F	117	LEU
5	F	155	GLU
5	F	166	ASP
7	H	33	VAL
7	H	57	ASN
7	H	122	GLN
8	I	10	LEU
8	I	11	GLN
8	I	48	ILE
9	J	30	THR
9	J	128	ASN
10	K	17	ARG

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Mol	Chain	Res	Type
10	K	32	TYR
10	K	58	LEU
10	K	67	LYS
10	K	123	LEU
11	L	42	SER
11	L	48	ARG
11	L	82	LEU
11	L	91	ASP
11	L	115	GLU
12	M	14	LYS
12	M	18	ARG
12	M	118	LYS
13	N	1	MET
13	N	17	ARG
13	N	24	MET
13	N	69	ARG
14	O	7	ARG
14	O	17	LYS
14	O	18	LEU
14	O	19	GLN
14	O	31	THR
14	O	53	THR
14	O	104	GLN
15	P	2	SER
15	P	102	GLU
15	P	114	LEU
16	Q	16	LYS
16	Q	18	LEU
16	Q	41	LYS
16	Q	51	ARG
16	Q	52	GLN
16	Q	91	ASP
16	Q	117	LEU
17	R	10	LYS
17	R	31	GLU
17	R	49	ILE
17	R	51	VAL
18	S	7	HIS
18	S	22	ASP
18	S	28	LYS
18	S	41	LYS
18	S	95	ARG

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Mol	Chain	Res	Type
18	S	96	ILE
19	T	2	ILE
19	T	3	ARG
19	T	30	ILE
19	T	49	LYS
19	T	50	LEU
19	T	77	ARG
20	U	46	GLN
20	U	72	ILE
20	U	99	ASN
21	V	10	LYS
21	V	14	LYS
21	V	24	ASN
21	V	40	ILE
21	V	53	LYS
24	Y	18	LEU
24	Y	57	LEU
24	Y	58	ASN
24	Y	60	LYS
25	Z	4	THR
25	Z	31	ARG
25	Z	45	ARG
26	a	44	PHE
27	b	27	SER
27	b	28	LEU
28	c	47	VAL
29	d	1	MET
29	d	3	ARG
29	d	22	MET
29	d	24	THR
29	d	41	ARG
29	d	44	VAL
30	e	13	ARG
30	e	30	ARG
30	e	47	LYS
30	e	54	ASP
30	e	55	LEU
31	f	3	VAL
31	f	4	ARG
31	f	12	ARG
31	f	26	ILE
32	g	23	TRP

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Mol	Chain	Res	Type
32	g	105	LYS
32	g	117	LEU
32	g	129	LEU
32	g	159	ASP
32	g	167	ASP
32	g	220	THR
33	h	3	GLN
33	h	55	ILE
33	h	64	ILE
33	h	107	ARG
33	h	126	ARG
33	h	152	GLU
33	h	156	ARG
33	h	185	ASN
33	h	200	VAL
33	h	206	GLU
34	i	26	ARG
34	i	58	LYS
34	i	105	MET
34	i	116	GLN
34	i	206	LYS
35	j	52	LYS
35	j	60	ILE
35	j	81	LEU
35	j	93	ARG
35	j	105	ILE
35	j	114	VAL
35	j	115	LEU
35	j	120	VAL
35	j	122	ASN
35	j	138	ARG
35	j	146	ASN
36	k	2	ARG
36	k	14	GLN
36	k	38	ARG
36	k	54	LEU
36	k	86	ARG
37	l	2	PRO
37	l	5	ARG
37	l	23	LEU
37	l	30	LEU
37	l	48	GLU

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Mol	Chain	Res	Type
37	l	50	LEU
37	l	59	LEU
37	l	77	SER
37	l	109	ARG
37	l	123	GLU
37	l	130	ASN
38	m	10	MET
38	m	13	ARG
38	m	27	MET
38	m	54	ASP
38	m	77	ARG
38	m	80	ARG
38	m	87	LYS
38	m	121	LEU
39	n	12	ARG
39	n	18	ARG
39	n	63	LEU
39	n	87	LEU
39	n	98	LEU
39	n	118	LEU
39	n	123	ARG
39	n	130	ARG
40	o	16	ARG
40	o	25	ILE
40	o	35	GLN
40	o	37	ARG
40	o	47	GLU
40	o	73	LEU
40	o	87	LEU
40	o	90	LEU
41	p	15	GLN
41	p	65	VAL
41	p	72	ASP
41	p	100	LEU
41	p	107	ILE
41	p	119	ASN
42	q	9	ARG
42	q	52	VAL
42	q	88	LYS
42	q	103	ASP
42	q	121	ARG
43	r	16	VAL

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Mol	Chain	Res	Type
43	r	27	LYS
43	r	29	ARG
43	r	48	LEU
43	r	59	GLU
43	r	60	VAL
43	r	104	THR
43	r	110	LYS
44	s	24	ARG
44	s	42	TRP
44	s	55	SER
44	s	89	MET
45	t	18	ASP
45	t	39	LEU
45	t	64	ARG
45	t	66	LEU
45	t	70	LEU
45	t	84	ARG
45	t	89	ARG
46	u	1	MET
46	u	46	LYS
46	u	51	ARG
46	u	55	ASP
46	u	77	GLU
46	u	80	LYS
47	v	21	ILE
47	v	38	ILE
47	v	40	ARG
47	v	55	ILE
47	v	73	TRP
47	v	75	LEU
47	v	81	LYS
48	w	43	ARG
48	w	52	GLN
49	x	13	LEU
49	x	32	ARG
49	x	49	ILE
50	y	6	SER
50	y	10	ARG
50	y	27	MET
50	y	54	MET
50	y	64	LYS
50	y	67	ILE

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Mol	Chain	Res	Type
51	z	20	LYS
51	z	24	GLU
51	z	34	ARG
51	z	44	GLU
59	8	15	PHE
59	8	16	ASP
59	8	18	GLU
59	8	39	TRP
59	8	41	TYR
59	8	49	HIS
59	8	84	LEU
59	8	88	ASN
59	8	112	ASP
59	8	116	ILE
59	8	122	THR
59	8	125	ASP
59	8	128	SER
59	8	134	ASN
59	8	135	VAL
59	8	159	HIS
59	8	163	VAL
59	8	164	LYS
59	8	179	THR
59	8	187	ASN
59	8	191	ILE
59	8	194	LEU
59	8	204	ARG
59	8	205	TYR
59	8	214	ILE
59	8	220	GLU
59	8	246	LYS
59	8	264	GLN
59	8	265	LYS
59	8	275	ASP
59	8	299	HIS
59	8	313	ASN
59	8	339	ARG
59	8	344	HIS
59	8	396	GLU
59	8	410	THR
59	8	430	HIS
59	8	457	MET

