



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:12 PM BST

PDB ID : 5AFI  
EMDB ID: : EMD-2847  
Title : 2.9A Structure of E. coli ribosome-EF-TU complex by cs-corrected cryo-EM  
Authors : fischer, N.; neumann, p.; konevega, a.l.; bock, l.v.; ficner, r.; rodnina, M.v.; stark, h.  
Deposited on : 2015-01-22  
Resolution : 2.90 Å(reported)

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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) : trunk27241

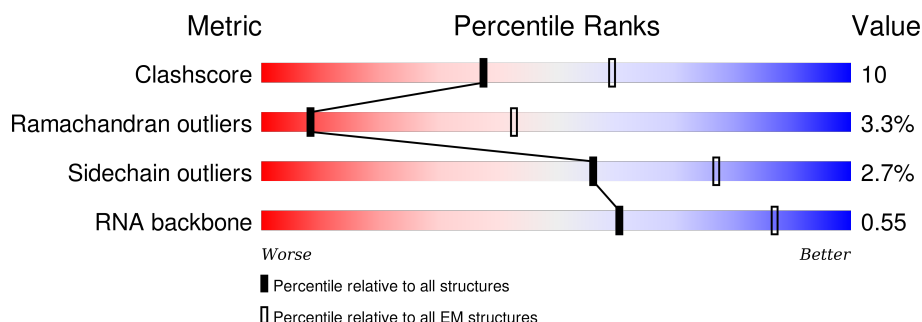
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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.














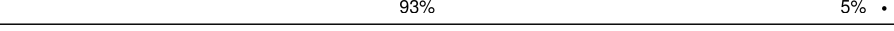







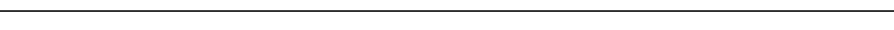

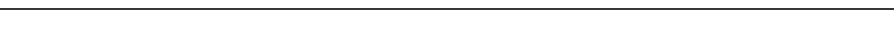
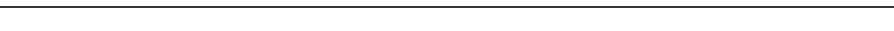


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	a	1539	84% 16%
2	b	240	85% 6% 9%
3	c	233	85% • 12%
4	d	206	92% 8%
5	e	167	84% 10% • 6%
6	f	135	68% • • 26%
7	g	179	78% 7% 16%
8	h	130	96% • •













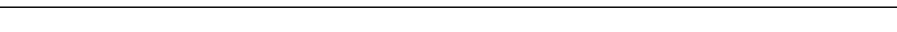

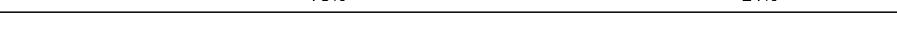

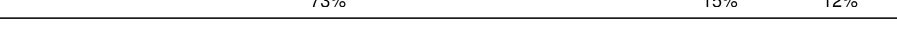








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Mol	Chain	Length	Quality of chain
9	i	130	 88% 10% .
10	j	103	 87% 8% 5%
11	k	129	 84% 6% 10%
12	l	124	 93% 6% .
13	m	118	 91% 6% .
14	n	102	 90% 9% .
15	o	89	 91% 8% .
16	p	82	 93% 7%
17	q	84	 86% 10% 5%
18	r	75	 79% 8% 13%
19	s	92	 85% . 14%
20	t	87	 93% 5% .
21	u	71	 82% 10% 8%
22	v	78	 77% 23%
23	w	77	 38% 49% 13%
24	x	11	 82% 18%
25	y	77	 74% 26%
26	z	393	 91% . 6%
27	A	2903	 53% 37% 9%
28	B	120	 55% 41% .
29	C	273	 77% 22% ..
30	D	209	 74% 25% .
31	E	201	 76% 23% .
32	F	179	 61% 34% . .
33	G	177	 80% 19% ..

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Mol	Chain	Length	Quality of chain
34	H	149	 80% 18% .
35	I	142	 63% 33% . .
36	J	142	 73% 26% .
37	K	123	 68% 28% . .
38	L	144	 63% 34% . .
39	M	136	 75% 24% .
40	N	127	 68% 26% . 6%
41	O	117	 82% 16% . .
42	P	115	 79% 19% . .
43	Q	118	 75% 25% .
44	R	103	 80% 20%
45	S	110	 70% 27% .
46	T	100	 67% 23% . 7%
47	U	104	 73% 24% . .
48	V	94	 71% 28% .
49	W	85	 73% 15% 12%
50	X	78	 78% 19% . .
51	Y	63	 75% 24% .
52	Z	59	 80% 19% .
53	0	57	 68% 26% . .
54	1	55	 78% 13% 9%
55	2	46	 70% 30%
56	3	65	 72% 25% . .
57	4	38	 61% 39%
58	5	165	 52% 25% . 21%

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Mol	Chain	Length	Quality of chain
59	6	70	<div><div></div><div>71%</div><div>21%</div><div>• 6%</div></div>

## 2 Entry composition

There are 66 unique types of molecules in this entry. The entry contains 152718 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			505	318	96	91		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.



Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 22 is a RNA chain called P-site fMet-tRNA<sup>fMet</sup>.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	78	Total	C	N	O	P	S	0	0
			1654	739	298	538	77	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	77	FME	-	initiating methionine	GB 147949

- Molecule 23 is a RNA chain called E-site tRNA<sup>fMet</sup>.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	w	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	x	11	Total	C	N	O	P	0	0
			234	105	41	77	11		

- Molecule 25 is a RNA chain called A/T-site Phe-tRNA<sup>Phe</sup>.

Mol	Chain	Residues	Atoms					AltConf	Trace	
25	y	77	Total	C	N	O	P	S	0	0
			1643	740	291	534	76	2		

- Molecule 26 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	z	371	Total	C	N	O	S	1	0
			2881	1824	495	549	13		

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A	2900	Total	C	N	O	P	0	0
			62276	27788	11460	20128	2900		

- Molecule 28 is a RNA chain called 5S ribosomal RNA (120-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

- Molecule 29 is a protein called 50S ribosomal protein L2.

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

- Molecule 30 is a protein called 50S ribosomal protein L3.

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

- Molecule 31 is a protein called 50S ribosomal protein L4.

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

- Molecule 32 is a protein called 50S ribosomal protein L5.

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

- Molecule 33 is a protein called 50S ribosomal protein L6.

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

- Molecule 34 is a protein called 50S ribosomal protein L9.

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

- Molecule 35 is a protein called 50S ribosomal protein L11.

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

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

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

- Molecule 38 is a protein called 50S ribosomal protein L15.

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

- Molecule 39 is a protein called 50S ribosomal protein L16.

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

- Molecule 40 is a protein called 50S ribosomal protein L17.

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

- Molecule 41 is a protein called 50S ribosomal protein L18.

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

- Molecule 42 is a protein called 50S ribosomal protein L19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

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

- Molecule 47 is a protein called 50S ribosomal protein L24.

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

- Molecule 48 is a protein called 50S ribosomal protein L25.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	W	75	Total	C	N	O	S	0
			575	356	116	102	1	0

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

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

- Molecule 51 is a protein called 50S ribosomal protein L29.

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

- Molecule 52 is a protein called 50S ribosomal protein L30.

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

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	0	56	Total	C	N	O	S	0
			444	269	94	80	1	0

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 58 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 59 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

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

Mol	Chain	Residues	Atoms		AltConf
60	0	1	Total	Mg	0
			1	1	
60	D	1	Total	Mg	0
			1	1	
60	B	7	Total	Mg	0
			7	7	

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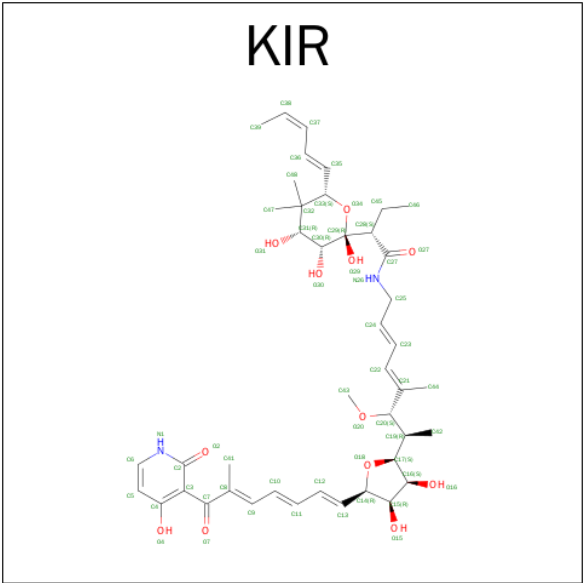
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Mol	Chain	Residues	Atoms		AltConf
60	a	83	Total	Mg	0
			83	83	
60	z	1	Total	Mg	0
			1	1	
60	A	234	Total	Mg	0
			234	234	
60	4	1	Total	Mg	0
			1	1	
60	v	4	Total	Mg	0
			4	4	
60	N	1	Total	Mg	0
			1	1	

- Molecule 61 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
61	A	1	Total	Cl	0
			1	1	
61	a	1	Total	Cl	0
			1	1	

- Molecule 62 is KIRROMYCIN (three-letter code: KIR) (formula: C<sub>43</sub>H<sub>60</sub>N<sub>2</sub>O<sub>12</sub>).