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Mol	Chain	Res	Type
59	8	467	LYS
59	8	470	ASN
59	8	487	ARG
59	8	594	ASN
59	8	602	VAL
59	8	611	ARG
59	8	616	ILE
59	8	622	VAL
59	8	629	ARG
59	8	632	SER
59	8	635	ARG
59	8	650	GLU
59	8	665	TYR
59	8	667	LEU
59	8	676	ARG
59	8	679	LEU
59	8	681	ARG
59	8	682	ASP
59	8	690	GLU
59	8	691	LYS
59	8	700	ARG
59	8	711	ASP
59	8	716	ILE
59	8	740	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	153	GLN
2	C	149	ASN
3	D	24	ASN
4	E	37	ASN
21	V	24	ASN
23	X	16	ASN
45	t	46	HIS
50	y	21	ASN
50	y	68	HIS
59	8	118	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	1	2891/2904 (99%)	610 (21%)	61 (2%)
53	2	1524/1533 (99%)	324 (21%)	24 (1%)
54	3	117/118 (99%)	19 (16%)	0
55	4	74/76 (97%)	22 (29%)	0
56	5	75/78 (96%)	37 (49%)	14 (18%)
57	6	73/76 (96%)	42 (57%)	11 (15%)
58	7	9/10 (90%)	0	0
All	All	4763/4795 (99%)	1054 (22%)	110 (2%)

All (1054) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	1	10	A
52	1	15	G
52	1	34	U
52	1	35	G
52	1	39	G
52	1	46	G
52	1	49	A
52	1	50	U
52	1	51	G
52	1	55	G
52	1	58	G
52	1	61	C
52	1	62	U
52	1	63	A
52	1	70	G
52	1	71	A
52	1	74	A
52	1	75	G
52	1	78	U
52	1	83	A
52	1	84	A
52	1	93	G
52	1	96	C
52	1	101	A
52	1	102	U
52	1	110	G
52	1	118	A
52	1	119	A
52	1	120	U
52	1	122	G
52	1	135	U

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Mol	Chain	Res	Type
52	1	137	U
52	1	138	U
52	1	139	U
52	1	140	C
52	1	141	G
52	1	142	A
52	1	149	A
52	1	154	U
52	1	158	U
52	1	163	C
52	1	165	A
52	1	181	A
52	1	196	A
52	1	199	A
52	1	215	G
52	1	216	A
52	1	222	A
52	1	228	C
52	1	233	A
52	1	234	U
52	1	241	A
52	1	248	G
52	1	249	C
52	1	264	C
52	1	265	A
52	1	266	G
52	1	271	G
52	1	272	A
52	1	273	G
52	1	276	U
52	1	277	G
52	1	278	A
52	1	285	G
52	1	291	G
52	1	294	A
52	1	311	A
52	1	315	G
52	1	321	U
52	1	322	A
52	1	327	G
52	1	329	G
52	1	330	A

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Mol	Chain	Res	Type
52	1	338	G
52	1	353	C
52	1	359	G
52	1	361	G
52	1	362	A
52	1	371	A
52	1	372	G
52	1	373	U
52	1	383	C
52	1	386	G
52	1	396	G
52	1	399	U
52	1	403	U
52	1	404	A
52	1	405	U
52	1	411	G
52	1	412	A
52	1	424	G
52	1	425	G
52	1	451	U
52	1	455	C
52	1	456	C
52	1	457	A
52	1	477	A
52	1	479	A
52	1	481	G
52	1	490	C
52	1	491	G
52	1	496	G
52	1	504	A
52	1	505	A
52	1	508	A
52	1	510	C
52	1	513	A
52	1	529	A
52	1	530	G
52	1	531	C
52	1	532	A
52	1	542	C
52	1	546	U
52	1	547	A
52	1	548	G

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Mol	Chain	Res	Type
52	1	549	G
52	1	555	G
52	1	556	A
52	1	558	U
52	1	563	A
52	1	569	U
52	1	573	U
52	1	575	A
52	1	577	G
52	1	580	U
52	1	582	A
52	1	588	U
52	1	603	A
52	1	613	A
52	1	614	A
52	1	615	U
52	1	616	A
52	1	620	G
52	1	621	A
52	1	627	A
52	1	637	A
52	1	645	C
52	1	646	U
52	1	647	G
52	1	651	G
52	1	654	A
52	1	655	A
52	1	656	G
52	1	664	G
52	1	668	A
52	1	677	A
52	1	678	C
52	1	685	A
52	1	686	U
52	1	695	G
52	1	698	C
52	1	710	U
52	1	717	C
52	1	724	U
52	1	730	A
52	1	738	G
52	1	747	5MU

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Mol	Chain	Res	Type
52	1	757	G
52	1	764	A
52	1	765	C
52	1	775	G
52	1	776	G
52	1	782	A
52	1	783	A
52	1	784	G
52	1	785	G
52	1	805	G
52	1	812	C
52	1	819	A
52	1	827	U
52	1	828	U
52	1	831	G
52	1	845	A
52	1	846	U
52	1	853	C
52	1	856	G
52	1	858	G
52	1	859	G
52	1	869	G
52	1	878	A
52	1	882	G
52	1	887	A
52	1	888	C
52	1	889	C
52	1	891	G
52	1	895	U
52	1	896	A
52	1	897	C
52	1	898	C
52	1	907	G
52	1	910	A
52	1	914	G
52	1	915	C
52	1	931	U
52	1	932	U
52	1	933	A
52	1	941	A
52	1	946	C
52	1	953	G

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Mol	Chain	Res	Type
52	1	961	C
52	1	973	A
52	1	974	G
52	1	983	A
52	1	990	A
52	1	995	C
52	1	996	A
52	1	999	U
52	1	1006	C
52	1	1012	U
52	1	1013	C
52	1	1022	G
52	1	1023	U
52	1	1025	G
52	1	1026	G
52	1	1033	U
52	1	1034	G
52	1	1036	G
52	1	1046	A
52	1	1047	G
52	1	1057	A
52	1	1065	U
52	1	1066	U
52	1	1067	A
52	1	1068	G
52	1	1070	A
52	1	1077	A
52	1	1083	U
52	1	1087	G
52	1	1088	A
52	1	1090	A
52	1	1096	A
52	1	1097	U
52	1	1110	G
52	1	1111	A
52	1	1112	G
52	1	1116	G
52	1	1117	C
52	1	1118	C
52	1	1119	U
52	1	1122	G
52	1	1128	G

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Mol	Chain	Res	Type
52	1	1130	U
52	1	1132	U
52	1	1133	A
52	1	1134	A
52	1	1135	C
52	1	1142	A
52	1	1143	A
52	1	1156	A
52	1	1171	G
52	1	1172	C
52	1	1175	A
52	1	1176	U
52	1	1178	C
52	1	1179	G
52	1	1180	U
52	1	1186	G
52	1	1201	U
52	1	1204	A
52	1	1210	G
52	1	1213	A
52	1	1218	G
52	1	1227	G
52	1	1236	G
52	1	1238	G
52	1	1248	G
52	1	1253	A
52	1	1256	G
52	1	1265	A
52	1	1266	G
52	1	1271	G
52	1	1272	A
52	1	1273	U
52	1	1275	A
52	1	1294	U
52	1	1300	G
52	1	1301	A
52	1	1302	A
52	1	1306	C
52	1	1321	A
52	1	1326	U
52	1	1327	A
52	1	1329	U