Mol	Chain	Residues	Atoms				AltConf
62	z	1	Total	C	N	O	0
			57	43	2	12	

- # GDP
- 
- The image displays the chemical structure of Guanosine Diphosphate (GDP). It consists of a guanine base (a purine ring system with an amino group at position 2) linked to a ribose sugar, which is in turn linked to two phosphate groups. The atoms are color-coded: carbon (grey), nitrogen (blue), oxygen (red), and phosphorus (purple). The structure is labeled with atom names (N1, N2, N3, N7, N9, C2, C4, C5, C6, C8, C9, O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779, O780, O781, O782, O783, O784, O785, O786, O787, O788, O789, O790, O791, O792, O793, O794, O795, O796, O797, O798, O799, O800, O801, O802, O803, O804, O805, O806, O807, O808

- Molecule 64 is SODIUM ION (three-letter code: NA) (formula: Na).

- Molecule 65 is ZINC ION (three-letter code: ZN) (formula:  $\text{Zn}$ ).

- Molecule 66 is water.

*Continued on next page...*

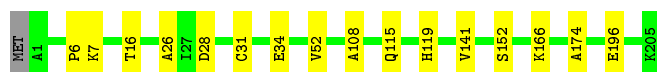


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Mol	Chain	Residues	Atoms		AltConf
66	A	9	Total 9	O 9	0
66	D	2	Total 2	O 2	0
66	K	1	Total 1	O 1	0



Chain d:  92% 8%



- Molecule 5: 30S ribosomal protein S5

Chain e:  84% 10% 6%




- Molecule 6: 30S ribosomal protein S6

Chain f:  68% 26%



- Molecule 7: 30S ribosomal protein S7

Chain g:  78% 7% 16%




- Molecule 8: 30S ribosomal protein S8

Chain h:  96%




- Molecule 9: 30S ribosomal protein S9

Chain i:  88% 10%




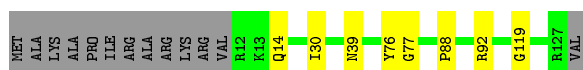
- Molecule 10: 30S ribosomal protein S10

Chain j:  87% 8% 5%



- Molecule 11: 30S ribosomal protein S11

Chain k:  84% 6% 10%



- Molecule 12: 30S ribosomal protein S12

Chain l: 93% 6% .



- Molecule 13: 30S ribosomal protein S13

Chain m: 91% 6% .



- Molecule 14: 30S ribosomal protein S14

Chain n: 90% 9% .



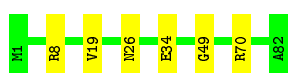
- Molecule 15: 30S ribosomal protein S15

Chain o: 91% 8% .



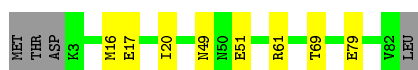
- Molecule 16: 30S ribosomal protein S16

Chain p: 93% 7% .



- Molecule 17: 30S ribosomal protein S17

Chain q: 86% 10% 5% .




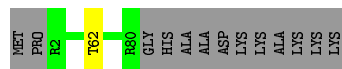
- Molecule 18: 30S ribosomal protein S18

Chain r: 79% 8% 13% .



- Molecule 19: 30S ribosomal protein S19

Chain s:  85% 14%




- Molecule 20: 30S ribosomal protein S20

Chain t:  93% 5%



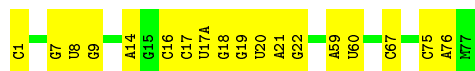
- Molecule 21: 30S ribosomal protein S21

Chain u:  82% 10% 8%



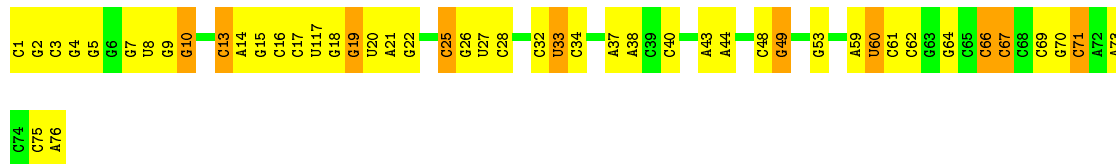
- Molecule 22: P-site fMet-tRNA<sup>fMet</sup>

Chain v:  77% 23%




- Molecule 23: E-site tRNA<sup>fMet</sup>

Chain w:  38% 49% 13%



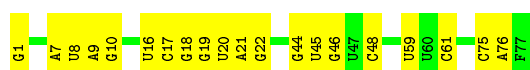
- Molecule 24: mRNA

Chain x:  82% 18%




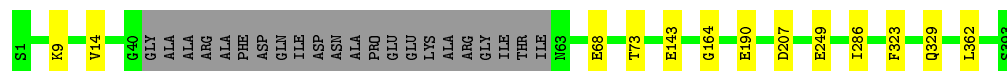
- Molecule 25: A/T-site Phe-tRNA<sup>Phe</sup>

Chain y:  74% 26%



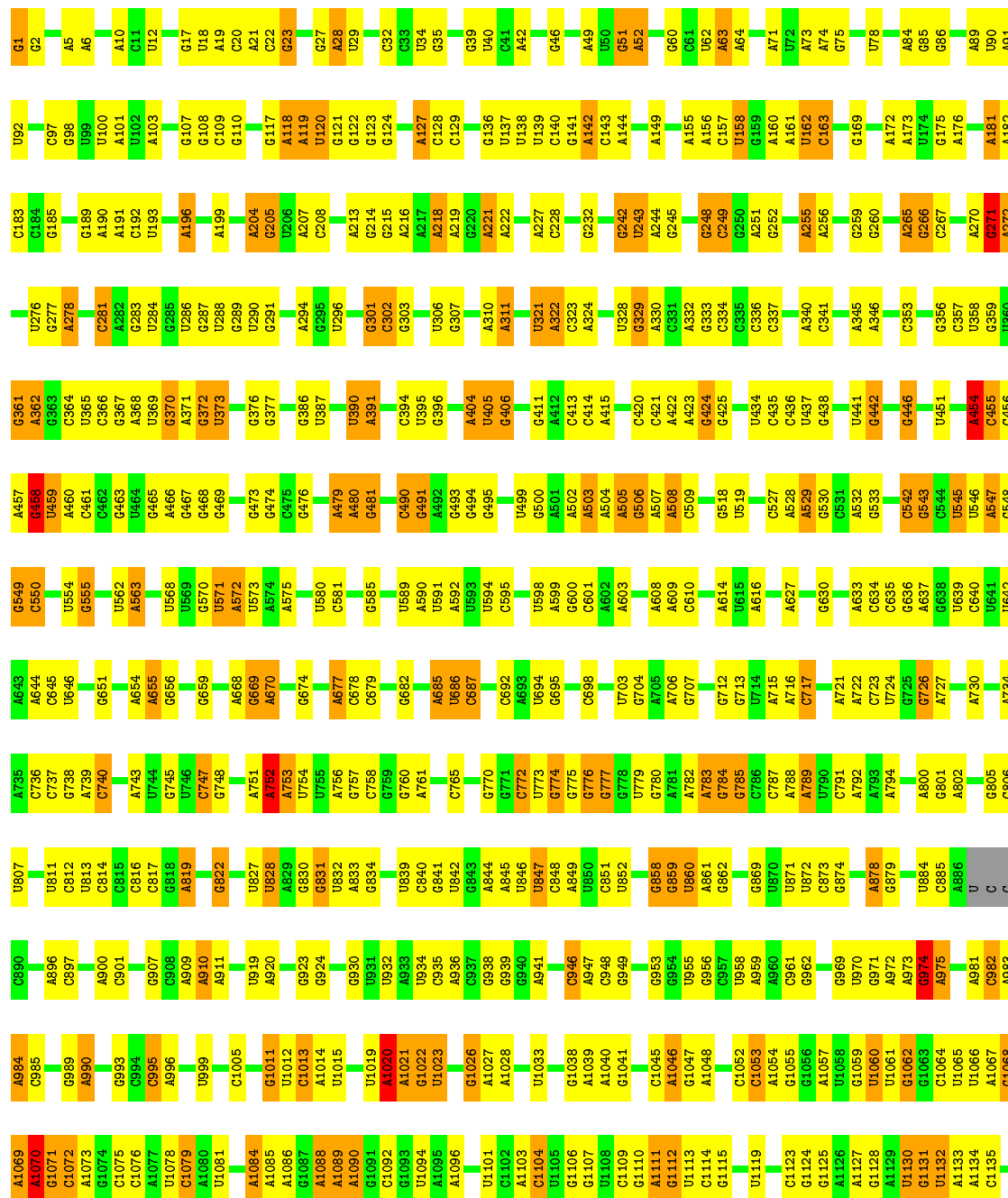
- Molecule 26: Elongation factor Tu 2

Chain z:  91% 6%

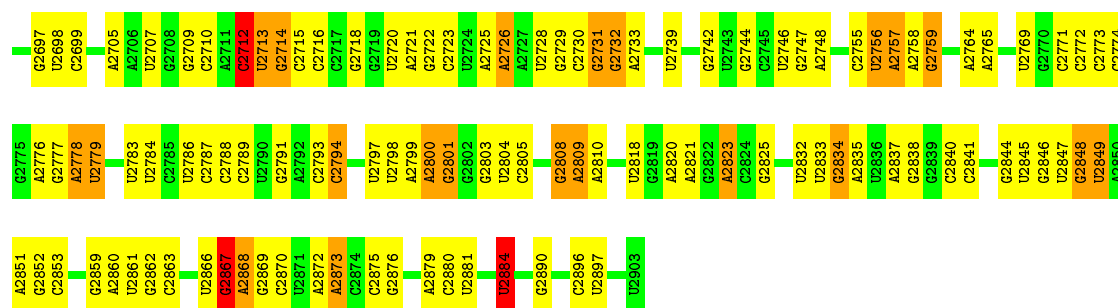


- Molecule 27: 23S ribosomal RNA

Chain A:  53% 37% 9%

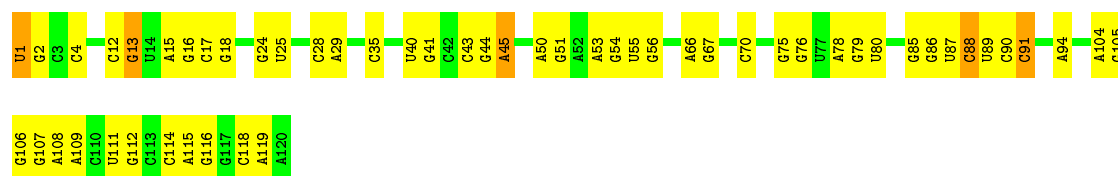


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U2585	U2586	U2587	A2587	C2590	C2591	C2592	C2501	C2502	C2503	G2205	U2299	U2393	C2490	C2393	U2299	A2205	A2117	G2038	C1942	G1845	U1647	C1646	U1539	G1435	U1340	U1249	C1140
U2586	U2587	A2587	A2587	C2590	C2591	C2592	C2501	C2502	C2503	G2206	U2299	U2393	C2490	C2393	U2299	A2206	A2118	U2039	C1943	G1846	C1748	U1648	U1539	G1435	U1341	G1250	U1141
U2587	A2587	A2587	A2587	C2590	C2591	C2592	C2501	C2502	C2503	G2207	G2303	C2394	C2494	C2394	U2398	C2207	A2119	U2040	C1944	G1847	G1649	U1542	U1443	U1342	G1251	A1142	
A2590	C2591	C2592	A2497	C2498	C2501	C2502	C2503	C2504	C2505	G2208	U2305	U2398	A2497	C2498	U2399	G2209	G2120	G2041	C1945	U1751	G1650	G1651	U1544	G1252	A1143		
C2591	C2592	U2402	C2399	C2498	C2501	C2502	C2503	C2504	C2505	U2210	G2306	C2399	C2498	C2501	U2402	U2211	G2121	A2042	U1951	G1857	G1652	C1345	G1256	A1151			
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U2532	U2533	U2431	C2434	C2435	U2436	U2437	U2438	U2439	U2440	U2248	U2156	A2433	A2434	A2435	A2436	U2248	U2157	C2077	U1983	U1797	A1292	G1292	U1190				
U2533	U2534	U2432	C2435	C2436	U2437	U2438	U2439	U2440	U2441	U2249	U2157	A2434	A2435	A2436	A2437	U2249	U2158	C2078	U1984	U1798	A1292	G1292	U1190				
U2534	U2535	U2433	C2436	C2437	U2438	U2439	U2440	U2441	U2442	U2250	U2158	A2435	A2436	A2437	A2438	U2250	U2159	C2079	U1985	U1799	A1292	G1292	U1190				
U2535	U2536	U2434	C2437	C2438	U2439	U2440	U2441	U2442	U2443	U2251	U2159	A2436	A2437	A2438	A2439	U2251	U2160	C2080	U1986	U1800	A1292	G1292	U1190				
U2536	U2537	U2435	C2438	C2439	U2440	U2441	U2442	U2443	U2444	U2252	U2160	A2437	A2438	A2439	A2440	U2252	U2161	C2081	U1987	U1801	A1292	G1292	U1190				
U2537	U2538	U2436	C2439	C2440	U2441	U2442	U2443	U2444	U2445	U2253	U2161	A2438	A2439	A2440	A2441	U2253	U2162	C2082	U1988	U1802	A1292	G1292	U1190				
U2538	U2539	U2437	C2440	C2441	U2442	U2443	U2444	U2445	U2446	U2254	U2162	A2439	A2440	A2441	A2442	U2254	U2163	C2083	U1989	U1803	A1292	G1292	U1190				
U2539	U2540	U2438	C2441	C2442	U2443	U2444	U2445	U2446	U2447	U2255	U2163	A2440	A2441	A2442	A2443	U2255	U2164	C2084	U1990	U1804	A1292	G1292	U1190				
U2540	U2541	U2439	C2442	C2443	U2444	U2445	U2446	U2447	U2448	U2256	U2164	A2441	A2442	A2443	A2444	U2256	U2165	C2085	U1991	U1805	A1292	G1292	U1190				
U2541	U2542	U2440	C2443	C2444	U2445	U2446	U2447	U2448	U2449	U2257	U2165	A2442	A2443	A2444	A2445	U2257	U2166	C2086	U1992	U1806	A1292	G1292	U1190				
U2542	U2543	U2441	C2444	C2445	U2446	U2447	U2448	U2449	U2450	U2258	U2166	A2443	A2444	A2445	A2446	U2258	U2167	C2087	U1993	U1807	A1292	G1292	U1190				
U2543	U2544	U2442	C2445	C2446	U2447	U2448	U2449	U2450	U2451	U2259	U2167	A2444	A2445	A2446	A2447	U2259	U2168	C2088	U1994	U1808	A1292	G1292	U1190				
U2544	U2545	U2443	C2446	C2447	U2448	U2449	U2450	U2451	U2452	U2260	U2168	A2445	A2446	A2447	A2448	U2260	U2169	C2089	U1995	U1809	A1292	G1292	U1190				
U2545	U2546	U2444	C2447	C2448	U2449	U2450	U2451	U2452	U2453	U2261	U2169	A2446	A2447	A2448	A2449	U2261	U2170	C2090	U1996	U1810	A1292	G1292	U1190				
U2546	U2547	U2445	C2448	C2449	U2450	U2451	U2452	U2453	U2454	U2262	U2170	A2447	A2448	A2449	A2450	U2262	U2171	C2091	U1997	U1811	A1292	G1292	U1190				
U2547	U2548	U2446	C2449	C2450	U2451	U																					



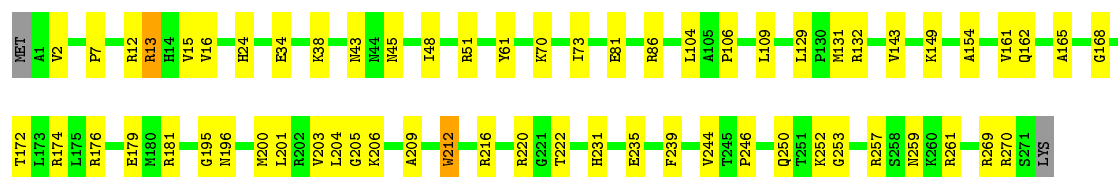
- Molecule 28: 5S ribosomal RNA (120-MER)