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Mol	Chain	Res	Type
52	1	1332	G
52	1	1333	G
52	1	1344	U
52	1	1345	C
52	1	1352	U
52	1	1359	A
52	1	1365	A
52	1	1378	A
52	1	1379	U
52	1	1380	G
52	1	1383	A
52	1	1386	C
52	1	1392	A
52	1	1395	A
52	1	1404	C
52	1	1408	G
52	1	1413	A
52	1	1414	C
52	1	1416	G
52	1	1417	C
52	1	1419	A
52	1	1427	A
52	1	1428	C
52	1	1434	A
52	1	1437	C
52	1	1451	C
52	1	1453	A
52	1	1455	G
52	1	1458	U
52	1	1461	C
52	1	1478	G
52	1	1482	G
52	1	1490	A
52	1	1493	C
52	1	1494	A
52	1	1497	U
52	1	1502	A
52	1	1504	A
52	1	1508	A
52	1	1509	A
52	1	1515	A
52	1	1529	G

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Mol	Chain	Res	Type
52	1	1532	A
52	1	1534	U
52	1	1535	A
52	1	1536	C
52	1	1537	G
52	1	1541	C
52	1	1544	A
52	1	1558	C
52	1	1566	A
52	1	1569	A
52	1	1578	U
52	1	1583	A
52	1	1584	U
52	1	1585	C
52	1	1588	G
52	1	1593	A
52	1	1608	A
52	1	1610	A
52	1	1616	A
52	1	1619	G
52	1	1627	G
52	1	1630	A
52	1	1639	C
52	1	1647	U
52	1	1648	U
52	1	1649	G
52	1	1651	G
52	1	1669	A
52	1	1674	G
52	1	1677	A
52	1	1700	A
52	1	1715	G
52	1	1721	G
52	1	1729	U
52	1	1730	C
52	1	1732	C
52	1	1738	G
52	1	1764	C
52	1	1773	A
52	1	1782	U
52	1	1791	A
52	1	1800	C

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Mol	Chain	Res	Type
52	1	1801	A
52	1	1808	A
52	1	1816	C
52	1	1829	A
52	1	1833	C
52	1	1842	G
52	1	1858	A
52	1	1859	U
52	1	1862	G
52	1	1867	G
52	1	1869	G
52	1	1870	C
52	1	1873	G
52	1	1882	U
52	1	1897	G
52	1	1906	G
52	1	1907	G
52	1	1913	A
52	1	1914	C
52	1	1916	A
52	1	1917	PSU
52	1	1927	A
52	1	1929	G
52	1	1930	G
52	1	1931	U
52	1	1936	A
52	1	1938	A
52	1	1955	U
52	1	1961	C
52	1	1962	5MC
52	1	1965	C
52	1	1967	C
52	1	1970	A
52	1	1971	U
52	1	1972	G
52	1	1982	U
52	1	1991	U
52	1	1993	U
52	1	1997	C
52	1	2002	G
52	1	2020	A
52	1	2022	U

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Mol	Chain	Res	Type
52	1	2023	C
52	1	2032	G
52	1	2033	A
52	1	2043	C
52	1	2052	A
52	1	2055	C
52	1	2056	G
52	1	2060	A
52	1	2061	G
52	1	2062	A
52	1	2069	G7M
52	1	2072	C
52	1	2076	U
52	1	2077	A
52	1	2087	G
52	1	2092	U
52	1	2093	G
52	1	2095	A
52	1	2102	G
52	1	2108	A
52	1	2110	G
52	1	2111	U
52	1	2112	G
52	1	2113	U
52	1	2115	G
52	1	2116	G
52	1	2117	A
52	1	2118	U
52	1	2120	G
52	1	2122	U
52	1	2124	G
52	1	2125	G
52	1	2126	A
52	1	2127	G
52	1	2128	G
52	1	2131	U
52	1	2132	U
52	1	2133	G
52	1	2134	A
52	1	2135	A
52	1	2139	U
52	1	2141	G

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Mol	Chain	Res	Type
52	1	2146	C
52	1	2147	A
52	1	2154	A
52	1	2157	G
52	1	2158	A
52	1	2159	G
52	1	2162	G
52	1	2163	A
52	1	2164	C
52	1	2165	C
52	1	2169	A
52	1	2171	A
52	1	2172	U
52	1	2182	U
52	1	2183	A
52	1	2189	U
52	1	2190	G
52	1	2193	G
52	1	2194	U
52	1	2198	A
52	1	2203	U
52	1	2204	G
52	1	2210	U
52	1	2211	A
52	1	2212	A
52	1	2225	A
52	1	2226	C
52	1	2229	U
52	1	2238	G
52	1	2239	G
52	1	2243	U
52	1	2250	G
52	1	2267	A
52	1	2268	A
52	1	2279	G
52	1	2283	C
52	1	2287	A
52	1	2288	A
52	1	2304	G
52	1	2305	U
52	1	2307	G
52	1	2309	A

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Mol	Chain	Res	Type
52	1	2310	C
52	1	2311	A
52	1	2312	U
52	1	2322	A
52	1	2325	G
52	1	2326	C
52	1	2327	A
52	1	2333	A
52	1	2335	A
52	1	2347	C
52	1	2350	C
52	1	2357	G
52	1	2361	G
52	1	2376	A
52	1	2383	G
52	1	2385	C
52	1	2394	C
52	1	2396	G
52	1	2402	U
52	1	2403	C
52	1	2406	A
52	1	2409	G
52	1	2410	G
52	1	2420	C
52	1	2423	U
52	1	2424	C
52	1	2425	A
52	1	2426	A
52	1	2428	G
52	1	2429	G
52	1	2430	A
52	1	2431	U
52	1	2435	A
52	1	2441	U
52	1	2447	G
52	1	2448	A
52	1	2459	A
52	1	2470	G
52	1	2476	A
52	1	2480	C
52	1	2484	G
52	1	2487	G

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Mol	Chain	Res	Type
52	1	2491	U
52	1	2494	G
52	1	2502	G
52	1	2504	PSU
52	1	2505	G
52	1	2506	U
52	1	2513	A
52	1	2518	A
52	1	2525	G
52	1	2529	G
52	1	2534	A
52	1	2535	G
52	1	2554	U
52	1	2562	U
52	1	2566	A
52	1	2567	G
52	1	2573	C
52	1	2574	G
52	1	2582	G
52	1	2585	U
52	1	2586	U
52	1	2602	A
52	1	2608	G
52	1	2609	U
52	1	2613	U
52	1	2615	U
52	1	2621	G
52	1	2629	U
52	1	2630	G
52	1	2634	A
52	1	2639	A
52	1	2663	G
52	1	2685	G
52	1	2689	U
52	1	2690	U
52	1	2691	C
52	1	2714	G
52	1	2716	C
52	1	2718	G
52	1	2724	U
52	1	2725	A
52	1	2726	A