Chain B: 55% 41%



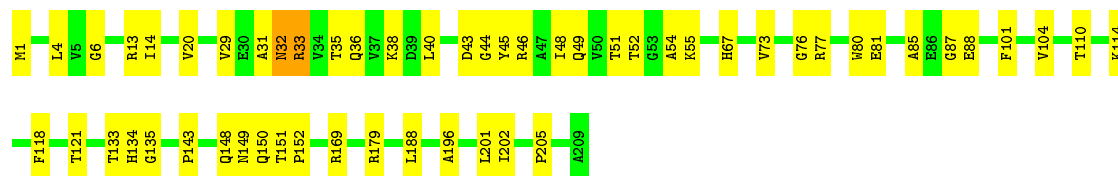
- Molecule 29: 50S ribosomal protein L2

Chain C: 77% 22%



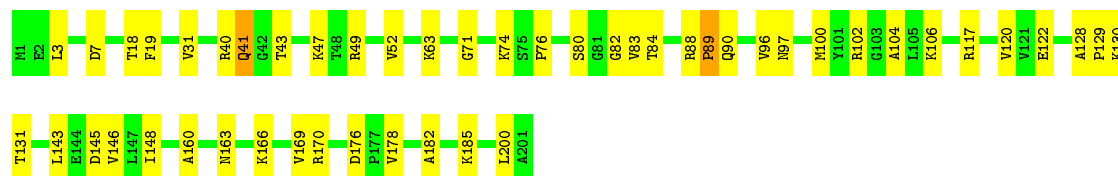
- Molecule 30: 50S ribosomal protein L3

Chain D: 74% 25%



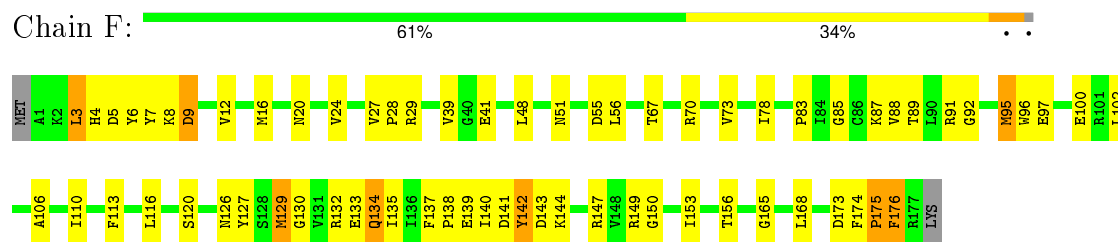
- Molecule 31: 50S ribosomal protein L4

Chain E: 76% 23%

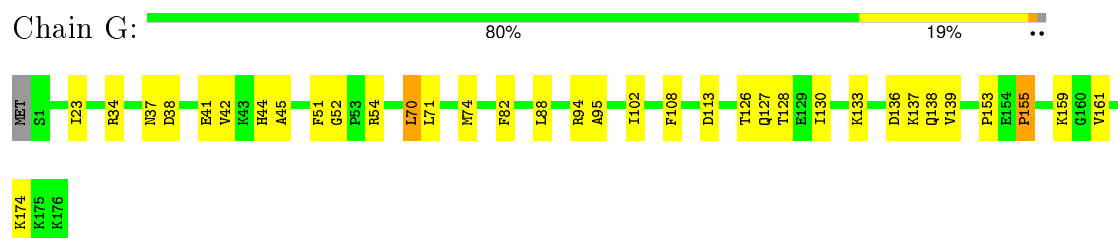


- Molecule 32: 50S ribosomal protein L5

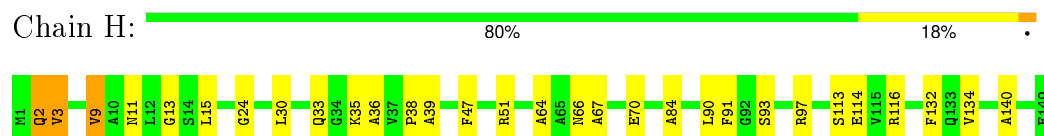




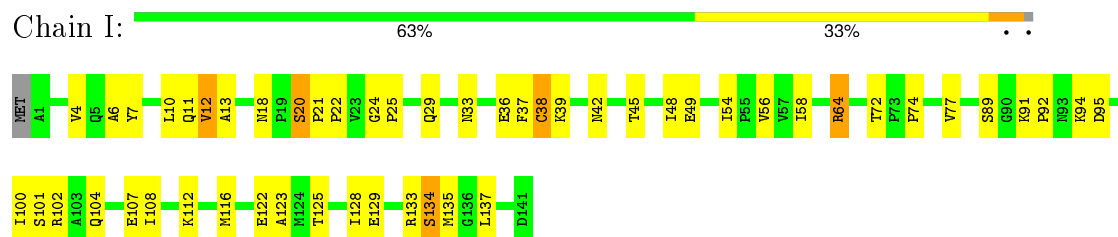
- Molecule 33: 50S ribosomal protein L6



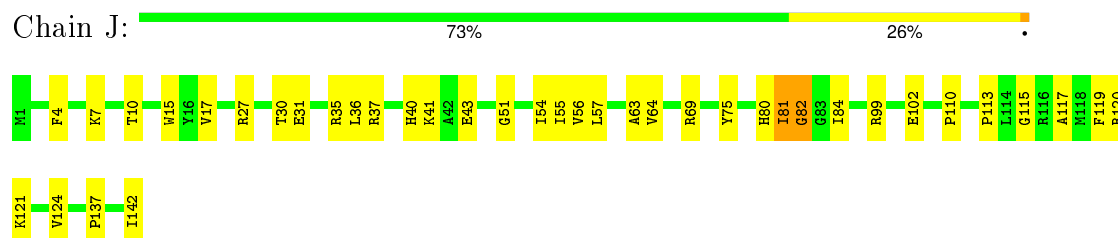
- Molecule 34: 50S ribosomal protein L9



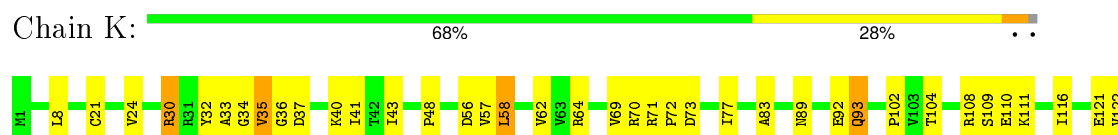
- Molecule 35: 50S ribosomal protein L11



- Molecule 36: 50S ribosomal protein L13

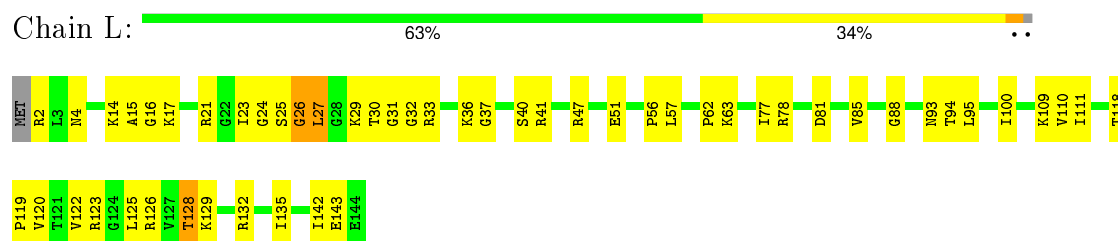


- Molecule 37: 50S ribosomal protein L14

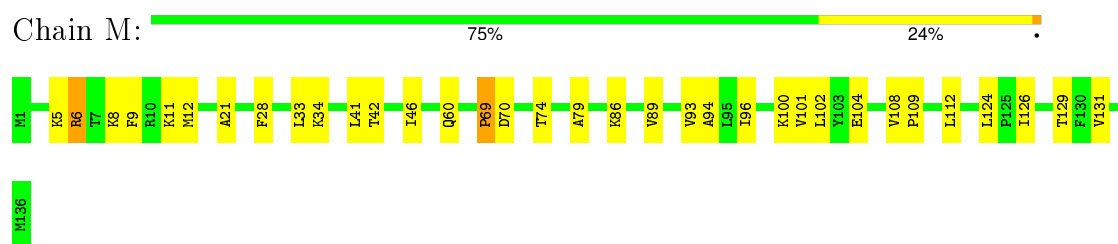


LEU

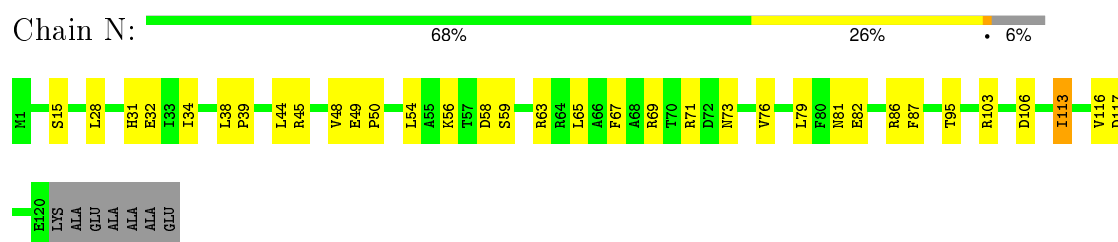
- Molecule 38: 50S ribosomal protein L15



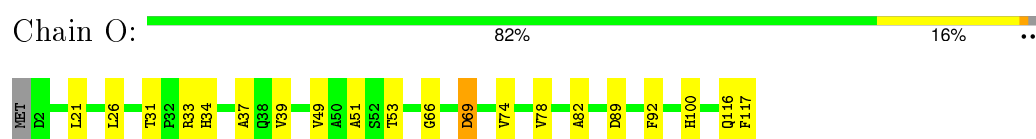
- Molecule 39: 50S ribosomal protein L16



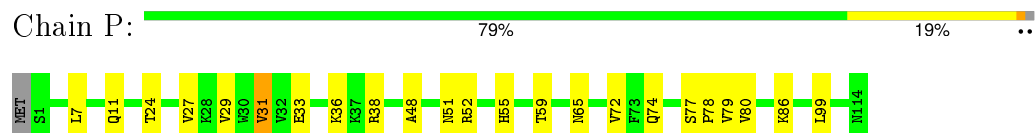
- Molecule 40: 50S ribosomal protein L17



- Molecule 41: 50S ribosomal protein L18



- Molecule 42: 50S ribosomal protein L19

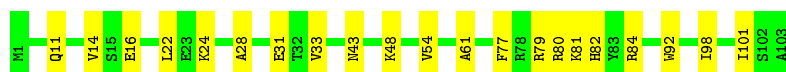
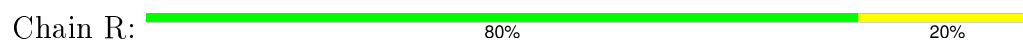


- Molecule 43: 50S ribosomal protein L20

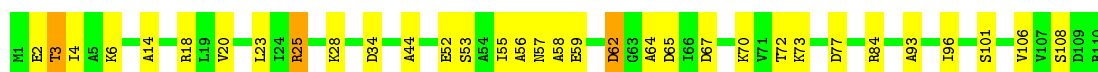




- Molecule 44: 50S ribosomal protein L21



- Molecule 45: 50S ribosomal protein L22



- Molecule 46: 50S ribosomal protein L23



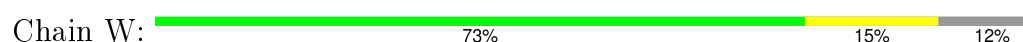
- Molecule 47: 50S ribosomal protein L24



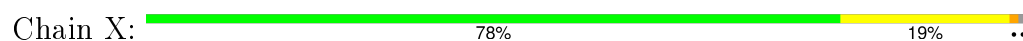
- Molecule 48: 50S ribosomal protein L25



- Molecule 49: 50S ribosomal protein L27



- Molecule 50: 50S ribosomal protein L28




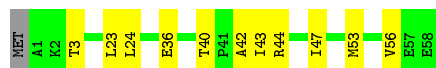
- Molecule 51: 50S ribosomal protein L29

Chain Y:  75% 24%



- Molecule 52: 50S ribosomal protein L30

Chain Z:  80% 19%




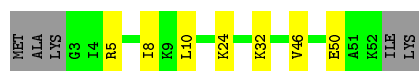
- Molecule 53: 50S ribosomal protein L32

Chain 0:  68% 26%



- Molecule 54: 50S ribosomal protein L33

Chain 1:  78% 13% 9%



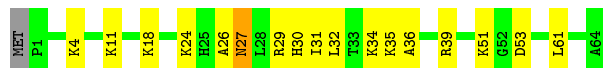
- Molecule 55: 50S ribosomal protein L34

Chain 2:  70% 30%



- Molecule 56: 50S ribosomal protein L35

Chain 3:  72% 25%



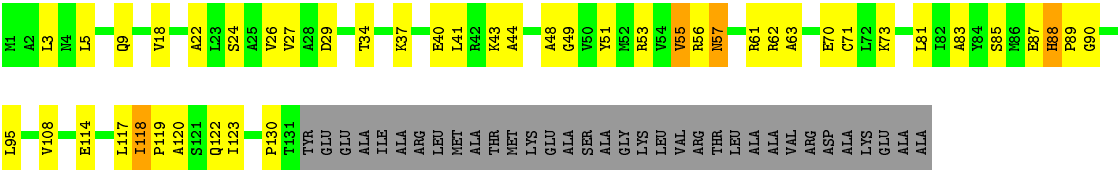
- Molecule 57: 50S ribosomal protein L36

Chain 4:  61% 39%

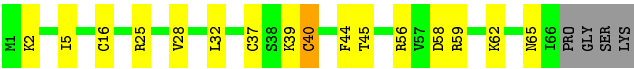


- Molecule 58: 50S ribosomal protein L10

Chain 5:  52% 25% 21%



• Molecule 59: 50S ribosomal protein L31



## 4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	LOCAL CTF CORRECTION	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	192000	Depositor
Image detector	FEI FALCON I (4K X 4K)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  > 2	RMSZ	# Z  > 2
1	a	0.39	1/36701 (0.0%)	0.85	12/57246 (0.0%)
10	j	0.36	0/796	0.54	0/1077
11	k	0.28	0/885	0.48	0/1195
12	l	0.29	0/969	0.47	0/1300
13	m	0.36	0/892	0.50	0/1193
14	n	0.27	0/811	0.40	0/1081
15	o	0.32	0/722	0.44	0/964
16	p	0.33	0/659	0.45	0/884
17	q	0.27	0/657	0.46	0/881
18	r	0.28	0/511	0.43	0/689
19	s	0.28	0/652	0.44	0/877
2	b	0.30	0/1735	0.44	0/2338
20	t	0.38	0/671	0.48	0/888
21	u	0.29	0/500	0.42	0/668
22	v	0.41	1/1747 (0.1%)	0.82	0/2721
23	w	0.98	1/1747 (0.1%)	1.40	24/2721 (0.9%)
24	x	0.62	1/261 (0.4%)	0.85	0/404
25	y	0.39	1/1618 (0.1%)	0.81	0/2514
26	z	0.34	0/2935	0.47	0/3970
27	A	0.46	1/69174 (0.0%)	0.90	50/107910 (0.0%)
28	B	0.38	1/2876 (0.0%)	0.86	0/4483
29	C	0.31	0/2121	0.47	0/2852
3	c	0.32	0/1651	0.46	0/2225
30	D	0.35	0/1586	0.48	0/2134
31	E	0.26	0/1571	0.41	0/2113
32	F	0.30	0/1434	0.47	0/1926
33	G	0.35	0/1343	0.47	0/1816
34	H	0.23	0/1122	0.40	0/1515
35	I	0.23	0/1046	0.44	0/1410
36	J	0.29	0/1152	0.43	0/1551
37	K	0.28	0/947	0.41	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
38	L	0.26	0/1054	0.45	0/1403
39	M	0.32	0/1093	0.46	0/1460
4	d	0.28	0/1665	0.44	0/2227
40	N	0.28	0/973	0.44	0/1301
41	O	0.33	0/902	0.44	0/1209
42	P	0.28	0/929	0.43	0/1242
43	Q	0.34	0/960	0.43	0/1278
44	R	0.34	0/829	0.52	0/1107
45	S	0.28	0/864	0.47	0/1156
46	T	0.29	0/744	0.45	0/994
47	U	0.35	0/787	0.44	0/1051
48	V	0.31	0/766	0.45	0/1025
49	W	0.33	0/582	0.47	0/769
5	e	0.31	0/1154	0.46	0/1554
50	X	0.28	0/635	0.40	0/848
51	Y	0.33	0/510	0.45	0/677
52	Z	0.25	0/453	0.41	0/605
53	0	0.26	0/450	0.41	0/599
54	1	0.26	0/416	0.41	0/554
55	2	0.29	0/380	0.44	0/498
56	3	0.27	0/513	0.43	0/676
57	4	0.28	0/303	0.40	0/397
58	5	0.25	0/1001	0.45	0/1350
59	6	0.33	0/531	0.54	0/709
6	f	0.35	0/835	0.48	0/1128
7	g	0.36	0/1195	0.50	0/1602
8	h	0.27	0/989	0.45	0/1326
9	i	0.27	0/1034	0.45	0/1375
All	All	0.41	7/164039 (0.0%)	0.80	86/244934 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	w	1	C	OP3-P	-10.97	1.48	1.61
28	B	1	U	OP3-P	-10.59	1.48	1.61
27	A	1	G	OP3-P	-10.58	1.48	1.61
22	v	1	C	OP3-P	-10.56	1.48	1.61
1	a	2	A	OP3-P	-10.52	1.48	1.61
25	y	1	G	OP3-P	-10.48	1.48	1.61
24	x	14	U	Cl'-N1	5.60	1.57	1.48