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Mol	Chain	Res	Type
52	1	2733	A
52	1	2744	G
52	1	2748	A
52	1	2754	U
52	1	2757	A
52	1	2758	A
52	1	2765	A
52	1	2777	G
52	1	2778	A
52	1	2791	G
52	1	2793	C
52	1	2794	C
52	1	2800	A
52	1	2801	G
52	1	2803	G
52	1	2805	C
52	1	2818	U
52	1	2820	A
52	1	2821	A
52	1	2825	G
52	1	2830	C
52	1	2835	A
52	1	2850	A
52	1	2860	A
52	1	2867	G
52	1	2874	C
52	1	2880	C
52	1	2884	U
52	1	2891	U
52	1	2893	A
52	1	2894	G
52	1	2902	C
52	1	2904	U
53	2	4	U
53	2	5	U
53	2	6	G
53	2	9	G
53	2	22	G
53	2	32	A
53	2	39	G
53	2	44	A
53	2	47	C

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Mol	Chain	Res	Type
53	2	48	C
53	2	51	A
53	2	52	C
53	2	54	C
53	2	66	A
53	2	70	U
53	2	71	A
53	2	73	C
53	2	74	A
53	2	76	G
53	2	77	A
53	2	80	A
53	2	81	A
53	2	82	G
53	2	83	C
53	2	84	U
53	2	87	C
53	2	88	U
53	2	90	C
53	2	95	C
53	2	96	U
53	2	108	G
53	2	120	A
53	2	128	G
53	2	130	A
53	2	131	A
53	2	134	G
53	2	137	U
53	2	138	G
53	2	143	A
53	2	144	G
53	2	147	G
53	2	149	A
53	2	157	U
53	2	158	G
53	2	161	A
53	2	163	C
53	2	164	G
53	2	168	G
53	2	173	U
53	2	177	G
53	2	182	A

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Mol	Chain	Res	Type
53	2	200	G
53	2	204	G
53	2	208	U
53	2	209	U
53	2	210	C
53	2	211	G
53	2	212	G
53	2	222	C
53	2	226	G
53	2	245	U
53	2	246	A
53	2	247	G
53	2	251	G
53	2	262	A
53	2	266	G
53	2	267	C
53	2	279	A
53	2	280	C
53	2	281	G
53	2	289	G
53	2	306	A
53	2	319	G
53	2	321	A
53	2	328	C
53	2	329	A
53	2	332	G
53	2	340	U
53	2	345	C
53	2	351	G
53	2	352	C
53	2	353	A
53	2	354	G
53	2	355	C
53	2	356	A
53	2	367	U
53	2	369	G
53	2	370	C
53	2	372	C
53	2	373	A
53	2	374	A
53	2	375	U
53	2	381	C

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Mol	Chain	Res	Type
53	2	382	A
53	2	392	C
53	2	397	A
53	2	406	G
53	2	410	G
53	2	411	A
53	2	412	A
53	2	413	G
53	2	414	A
53	2	420	U
53	2	421	U
53	2	422	C
53	2	423	G
53	2	424	G
53	2	425	G
53	2	426	U
53	2	429	U
53	2	445	G
53	2	446	G
53	2	451	A
53	2	458	U
53	2	463	U
53	2	464	U
53	2	467	U
53	2	468	A
53	2	469	C
53	2	476	U
53	2	478	A
53	2	479	U
53	2	484	G
53	2	485	U
53	2	486	U
53	2	495	A
53	2	496	A
53	2	499	A
53	2	501	C
53	2	505	G
53	2	511	C
53	2	515	G
53	2	516	PSU
53	2	517	G
53	2	518	C

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Mol	Chain	Res	Type
53	2	519	C
53	2	521	G
53	2	527	G7M
53	2	530	G
53	2	531	U
53	2	532	A
53	2	533	A
53	2	534	U
53	2	536	C
53	2	542	G
53	2	545	C
53	2	547	A
53	2	559	A
53	2	560	A
53	2	562	U
53	2	567	G
53	2	568	G
53	2	572	A
53	2	573	A
53	2	576	C
53	2	579	A
53	2	596	A
53	2	615	G
53	2	620	C
53	2	628	G
53	2	633	G
53	2	642	A
53	2	650	G
53	2	653	U
53	2	665	A
53	2	703	G
53	2	723	U
53	2	724	G
53	2	731	G
53	2	734	G
53	2	747	A
53	2	755	G
53	2	777	A
53	2	790	A
53	2	793	U
53	2	794	A
53	2	799	G

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Mol	Chain	Res	Type
53	2	815	A
53	2	817	C
53	2	828	U
53	2	841	C
53	2	843	U
53	2	844	G
53	2	845	A
53	2	846	G
53	2	849	G
53	2	851	G
53	2	855	U
53	2	857	C
53	2	876	C
53	2	902	G
53	2	914	A
53	2	915	A
53	2	926	G
53	2	934	C
53	2	935	A
53	2	942	G
53	2	960	U
53	2	966	2MG
53	2	969	A
53	2	972	C
53	2	975	A
53	2	976	G
53	2	978	A
53	2	982	U
53	2	983	A
53	2	987	G
53	2	993	G
53	2	1004	A
53	2	1005	A
53	2	1008	U
53	2	1009	U
53	2	1012	A
53	2	1013	G
53	2	1017	U
53	2	1018	G
53	2	1020	G
53	2	1021	A
53	2	1023	U

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Mol	Chain	Res	Type
53	2	1024	G
53	2	1026	G
53	2	1028	C
53	2	1030	U
53	2	1031	C
53	2	1032	G
53	2	1033	G
53	2	1037	C
53	2	1043	G
53	2	1046	A
53	2	1065	U
53	2	1070	U
53	2	1086	U
53	2	1088	G
53	2	1092	A
53	2	1094	G
53	2	1095	U
53	2	1097	C
53	2	1101	A
53	2	1108	G
53	2	1124	G
53	2	1133	G
53	2	1135	U
53	2	1136	C
53	2	1137	C
53	2	1139	G
53	2	1140	C
53	2	1141	C
53	2	1142	G
53	2	1145	A
53	2	1146	A
53	2	1151	A
53	2	1152	A
53	2	1159	U
53	2	1160	G
53	2	1164	G
53	2	1167	A
53	2	1168	U
53	2	1171	A
53	2	1184	G
53	2	1187	G
53	2	1196	A

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Mol	Chain	Res	Type
53	2	1197	A
53	2	1201	A
53	2	1202	U
53	2	1206	G
53	2	1212	U
53	2	1213	A
53	2	1214	C
53	2	1225	A
53	2	1227	A
53	2	1228	C
53	2	1236	A
53	2	1238	A
53	2	1240	U
53	2	1253	G
53	2	1256	A
53	2	1257	A
53	2	1260	G
53	2	1275	A
53	2	1278	G
53	2	1280	A
53	2	1285	A
53	2	1286	U
53	2	1287	A
53	2	1299	A
53	2	1302	C
53	2	1305	G
53	2	1312	G
53	2	1317	C
53	2	1318	A
53	2	1320	C
53	2	1332	A
53	2	1338	G
53	2	1346	A
53	2	1353	G
53	2	1363	A
53	2	1368	A
53	2	1370	G
53	2	1379	G
53	2	1381	U
53	2	1394	A
53	2	1398	A
53	2	1419	G