All (86) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	974	G	N1-C6-O6	9.46	125.57	119.90
27	A	1936	A	N1-C6-N6	9.14	124.09	118.60
23	w	13	C	C6-N1-C2	-8.20	117.02	120.30
23	w	62	C	C6-N1-C2	-8.13	117.05	120.30
23	w	62	C	C5-C6-N1	7.73	124.87	121.00
23	w	62	C	N1-C2-O2	7.54	123.42	118.90
23	w	62	C	C2-N1-C1'	7.33	126.86	118.80
27	A	1936	A	C2-N3-C4	-7.29	106.95	110.60
27	A	783	A	N7-C8-N9	7.27	117.44	113.80
1	a	1297	G	P-O3'-C3'	7.20	128.34	119.70
27	A	783	A	C5-N7-C8	-7.14	100.33	103.90
27	A	62	U	C2-N1-C1'	6.93	126.02	117.70
27	A	974	G	C6-C5-N7	-6.73	126.36	130.40
23	w	71	C	C5-C4-N4	-6.56	115.61	120.20
27	A	62	U	N1-C2-O2	6.55	127.38	122.80
23	w	66	C	C6-N1-C2	-6.54	117.68	120.30
27	A	783	A	N1-C6-N6	6.49	122.49	118.60
27	A	1779	U	C5-C6-N1	-6.44	119.48	122.70
27	A	2884	U	C2-N1-C1'	6.41	125.39	117.70
27	A	984	A	C2-N3-C4	-6.39	107.41	110.60
27	A	2884	U	N1-C2-O2	6.27	127.19	122.80
23	w	71	C	N3-C4-C5	6.12	124.35	121.90
27	A	2076	U	C2-N1-C1'	6.09	125.01	117.70
27	A	62	U	N3-C2-O2	-6.00	118.00	122.20
27	A	1313	U	C2-N1-C1'	5.95	124.83	117.70
23	w	71	C	C6-N1-C1'	-5.90	113.72	120.80
23	w	66	C	C5-C6-N1	5.88	123.94	121.00
23	w	71	C	C2-N1-C1'	5.81	125.19	118.80
23	w	49	G	C6-C5-N7	-5.74	126.96	130.40
1	a	1158	C	C2-N1-C1'	5.72	125.09	118.80
27	A	974	G	N7-C8-N9	5.71	115.95	113.10
23	w	61	C	N1-C2-O2	5.68	122.31	118.90
27	A	2682	A	C8-N9-C4	5.68	108.07	105.80
27	A	2501	C	C2-N1-C1'	-5.65	112.58	118.80
27	A	2884	U	N3-C2-O2	-5.63	118.26	122.20
27	A	2542	A	C8-N9-C4	5.62	108.05	105.80
23	w	33	U	C5-C6-N1	5.62	125.51	122.70
27	A	458	G	C4-N9-C1'	-5.58	119.24	126.50
23	w	4	G	N3-C4-N9	-5.58	122.65	126.00
23	w	49	G	C4-N9-C1'	5.58	133.75	126.50
23	w	25	C	N3-C4-C5	5.57	124.13	121.90
27	A	2867	G	N3-C4-N9	-5.56	122.66	126.00
1	a	246	A	P-O3'-C3'	5.55	126.36	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1399	C	P-O3'-C3'	5.54	126.35	119.70
27	A	2867	G	C6-C5-N7	5.50	133.70	130.40
27	A	669	G	C8-N9-C1'	-5.48	119.87	127.00
27	A	2867	G	C4-N9-C1'	-5.48	119.37	126.50
23	w	62	C	N3-C2-O2	-5.45	118.09	121.90
23	w	67	C	C5-C6-N1	5.42	123.71	121.00
27	A	974	G	C4-C5-N7	5.40	112.96	110.80
23	w	10	G	C5-C6-O6	-5.39	125.37	128.60
27	A	1142	A	OP1-P-O3'	5.38	117.04	105.20
27	A	783	A	C8-N9-C4	-5.38	103.65	105.80
27	A	783	A	C5-C6-N1	-5.37	115.02	117.70
23	w	60	U	N1-C2-O2	5.36	126.55	122.80
27	A	752	A	P-O3'-C3'	5.33	126.09	119.70
27	A	1936	A	C4-C5-N7	5.28	113.34	110.70
27	A	669	G	C4-N9-C1'	5.28	133.36	126.50
27	A	1936	A	C5-N7-C8	-5.25	101.27	103.90
27	A	2501	C	C5-C6-N1	-5.25	118.38	121.00
27	A	974	G	C5-C6-O6	-5.22	125.47	128.60
1	a	1306	A	N7-C8-N9	5.18	116.39	113.80
27	A	783	A	C2-N3-C4	-5.17	108.01	110.60
27	A	2712	C	P-O3'-C3'	5.17	125.90	119.70
27	A	1020	A	P-O3'-C3'	5.16	125.89	119.70
27	A	271	G	OP1-P-O3'	5.15	116.54	105.20
1	a	1201	A	P-O3'-C3'	5.14	125.87	119.70
27	A	1475	G	OP2-P-O3'	5.11	116.44	105.20
1	a	246	A	OP1-P-O3'	5.10	116.43	105.20
27	A	974	G	C5-C6-N1	-5.08	108.96	111.50
23	w	19	G	C4'-C3'-O3'	-5.08	98.72	109.40
1	a	16	A	C8-N9-C4	5.08	107.83	105.80
27	A	2759	G	N1-C2-N3	5.07	126.94	123.90
1	a	1158	C	N1-C2-O2	5.06	121.94	118.90
23	w	27	U	OP1-P-O3'	5.05	116.31	105.20
27	A	458	G	O4'-C1'-N9	5.05	112.24	108.20
27	A	1652	A	C8-N9-C4	5.04	107.82	105.80
27	A	451	U	C5-C6-N1	-5.03	120.19	122.70
1	a	754	C	C2-N1-C1'	5.03	124.33	118.80
1	a	960	U	P-O3'-C3'	5.02	125.73	119.70
23	w	13	C	C5-C6-N1	5.01	123.51	121.00
27	A	1936	A	C6-C5-N7	-5.01	128.79	132.30
27	A	454	A	OP2-P-O3'	5.01	116.23	105.20
27	A	2076	U	N1-C2-O2	5.01	126.31	122.80
27	A	1070	A	P-O3'-C3'	5.01	125.71	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1346	A	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	33029	0	16645	0	0
2	b	1704	0	1732	0	0
3	c	1624	0	1699	0	0
4	d	1643	0	1710	0	0
5	e	1141	0	1170	0	0
6	f	817	0	808	0	0
7	g	1181	0	1240	0	0
8	h	979	0	1034	0	0
9	i	1022	0	1070	0	0
10	j	786	0	828	0	0
11	k	869	0	878	0	0
12	l	955	0	1019	0	0
13	m	883	0	944	0	0
14	n	799	0	841	0	0
15	o	714	0	737	0	0
16	p	649	0	666	0	0
17	q	648	0	691	0	0
18	r	505	0	502	0	0
19	s	637	0	665	0	0
20	t	665	0	714	0	0
21	u	495	0	486	0	0
22	v	1654	0	849	0	0
23	w	1644	0	840	0	0
24	x	234	0	118	0	0
25	y	1643	0	850	0	0
26	z	2881	0	2894	0	0
27	A	62276	0	31346	830	0
28	B	2572	0	1302	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	C	2082	0	2157	39	0
30	D	1565	0	1616	37	0
31	E	1552	0	1619	28	0
32	F	1410	0	1447	47	0
33	G	1323	0	1374	22	0
34	H	1111	0	1148	18	0
35	I	1032	0	1088	34	0
36	J	1129	0	1162	31	0
37	K	938	0	1012	22	0
38	L	1045	0	1117	36	0
39	M	1074	0	1157	20	0
40	N	960	0	1000	24	0
41	O	892	0	923	12	0
42	P	917	0	965	16	0
43	Q	947	0	1022	22	0
44	R	816	0	839	13	0
45	S	857	0	922	23	0
46	T	738	0	807	17	0
47	U	779	0	834	17	0
48	V	753	0	780	16	0
49	W	575	0	592	9	0
50	X	625	0	655	12	0
51	Y	509	0	543	11	0
52	Z	449	0	491	7	0
53	0	444	0	461	15	0
54	1	409	0	440	4	0
55	2	377	0	418	18	0
56	3	504	0	574	16	0
57	4	302	0	341	12	0
58	5	988	0	1025	31	0
59	6	522	0	520	12	0
60	0	1	0	0	0	0
60	4	1	0	0	0	0
60	A	234	0	0	0	0
60	B	7	0	0	0	0
60	D	1	0	0	0	0
60	N	1	0	0	0	0
60	a	83	0	0	0	0
60	v	4	0	0	0	0
60	z	1	0	0	0	0
61	A	1	0	0	0	0
61	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	z	57	0	60	0	0
63	z	28	0	12	0	0
64	A	1	0	0	0	0
64	B	1	0	0	0	0
65	4	1	0	0	0	0
65	6	1	0	0	0	0
66	A	9	0	0	1	0
66	D	2	0	0	0	0
66	K	1	0	0	0	0
66	a	9	0	0	0	0
All	All	152718	0	103399	1338	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 10.