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Mol	Chain	Res	Type
53	2	1429	A
53	2	1432	G
53	2	1441	A
53	2	1446	A
53	2	1448	C
53	2	1452	C
53	2	1453	G
53	2	1455	G
53	2	1487	G
53	2	1491	G
53	2	1492	A
53	2	1493	A
53	2	1499	A
53	2	1503	A
53	2	1505	G
53	2	1506	U
53	2	1517	G
53	2	1529	G
53	2	1530	G
53	2	1533	C
53	2	1534	A
54	3	9	G
54	3	13	G
54	3	15	A
54	3	16	G
54	3	17	C
54	3	30	C
54	3	35	C
54	3	44	G
54	3	45	A
54	3	56	G
54	3	64	G
54	3	66	A
54	3	67	G
54	3	68	C
54	3	88	C
54	3	89	U
54	3	90	C
54	3	99	A
54	3	109	A
55	4	3	C
55	4	6	G

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Mol	Chain	Res	Type
55	4	9	A
55	4	18	G
55	4	19	G
55	4	21	A
55	4	22	G
55	4	34	G
55	4	39	U
55	4	41	C
55	4	43	C
55	4	44	G
55	4	45	U
55	4	47	U
55	4	48	C
55	4	50	U
55	4	58	A
55	4	59	U
55	4	60	U
55	4	61	C
55	4	65	G
55	4	76	A
56	5	1	G
56	5	2	C
56	5	3	G
56	5	7	U
56	5	8	4SU
56	5	9	G
56	5	13	A
56	5	14	G
56	5	15	C
56	5	16	C
56	5	18	G
56	5	19	G
56	5	20	H2U
56	5	21	A
56	5	23	C
56	5	33	U
56	5	35	A
56	5	37	A
56	5	44	A
56	5	45	G
56	5	46	A
56	5	47	U

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Mol	Chain	Res	Type
56	5	48	C
56	5	49	G
56	5	53	G
56	5	55	PSU
56	5	56	C
56	5	58	A
56	5	59	A
56	5	60	U
56	5	61	C
56	5	64	G
56	5	69	C
56	5	71	C
56	5	72	A
56	5	74	C
56	5	75	C
57	6	3	C
57	6	5	G
57	6	7	A
57	6	8	4SU
57	6	9	A
57	6	10	G
57	6	11	C
57	6	13	C
57	6	15	G
57	6	16	H2U
57	6	17	U
57	6	18	G
57	6	19	G
57	6	20	H2U
57	6	21	A
57	6	22	G
57	6	23	A
57	6	29	G
57	6	32	PSU
57	6	33	U
57	6	36	A
57	6	38	A
57	6	41	C
57	6	44	G
57	6	45	U
57	6	46	7MG
57	6	48	C

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Mol	Chain	Res	Type
57	6	49	C
57	6	52	G
57	6	57	G
57	6	59	U
57	6	60	U
57	6	62	C
57	6	63	G
57	6	64	A
57	6	65	G
57	6	70	G
57	6	71	G
57	6	73	A
57	6	74	C
57	6	75	C
57	6	76	A

All (110) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	1	62	U
52	1	70	G
52	1	84	A
52	1	100	U
52	1	102	U
52	1	177	G
52	1	199	A
52	1	247	G
52	1	271	G
52	1	272	A
52	1	310	A
52	1	403	U
52	1	404	A
52	1	446	G
52	1	474	G
52	1	504	A
52	1	529	A
52	1	555	G
52	1	614	A
52	1	620	G
52	1	645	C
52	1	685	A
52	1	784	G

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Mol	Chain	Res	Type
52	1	894	U
52	1	896	A
52	1	974	G
52	1	995	C
52	1	1065	U
52	1	1067	A
52	1	1070	A
52	1	1288	G
52	1	1332	G
52	1	1344	U
52	1	1358	G
52	1	1379	U
52	1	1415	U
52	1	1508	A
52	1	1509	A
52	1	1543	G
52	1	1608	A
52	1	1784	A
52	1	2133	G
52	1	2146	C
52	1	2162	G
52	1	2182	U
52	1	2193	G
52	1	2211	A
52	1	2225	A
52	1	2286	G
52	1	2308	G
52	1	2311	A
52	1	2319	G
52	1	2326	C
52	1	2425	A
52	1	2447	G
52	1	2581	G
52	1	2629	U
52	1	2751	G
52	1	2756	U
52	1	2830	C
52	1	2873	A
53	2	73	C
53	2	243	A
53	2	246	A
53	2	279	A

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Mol	Chain	Res	Type
53	2	280	C
53	2	328	C
53	2	329	A
53	2	351	G
53	2	428	G
53	2	517	G
53	2	518	C
53	2	530	G
53	2	531	U
53	2	532	A
53	2	533	A
53	2	641	U
53	2	965	U
53	2	974	A
53	2	982	U
53	2	1109	C
53	2	1145	A
53	2	1201	A
53	2	1211	U
53	2	1363	A
56	5	8	4SU
56	5	14	G
56	5	15	C
56	5	16	C
56	5	17	U
56	5	18	G
56	5	19	G
56	5	20	H2U
56	5	21	A
56	5	47	U
56	5	48	C
56	5	58	A
56	5	59	A
56	5	60	U
57	6	10	G
57	6	16	H2U
57	6	17	U
57	6	18	G
57	6	19	G
57	6	32	PSU
57	6	45	U
57	6	56	C

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Mol	Chain	Res	Type
57	6	59	U
57	6	70	G
57	6	75	C