All (1338) 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)
50:X:17:ARG:HE	50:X:23:ALA:HB2	1.29	0.97
27:A:704:G:H2'	27:A:726:G:H22	1.31	0.94
27:A:1055:G:H1	27:A:1104:C:H42	1.11	0.94
32:F:134:GLN:NE2	32:F:149:ARG:O	2.06	0.87
27:A:585:G:N7	43:Q:5:ARG:NH1	2.26	0.83
44:R:14:VAL:HG21	44:R:98:ILE:HG13	1.61	0.82
47:U:65:GLN:HB2	47:U:68:ASN:OD1	1.80	0.82
27:A:2848:G:H2'	27:A:2867:G:N2	1.95	0.82
30:D:13:ARG:HH11	42:P:55:HIS:HA	1.44	0.82
27:A:2333:A:H4'	27:A:2334:U:O5'	1.81	0.81
27:A:1060:U:H5'	27:A:1062:G:H5'	1.63	0.80
27:A:1103:A:H3'	27:A:1104:C:H5''	1.62	0.80
31:E:146:VAL:HG12	31:E:185:LYS:HB2	1.65	0.79
27:A:1041:G:H1	27:A:1114:C:H42	1.31	0.78
29:C:106:PRO:HD2	29:C:109:LEU:HD22	1.66	0.78
27:A:2220:U:H4'	34:H:97:ARG:HH21	1.48	0.77
45:S:53:SER:O	45:S:57:ASN:HB2	1.83	0.77
30:D:35:THR:OG1	30:D:49:GLN:HG2	1.86	0.76
36:J:80:HIS:O	36:J:82:GLY:N	2.15	0.76
36:J:117:ALA:HA	36:J:120:ARG:HH21	1.49	0.76
27:A:1936:A:H2	27:A:1943:U:H3	1.31	0.76
27:A:2345:G:H4'	27:A:2346:A:H5''	1.67	0.75
58:5:87:GLU:HG2	58:5:95:LEU:HD12	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2848:G:H2'	27:A:2867:G:H22	1.50	0.75
27:A:1090:A:H61	27:A:1101:U:H3	1.35	0.75
27:A:1845:G:N2	27:A:1895:C:O2	2.14	0.74
35:I:91:LYS:HG3	35:I:94:LYS:HE2	1.70	0.74
27:A:1532:A:H2	27:A:1539:U:H3	1.34	0.73
27:A:947:A:HO2'	27:A:984:A:H2	1.37	0.73
27:A:2808:G:H4'	27:A:2809:A:O5'	1.88	0.72
27:A:458:G:O2'	27:A:459:U:OP2	2.06	0.72
27:A:572:A:OP2	44:R:80:ARG:NH2	2.22	0.72
54:1:8:ILE:HD13	54:1:24:LYS:HE3	1.70	0.72
51:Y:6:LEU:HD13	51:Y:56:LEU:HD22	1.72	0.72
45:S:73:LYS:HB2	45:S:106:VAL:HB	1.70	0.72
27:A:1022:G:H4'	27:A:1023:U:O5'	1.88	0.72
42:P:33:GLU:HB2	42:P:36:LYS:HB2	1.71	0.71
27:A:1059:G:H22	35:I:128:ILE:HG12	1.53	0.71
27:A:2682:A:H61	27:A:2728:U:H1'	1.55	0.71
27:A:1188:U:C2'	27:A:1189:A:H5'	2.21	0.71
27:A:568:U:H1'	27:A:2030:6MZ:H9C1	1.72	0.70
27:A:704:G:H1'	27:A:727:A:N6	2.05	0.70
32:F:3:LEU:HA	32:F:6:TYR:HB3	1.73	0.70
45:S:4:ILE:HG22	45:S:106:VAL:HG22	1.71	0.70
37:K:69:VAL:HG21	37:K:104:THR:HG21	1.72	0.70
27:A:1213:A:N6	27:A:1236:G:H1'	2.07	0.70
27:A:2644:G:C2'	27:A:2645:G:H5'	2.22	0.69
27:A:328:U:H4'	47:U:65:GLN:HE21	1.56	0.69
47:U:32:LYS:HB3	47:U:63:ALA:HB1	1.73	0.69
27:A:1341:G:N3	46:T:59:ASN:OD1	2.25	0.69
48:V:20:LEU:HD11	48:V:41:GLU:HG3	1.73	0.69
27:A:284:U:H3	27:A:356:G:H1	1.40	0.69
38:L:62:PRO:HB2	56:3:29:ARG:HH11	1.56	0.69
55:2:12:ARG:HE	55:2:44:VAL:HG21	1.58	0.69
27:A:1046:A:H4'	58:5:61:ARG:HB3	1.75	0.68
29:C:131:MET:HE1	29:C:143:VAL:HG13	1.74	0.68
27:A:107:G:H2'	27:A:108:G:H8	1.58	0.68
29:C:196:ASN:OD1	29:C:196:ASN:O	2.11	0.68
27:A:1565:C:O2'	27:A:1566:A:H8	1.77	0.68
27:A:776:G:H4'	27:A:777:G:O5'	1.94	0.68
27:A:1613:G:H4'	55:2:3:ARG:HE	1.58	0.67
27:A:2133:G:H21	27:A:2158:A:H61	1.41	0.67
27:A:1011:G:O2'	27:A:1013:C:H5''	1.93	0.67
27:A:703:U:H2'	27:A:704:G:O4'	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2331:G:H4'	49:W:39:THR:H	1.57	0.67
37:K:40:LYS:HE3	37:K:57:VAL:HG12	1.76	0.67
27:A:2291:U:H2'	27:A:2292:U:C6	2.29	0.67
27:A:2564:A:OP1	27:A:2648:G:H4'	1.95	0.67
27:A:189:G:H1	27:A:205:G:HO2'	1.39	0.67
27:A:655:A:H4'	27:A:656:G:H5'	1.77	0.67
27:A:910:A:H62	39:M:12:MET:HA	1.58	0.67
27:A:2339:C:H2'	27:A:2340:A:H8	1.59	0.66
27:A:1478:G:H1	27:A:1513:U:H3	1.42	0.66
27:A:2759:G:H21	33:G:138:GLN:NE2	1.93	0.66
27:A:1701:A:H2'	27:A:1702:G:H5'	1.78	0.66
32:F:28:PRO:HB2	32:F:168:LEU:HD22	1.77	0.66
48:V:21:ARG:HA	48:V:25:LYS:O	1.95	0.66
27:A:545:U:H3	27:A:548:G:H1	1.41	0.66
27:A:753:A:OP2	27:A:753:A:H8	1.79	0.66
27:A:499:U:H5''	47:U:42:LYS:HE2	1.78	0.66
55:2:3:ARG:HG3	55:2:5:PHE:H	1.60	0.66
27:A:1999:C:H5''	27:A:2723:C:O2'	1.95	0.66
27:A:5:A:H2'	27:A:6:A:C8	2.31	0.66
27:A:2800:A:H3'	27:A:2801:G:H5'	1.77	0.66
27:A:1530:G:N2	27:A:1542:U:H1'	2.11	0.66
32:F:140:ILE:HG22	32:F:142:TYR:H	1.60	0.65
36:J:17:VAL:HG23	36:J:137:PRO:HB2	1.78	0.65
29:C:165:ALA:HB3	29:C:172:THR:HB	1.76	0.65
27:A:948:C:O2	27:A:984:A:O2'	2.14	0.65
27:A:503:A:H1'	27:A:506:G:OP2	1.96	0.65
27:A:2428:G:H5''	27:A:2429:G:O5'	1.96	0.65
35:I:101:SER:HB3	35:I:104:GLN:OE1	1.97	0.65
27:A:2638:G:HO2'	27:A:2639:A:H8	1.43	0.65
27:A:841:G:H2'	27:A:842:U:C6	2.31	0.65
27:A:248:G:O5'	27:A:249:C:H5'	1.96	0.65
27:A:218:A:H8	27:A:218:A:OP2	1.79	0.65
27:A:1212:G:O2'	27:A:1236:G:N2	2.29	0.65
27:A:2786:U:H2'	27:A:2787:C:H6	1.60	0.65
27:A:2788:C:H2'	27:A:2789:C:C6	2.32	0.64
27:A:5:A:H2'	27:A:6:A:H8	1.62	0.64
27:A:923:G:H2'	27:A:924:G:H8	1.63	0.64
27:A:2131:U:O5'	27:A:2133:G:H4'	1.97	0.64
27:A:51:G:H4'	27:A:52:A:H5'	1.78	0.64
36:J:117:ALA:HA	36:J:120:ARG:NH2	2.12	0.64
27:A:1930:G:O2'	27:A:1931:U:P	2.55	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:I:122:GLU:O	35:I:125:THR:HB	1.97	0.64
53:O:54:ILE:HG13	53:O:56:LYS:HB3	1.80	0.64
34:H:9:VAL:HB	34:H:13:GLY:HA3	1.78	0.64
29:C:48:ILE:HD11	29:C:51:ARG:HA	1.78	0.64
27:A:704:G:H2'	27:A:726:G:N2	2.10	0.64
27:A:859:G:O2'	27:A:860:U:P	2.56	0.64
38:L:93:ASN:O	38:L:95:LEU:N	2.30	0.63
27:A:2584:U:H3'	27:A:2585:U:H5''	1.80	0.63
40:N:73:ASN:HA	40:N:76:VAL:HG12	1.80	0.63