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

48 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	$\#\|Z\| > 2$
52	6MZ	1	1618	52	17,25,26	0.57	0	15,36,39	1.15	2 (13%)
52	2MG	1	1835	52	18,26,27	1.09	1 (5%)	21,38,41	2.44	5 (23%)
52	PSU	1	1911	52	15,21,22	1.07	1 (6%)	16,30,33	2.66	1 (6%)
52	3TD	1	1915	52	15,22,23	0.89	1 (6%)	17,32,35	0.89	1 (5%)
52	PSU	1	1917	52	15,21,22	1.06	1 (6%)	16,30,33	2.75	1 (6%)
52	5MU	1	1939	52	13,22,23	1.08	2 (15%)	16,32,35	4.14	2 (12%)
52	5MC	1	1962	52	14,22,23	0.73	1 (7%)	17,32,35	0.47	0
52	6MZ	1	2030	52	17,25,26	0.62	0	15,36,39	1.21	1 (6%)
52	G7M	1	2069	52	18,26,27	1.18	2 (11%)	21,39,42	2.70	3 (14%)
52	OMG	1	2251	56,52	18,26,27	1.06	1 (5%)	21,38,41	2.56	3 (14%)
52	2MG	1	2445	52	18,26,27	1.10	1 (5%)	21,38,41	2.48	5 (23%)
52	PSU	1	2457	52	15,21,22	1.10	1 (6%)	16,30,33	2.69	2 (12%)
52	OMC	1	2498	60,52	15,22,23	0.69	0	20,31,34	0.89	1 (5%)
52	2MA	1	2503	60,52	17,25,26	1.08	2 (11%)	18,37,40	2.17	2 (11%)
52	PSU	1	2504	52	15,21,22	1.05	1 (6%)	16,30,33	2.77	3 (18%)
52	OMU	1	2552	60,52	14,22,23	1.00	1 (7%)	19,31,34	2.57	2 (10%)
52	PSU	1	2580	52	15,21,22	1.03	1 (6%)	16,30,33	2.75	1 (6%)
52	PSU	1	2605	52	15,21,22	1.06	1 (6%)	16,30,33	2.72	2 (12%)
52	1MG	1	745	52	17,26,27	0.85	1 (5%)	19,39,42	0.85	1 (5%)
52	PSU	1	746	60,52	15,21,22	1.08	1 (6%)	16,30,33	2.64	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
52	5MU	1	747	52	13,22,23	1.04	2 (15%)	16,32,35	4.26	2 (12%)
52	PSU	1	955	52	15,21,22	1.07	1 (6%)	16,30,33	2.62	1 (6%)
53	2MG	2	1207	53	18,26,27	1.12	1 (5%)	21,38,41	2.52	5 (23%)
53	4OC	2	1402	53	15,23,24	0.69	0	21,32,35	1.25	2 (9%)
53	5MC	2	1407	53	14,22,23	0.71	0	17,32,35	0.70	0
53	UR3	2	1498	53	13,22,23	0.76	0	18,32,35	0.54	0
53	2MG	2	1516	53	18,26,27	1.14	1 (5%)	21,38,41	2.37	3 (14%)
53	MA6	2	1518	53	18,26,27	0.55	0	15,38,41	1.20	2 (13%)
53	MA6	2	1519	53	18,26,27	0.60	0	15,38,41	1.16	2 (13%)
53	PSU	2	516	53	15,21,22	1.07	1 (6%)	16,30,33	2.89	2 (12%)
53	G7M	2	527	53	18,26,27	1.20	2 (11%)	21,39,42	2.61	3 (14%)
53	2MG	2	966	53	18,26,27	1.13	1 (5%)	21,38,41	2.47	5 (23%)
53	5MC	2	967	53	14,22,23	0.74	1 (7%)	17,32,35	0.52	0
56	H2U	5	20	56	17,21,22	0.56	0	23,30,33	0.77	0
56	4OC	5	32	56	15,23,24	0.67	0	21,32,35	1.11	2 (9%)
56	5MU	5	54	56	13,22,23	1.03	1 (7%)	16,32,35	4.38	2 (12%)
56	PSU	5	55	56	15,21,22	1.07	1 (6%)	16,30,33	2.63	2 (12%)
56	4SU	5	8	56	12,21,22	1.04	1 (8%)	15,30,33	1.80	2 (13%)
57	H2U	6	16	57	17,21,22	0.57	0	23,30,33	2.30	6 (26%)
57	H2U	6	20	57	17,21,22	0.62	0	23,30,33	1.56	4 (17%)
57	PSU	6	32	57	15,21,22	1.23	1 (6%)	16,30,33	3.55	5 (31%)
57	6IA	6	37	57,58	20,29,30	0.55	0	22,41,44	1.85	5 (22%)
57	7MG	6	46	57	20,26,27	1.03	1 (5%)	23,39,42	2.33	4 (17%)
57	3AU	6	47	57	16,28,29	0.86	1 (6%)	16,40,43	0.55	0
57	5MU	6	54	57	13,22,23	1.06	1 (7%)	16,32,35	4.24	2 (12%)
57	PSU	6	55	57	15,21,22	1.26	1 (6%)	16,30,33	3.61	5 (31%)
57	4SU	6	8	57	12,21,22	1.05	1 (8%)	15,30,33	1.54	1 (6%)
42	D2T	q	89	42	4,9,10	0.54	0	4,11,13	2.13	2 (50%)

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
52	6MZ	1	1618	52	-	0/5/27/28	0/3/3/3
52	2MG	1	1835	52	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	1	1911	52	-	0/7/25/26	0/2/2/2
52	3TD	1	1915	52	-	0/7/25/26	0/2/2/2
52	PSU	1	1917	52	-	0/7/25/26	0/2/2/2
52	5MU	1	1939	52	-	0/3/25/26	0/2/2/2
52	5MC	1	1962	52	-	0/3/25/26	0/2/2/2
52	6MZ	1	2030	52	-	0/5/27/28	0/3/3/3
52	G7M	1	2069	52	-	0/3/25/26	0/3/3/3
52	OMG	1	2251	56,52	-	0/5/27/28	0/3/3/3
52	2MG	1	2445	52	-	0/5/27/28	0/3/3/3
52	PSU	1	2457	52	-	0/7/25/26	0/2/2/2
52	OMC	1	2498	60,52	-	0/5/27/28	0/2/2/2
52	2MA	1	2503	60,52	-	0/3/25/26	0/3/3/3
52	PSU	1	2504	52	-	0/7/25/26	0/2/2/2
52	OMU	1	2552	60,52	-	0/5/27/28	0/2/2/2
52	PSU	1	2580	52	-	0/7/25/26	0/2/2/2
52	PSU	1	2605	52	-	0/7/25/26	0/2/2/2
52	1MG	1	745	52	-	0/3/25/26	0/3/3/3
52	PSU	1	746	60,52	-	0/7/25/26	0/2/2/2
52	5MU	1	747	52	-	0/3/25/26	0/2/2/2
52	PSU	1	955	52	-	0/7/25/26	0/2/2/2
53	2MG	2	1207	53	-	0/5/27/28	0/3/3/3
53	4OC	2	1402	53	-	0/7/29/30	0/2/2/2
53	5MC	2	1407	53	-	0/3/25/26	0/2/2/2
53	UR3	2	1498	53	-	0/3/25/26	0/2/2/2
53	2MG	2	1516	53	-	0/5/27/28	0/3/3/3
53	MA6	2	1518	53	-	0/7/29/30	0/3/3/3
53	MA6	2	1519	53	-	0/7/29/30	0/3/3/3
53	PSU	2	516	53	-	0/7/25/26	0/2/2/2
53	G7M	2	527	53	-	0/3/25/26	0/3/3/3
53	2MG	2	966	53	-	0/5/27/28	0/3/3/3
53	5MC	2	967	53	-	0/3/25/26	0/2/2/2
56	H2U	5	20	56	-	0/7/38/39	0/2/2/2
56	4OC	5	32	56	-	0/7/29/30	0/2/2/2
56	5MU	5	54	56	-	0/3/25/26	0/2/2/2
56	PSU	5	55	56	-	0/7/25/26	0/2/2/2
56	4SU	5	8	56	-	0/3/25/26	0/2/2/2
57	H2U	6	16	57	3/3/8/9	0/7/38/39	0/2/2/2
57	H2U	6	20	57	2/2/8/9	0/7/38/39	0/2/2/2
57	PSU	6	32	57	1/1/5/5	0/7/25/26	0/2/2/2
57	6IA	6	37	57,58	1/1/6/7	0/9/31/32	0/3/3/3
57	7MG	6	46	57	-	0/7/37/38	0/3/3/3
57	3AU	6	47	57	-	0/8/34/35	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	5MU	6	54	57	-	0/3/25/26	0/2/2/2
57	PSU	6	55	57	1/1/5/5	0/7/25/26	0/2/2/2
57	4SU	6	8	57	-	0/3/25/26	0/2/2/2
42	D2T	q	89	42	-	0/2/12/14	0/0/0/0

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	1	747	5MU	C6-C5	-2.05	1.34	1.40
53	2	967	5MC	C6-C5	-2.05	1.34	1.40
52	1	1962	5MC	C6-C5	-2.04	1.34	1.40
52	1	1939	5MU	C6-C5	-2.02	1.34	1.40
52	1	2069	G7M	C8-N9	2.27	1.37	1.33
52	1	2503	2MA	C6-N1	2.28	1.39	1.34
53	2	527	G7M	C8-N9	2.28	1.37	1.33
52	1	1915	3TD	C4-N3	2.31	1.41	1.38
52	1	745	1MG	C6-N1	2.36	1.41	1.38
52	1	2503	2MA	C2-N1	2.46	1.38	1.34
57	6	47	3AU	C4-N3	2.49	1.42	1.38
56	5	8	4SU	C5-C4	2.94	1.42	1.38
52	1	2552	OMU	C4-N3	2.96	1.38	1.33
52	1	747	5MU	C4-N3	2.99	1.38	1.33
57	6	8	4SU	C5-C4	3.02	1.42	1.38
56	5	54	5MU	C4-N3	3.04	1.38	1.33
52	1	2504	PSU	C4-N3	3.07	1.38	1.33
52	1	2580	PSU	C4-N3	3.09	1.38	1.33
52	1	2457	PSU	C4-N3	3.12	1.38	1.33
52	1	1939	5MU	C4-N3	3.14	1.38	1.33
57	6	54	5MU	C4-N3	3.15	1.38	1.33
52	1	2605	PSU	C4-N3	3.16	1.38	1.33
52	1	746	PSU	C4-N3	3.20	1.38	1.33
52	1	1911	PSU	C4-N3	3.21	1.38	1.33
52	1	955	PSU	C4-N3	3.21	1.38	1.33
56	5	55	PSU	C4-N3	3.24	1.38	1.33
53	2	516	PSU	C4-N3	3.27	1.38	1.33
52	1	1917	PSU	C4-N3	3.29	1.39	1.33
57	6	32	PSU	C4-N3	3.39	1.39	1.33
57	6	55	PSU	C4-N3	3.43	1.39	1.33
52	1	2069	G7M	C6-N1	3.50	1.39	1.33
53	2	527	G7M	C6-N1	3.64	1.39	1.33
52	1	2251	OMG	C6-N1	3.73	1.39	1.33
57	6	46	7MG	C6-N1	3.74	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	1	2445	2MG	C6-N1	3.85	1.40	1.33
52	1	1835	2MG	C6-N1	3.85	1.40	1.33
53	2	1207	2MG	C6-N1	3.96	1.40	1.33
53	2	966	2MG	C6-N1	4.03	1.40	1.33
53	2	1516	2MG	C6-N1	4.05	1.40	1.33

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	1	747	5MU	C5-C4-N3	-11.50	115.70	125.35
56	5	54	5MU	C5-C4-N3	-11.43	115.75	125.35
57	6	54	5MU	C5-C4-N3	-11.04	116.08	125.35
52	1	1939	5MU	C5-C4-N3	-10.90	116.20	125.35
52	1	2069	G7M	C5-C6-N1	-8.57	112.32	123.52
53	2	527	G7M	C5-C6-N1	-8.41	112.53	123.52
52	1	1835	2MG	C5-C6-N1	-8.08	112.95	123.52
53	2	1207	2MG	C5-C6-N1	-8.03	113.02	123.52
52	1	2251	OMG	C5-C6-N1	-8.03	113.03	123.52
53	2	1516	2MG	C5-C6-N1	-8.00	113.06	123.52
52	1	2445	2MG	C5-C6-N1	-7.97	113.11	123.52
53	2	966	2MG	C5-C6-N1	-7.86	113.25	123.52
57	6	46	7MG	C5-C6-N1	-7.42	112.34	123.39
56	5	8	4SU	C5-C4-N3	-5.50	117.72	123.56
57	6	8	4SU	C5-C4-N3	-5.50	117.73	123.56
52	1	2069	G7M	N3-C2-N1	-4.14	121.93	127.56
53	2	527	G7M	N3-C2-N1	-4.04	122.06	127.56
57	6	55	PSU	C3'-C2'-C1'	-4.04	96.93	101.71
57	6	32	PSU	C3'-C2'-C1'	-3.86	97.13	101.71
52	1	2251	OMG	N3-C2-N1	-3.71	122.51	127.56
57	6	55	PSU	C4'-O4'-C1'	-3.42	106.02	109.54
57	6	16	H2U	C3'-C2'-C1'	-3.40	94.61	101.44
52	1	2552	OMU	C5-C4-N3	-3.09	115.70	123.28
57	6	32	PSU	C4'-O4'-C1'	-2.68	106.78	109.54
57	6	46	7MG	C5-C4-N3	-2.45	124.25	126.74
42	q	89	D2T	O-C-CA	-2.30	119.40	125.69
52	1	2445	2MG	N3-C2-N1	-2.28	122.78	126.19
53	2	1518	MA6	N3-C2-N1	-2.25	127.11	128.87
52	1	1835	2MG	N3-C2-N1	-2.23	122.85	126.19
53	2	1207	2MG	N3-C2-N1	-2.23	122.86	126.19
53	2	966	2MG	N3-C2-N1	-2.13	123.00	126.19
53	2	1516	2MG	N3-C2-N1	-2.13	123.00	126.19
53	2	1519	MA6	N3-C2-N1	-2.12	127.20	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	5	55	PSU	C5-C6-N1	-2.12	121.42	124.38
52	1	745	1MG	C5-C6-N1	-2.08	115.62	118.35
52	1	2605	PSU	C5-C6-N1	-2.08	121.48	124.38
57	6	46	7MG	N1-C2-N3	-2.07	122.12	125.51
52	1	1915	3TD	C5-C6-N1	-2.05	121.52	124.38
52	1	2457	PSU	C5-C6-N1	-2.05	121.52	124.38
52	1	2504	PSU	C2'-C3'-C4'	-2.04	98.46	102.64
52	1	2504	PSU	C5-C6-N1	-2.02	121.56	124.38
52	1	1618	6MZ	N3-C2-N1	-2.01	127.29	128.87
56	5	32	4OC	C6-C5-C4	2.01	118.21	117.42
52	1	1835	2MG	CM2-N2-C2	2.02	125.31	123.03
57	6	37	6IA	C2'-C3'-C4'	2.03	106.79	102.64
57	6	16	H2U	O4'-C1'-C2'	2.07	111.30	106.61
52	1	2445	2MG	CM2-N2-C2	2.10	125.39	123.03
57	6	20	H2U	O4'-C1'-C2'	2.11	111.38	106.61
52	1	2445	2MG	N2-C2-N3	2.25	119.55	116.94
52	1	2503	2MA	CM2-C2-N1	2.25	121.05	117.20
57	6	55	PSU	O3'-C3'-C4'	2.29	117.85	111.01
57	6	20	H2U	C5-C6-N1	2.38	113.37	110.76
53	2	1402	4OC	C6-C5-C4	2.50	118.40	117.42
52	1	1835	2MG	N2-C2-N3	2.51	119.86	116.94
53	2	966	2MG	N2-C2-N3	2.51	119.86	116.94
53	2	1207	2MG	N2-C2-N3	2.60	119.96	116.94
52	1	2498	OMC	C6-C5-C4	2.75	118.51	117.44
57	6	16	H2U	O3'-C3'-C2'	3.03	121.66	111.86
53	2	1519	MA6	C2-N1-C6	3.10	118.96	111.64
57	6	37	6IA	C2-N1-C6	3.13	118.72	116.47
53	2	1207	2MG	CM2-N2-C2	3.13	126.56	123.03
42	q	89	D2T	CB-CA-N	3.18	116.20	109.83
57	6	32	PSU	O3'-C3'-C4'	3.39	121.13	111.01
53	2	1518	MA6	C2-N1-C6	3.43	119.72	111.64
52	1	2030	6MZ	C2-N1-C6	3.43	118.94	116.47
52	1	1618	6MZ	C2-N1-C6	3.47	118.96	116.47
57	6	37	6IA	C12-N6-C6	3.52	127.53	123.46
57	6	20	H2U	O2'-C2'-C3'	3.61	123.54	111.86
53	2	966	2MG	CM2-N2-C2	3.70	127.20	123.03
56	5	8	4SU	C2'-C1'-N1	3.75	123.54	113.46
56	5	32	4OC	C2-N3-C4	3.81	120.27	115.43
53	2	1402	4OC	C2-N3-C4	3.82	120.29	115.43
53	2	516	PSU	C3'-C2'-C1'	3.87	106.30	101.71
57	6	16	H2U	O2'-C2'-C3'	4.12	125.18	111.86
57	6	37	6IA	O3'-C3'-C4'	4.44	124.28	111.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	6	37	6IA	O3'-C3'-C2'	4.59	126.70	111.86
57	6	20	H2U	O2'-C2'-C1'	4.66	126.18	109.98
57	6	16	H2U	O2'-C2'-C1'	5.18	127.99	109.98
53	2	966	2MG	C6-N1-C2	5.88	123.66	115.24
53	2	1516	2MG	C6-N1-C2	5.94	123.74	115.24
53	2	1207	2MG	C6-N1-C2	6.12	124.00	115.24
52	1	1835	2MG	C6-N1-C2	6.19	124.11	115.24
52	1	2445	2MG	C6-N1-C2	6.20	124.12	115.24
57	6	16	H2U	O3'-C3'-C4'	6.55	130.56	111.01
57	6	32	PSU	C5-C1'-C2'	6.96	127.26	115.44
57	6	46	7MG	C6-N1-C2	6.99	124.07	115.88
53	2	527	G7M	C6-N1-C2	7.01	124.10	115.88
52	1	2069	G7M	C6-N1-C2	7.15	124.26	115.88
52	1	2251	OMG	C6-N1-C2	7.18	124.30	115.88
57	6	55	PSU	C5-C1'-C2'	7.83	128.73	115.44
52	1	2503	2MA	C2-N3-C4	8.48	119.37	115.29
56	5	55	PSU	C4-N3-C2	10.00	123.50	115.16
52	1	955	PSU	C4-N3-C2	10.07	123.56	115.16
52	1	746	PSU	C4-N3-C2	10.13	123.61	115.16
52	1	2605	PSU	C4-N3-C2	10.14	123.61	115.16
52	1	1911	PSU	C4-N3-C2	10.17	123.64	115.16
53	2	516	PSU	C4-N3-C2	10.23	123.69	115.16
57	6	55	PSU	C4-N3-C2	10.25	123.71	115.16
52	1	2504	PSU	C4-N3-C2	10.30	123.75	115.16
52	1	2457	PSU	C4-N3-C2	10.30	123.75	115.16
52	1	2552	OMU	C4-N3-C2	10.35	125.11	114.21
52	1	2580	PSU	C4-N3-C2	10.36	123.80	115.16
57	6	32	PSU	C4-N3-C2	10.37	123.81	115.16
52	1	1917	PSU	C4-N3-C2	10.63	124.02	115.16
52	1	1939	5MU	C4-N3-C2	12.12	125.27	115.16
52	1	747	5MU	C4-N3-C2	12.25	125.38	115.16
57	6	54	5MU	C4-N3-C2	12.49	125.58	115.16
56	5	54	5MU	C4-N3-C2	12.86	125.89	115.16

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
57	6	16	H2U	C2'
57	6	16	H2U	C3'
57	6	16	H2U	C1'
57	6	55	PSU	C1'
57	6	32	PSU	C1'

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Mol	Chain	Res	Type	Atom
57	6	20	H2U	C2'
57	6	20	H2U	C1'
57	6	37	6IA	C3'

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	1	1915	3TD	1	0
52	1	1939	5MU	1	0
52	1	2030	6MZ	3	0
52	1	2445	2MG	2	0
52	1	2498	OMC	1	0
52	1	2503	2MA	2	0
52	1	2552	OMU	1	0
52	1	745	1MG	1	0
52	1	747	5MU	1	0
53	2	1207	2MG	1	0
53	2	1402	4OC	1	0
53	2	1518	MA6	1	0
53	2	1519	MA6	1	0
53	2	516	PSU	1	0
53	2	966	2MG	2	0
53	2	967	5MC	2	0
56	5	20	H2U	3	0
56	5	32	4OC	1	0
56	5	54	5MU	2	0
56	5	8	4SU	1	0
57	6	16	H2U	1	0
57	6	32	PSU	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 304 ligands modelled in this entry, 302 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
62	PAR	2	1665	-	45,45,45	0.82	2 (4%)	60,67,67	0.67	1 (1%)
63	MET	5	101	-	5,7,8	0.42	0	4,7,9	0.96	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PAR	2	1665	-	-	0/18/94/94	0/4/4/4
63	MET	5	101	-	-	0/4/6/8	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	2	1665	PAR	O51-C11	-3.72	1.32	1.41
62	2	1665	PAR	C14-C24	-2.27	1.48	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	2	1665	PAR	O51-C11-C21	2.40	115.36	109.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	2	1665	PAR	1	0
63	5	101	MET	1	0

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
52	1	8
53	2	4
55	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	1588:G	O3'	1589:U	P	4.95
1	4	1:G	O3'	2:C	P	4.28
1	1	2098:U	O3'	2099:U	P	3.58
1	2	480:U	O3'	481:G	P	3.44
1	1	1408:G	O3'	1409:U	P	3.41
1	1	1169:A	O3'	1170:C	P	3.38
1	2	147:G	O3'	148:G	P	3.36
1	1	2314:A	O3'	2315:G	P	3.34
1	1	1579:A	O3'	1580:A	P	3.31
1	1	1167:C	O3'	1168:G	P	3.25
1	2	197:A	O3'	198:G	P	3.24
1	1	2196:C	O3'	2197:U	P	3.12
1	2	1383:C	O3'	1384:C	P	3.09