27:A:404:A:H1'	27:A:406:G:C4	2.33	0.63
27:A:2097:A:H2'	27:A:2098:U:O4'	1.98	0.63
27:A:454:A:H4'	27:A:455:C:OP2	1.97	0.63
44:R:82:HIS:O	44:R:82:HIS:ND1	2.31	0.63
27:A:1542:U:H2'	27:A:1543:G:O4'	1.99	0.63
27:A:2712:C:O2'	27:A:2713:U:H5'	1.99	0.63
27:A:1186:G:H2'	27:A:1187:G:O4'	1.99	0.63
27:A:370:G:O2'	27:A:424:G:OP1	2.17	0.63
27:A:1028:A:N6	27:A:1125:G:H2'	2.13	0.63
28:B:94:A:OP1	48:V:19:ARG:HD3	1.99	0.63
27:A:2537:U:H2'	27:A:2538:C:C6	2.33	0.63
27:A:120:U:H5''	27:A:122:G:OP2	1.98	0.63
27:A:1055:G:H1	27:A:1104:C:N4	1.90	0.62
28:B:118:C:H2'	28:B:119:A:C8	2.34	0.62
31:E:145:ASP:HA	31:E:166:LYS:HB3	1.81	0.62
27:A:1062:G:H22	35:I:134:SER:HB2	1.65	0.62
35:I:33:ASN:HB2	35:I:64:ARG:HH22	1.64	0.62
27:A:2394:C:H5''	38:L:63:LYS:HE3	1.81	0.62
27:A:1385:A:OP1	27:A:1385:A:H4'	1.98	0.62
27:A:2391:G:H2'	27:A:2424:C:H41	1.65	0.62
27:A:221:A:N1	27:A:265:A:O2'	2.33	0.62
46:T:58:VAL:HG22	46:T:85:VAL:HG13	1.80	0.62
27:A:1188:U:H2'	27:A:1189:A:H5'	1.82	0.62
27:A:1816:C:N4	29:C:34:GLU:OE2	2.33	0.62
27:A:878:A:H3'	27:A:879:G:H8	1.64	0.62
27:A:2867:G:O2'	27:A:2868:A:H8	1.82	0.62
27:A:839:U:H2'	27:A:840:C:C6	2.35	0.62
27:A:2346:A:H3'	27:A:2347:C:C5'	2.30	0.61
49:W:33:ILE:HD11	49:W:78:ILE:HD11	1.82	0.61
58:5:53:ARG:HB3	58:5:55:VAL:HG13	1.82	0.61
30:D:4:LEU:HD23	30:D:29:VAL:HG11	1.82	0.61
27:A:2786:U:H2'	27:A:2787:C:C6	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1026:G:H2'	27:A:1027:A:H8	1.65	0.61
27:A:1019:U:H3	27:A:1142:A:N6	1.98	0.61
27:A:242:G:O2'	27:A:243:U:P	2.59	0.61
40:N:28:LEU:HD23	40:N:48:VAL:HG21	1.82	0.61
58:5:73:LYS:HB3	58:5:117:LEU:HD11	1.81	0.61
42:P:59:THR:HG22	42:P:72:VAL:HG12	1.82	0.61
27:A:704:G:H1'	27:A:727:A:H61	1.64	0.61
39:M:21:ALA:HB1	39:M:100:LYS:HD3	1.83	0.61
27:A:2267:A:H5''	27:A:2268:A:H5'	1.83	0.61
27:A:2517:C:O3'	27:A:2518:A:H3'	2.00	0.61
27:A:1019:U:H2'	27:A:1020:A:H8	1.66	0.61
27:A:2655:G:O2'	27:A:2656:U:P	2.59	0.61
48:V:76:ASP:HB3	48:V:90:ASP:HB2	1.83	0.60
27:A:1081:U:H4'	35:I:123:ALA:HB1	1.81	0.60
51:Y:24:GLU:O	51:Y:28:LEU:HB2	2.01	0.60
27:A:1490:A:H62	29:C:73:ILE:HG23	1.67	0.60
30:D:54:ALA:HA	30:D:76:GLY:HA2	1.83	0.60
27:A:1086:A:N3	27:A:1086:A:H2'	2.17	0.60
45:S:59:GLU:HA	45:S:64:ALA:HA	1.83	0.60
27:A:242:G:HO2'	27:A:243:U:P	2.24	0.60
48:V:4:ILE:HD13	48:V:47:VAL:HG22	1.84	0.60
27:A:2104:C:H2'	27:A:2105:U:C6	2.36	0.60
27:A:828:U:O4	27:A:858:G:N2	40.59	0.60
27:A:144:A:H4'	46:T:2:ILE:HD11	1.83	0.60
57:4:36:ARG:HG2	57:4:37:GLN:H	1.66	0.60
59:6:62:LYS:C	59:6:65:ASN:HD21	2.04	0.60
27:A:2271:G:H5'	49:W:16:ARG:HD3	1.84	0.59
27:A:2427:C:H5'	27:A:2429:G:H5'	1.84	0.59
27:A:100:U:H4'	27:A:101:A:O4'	2.01	0.59
27:A:2074:U:H2'	27:A:2075:U:C6	2.36	0.59
27:A:476:G:N1	27:A:479:A:OP2	2.36	0.59
27:A:546:U:H2'	27:A:547:A:H4'	1.84	0.59
27:A:2557:G:H2'	27:A:2558:C:C6	2.38	0.59
27:A:2238:G:N3	27:A:2238:G:H2'	2.17	0.59
27:A:2115:G:H4'	27:A:2166:U:O2	2.03	0.59
27:A:434:U:O2'	27:A:436:C:N4	2.36	0.59
27:A:437:U:H2'	27:A:438:G:H8	1.67	0.59
27:A:1779:U:H5	27:A:1784:A:N7	2.01	0.59
37:K:109:SER:O	37:K:111:LYS:N	2.35	0.59
27:A:633:A:H2'	27:A:634:C:H5'	1.85	0.59
27:A:2267:A:H5''	27:A:2268:A:C5'	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:639:U:H2'	27:A:640:C:C6	2.38	0.59
35:I:102:ARG:HA	35:I:129:GLU:OE2	2.03	0.59
27:A:271:G:H4'	27:A:272:A:OP1	2.03	0.59
27:A:1386:C:H2'	27:A:1387:A:C8	2.38	0.59
30:D:121:THR:HG21	30:D:143:PRO:HB3	1.85	0.58
27:A:283:G:H1	27:A:357:C:H42	1.51	0.58
38:L:78:ARG:HB2	38:L:81:ASP:OD1	2.03	0.58
29:C:203:VAL:O	29:C:205:GLY:N	2.36	0.58
27:A:372:G:O2'	27:A:373:U:P	2.60	0.58
40:N:58:ASP:OD1	40:N:63:ARG:NH2	2.33	0.58
27:A:847:U:O2	27:A:934:U:H1'	2.03	0.58
46:T:13:ALA:HB3	46:T:33:LYS:HD3	1.85	0.58
27:A:302:C:H2'	27:A:303:G:H8	1.69	0.58
27:A:770:G:H5''	55:2:10:LEU:HD23	1.86	0.58
29:C:244:VAL:HG12	29:C:250:GLN:HA	1.86	0.58
31:E:88:ARG:O	31:E:90:GLN:N	2.37	0.58
27:A:2233:U:H2'	27:A:2234:G:C8	2.38	0.58
27:A:2427:C:H5''	27:A:2428:G:OP1	2.03	0.58
27:A:302:C:H2'	27:A:303:G:C8	2.39	0.58
40:N:69:ARG:O	40:N:71:ARG:N	2.28	0.58
27:A:2326:C:O2'	27:A:2327:A:OP1	2.20	0.58
27:A:84:A:H4'	27:A:85:G:O5'	2.03	0.58
27:A:265:A:H4'	27:A:266:G:OP1	2.03	0.58
27:A:2305:U:H5''	32:F:130:GLY:HA3	1.85	0.58
27:A:1956:U:H2'	27:A:1957:C:H5'	1.86	0.58
27:A:2776:A:H4'	27:A:2777:G:O5'	2.04	0.58
31:E:117:ARG:HH12	38:L:2:ARG:HG2	1.68	0.57
27:A:2591:C:H2'	27:A:2592:G:C8	2.39	0.57
27:A:479:A:H4'	27:A:480:A:OP1	2.03	0.57
27:A:686:U:O2'	55:2:5:PHE:HA	2.05	0.57
31:E:88:ARG:HD3	31:E:89:PRO:HD2	1.86	0.57
45:S:3:THR:HG21	45:S:58:ALA:HB2	1.87	0.57
40:N:45:ARG:HG2	40:N:95:THR:HG21	1.86	0.57
27:A:1055:G:O2'	27:A:1084:A:N6	2.36	0.57
50:X:17:ARG:NE	50:X:23:ALA:HB2	2.11	0.57
32:F:141:ASP:HB2	32:F:144:LYS:HD3	1.85	0.57
37:K:121:GLU:HG2	37:K:122:VAL:HG23	1.86	0.57
38:L:132:ARG:HG3	38:L:142:ILE:HD12	1.86	0.57
27:A:466:A:OP1	55:2:34:ARG:NH1	2.37	0.57
27:A:2391:G:H2'	27:A:2424:C:N4	2.20	0.57
42:P:29:VAL:HG22	42:P:80:VAL:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:172:A:H2'	27:A:173:A:C8	2.40	0.57
27:A:2339:C:H2'	27:A:2340:A:C8	2.39	0.57
27:A:495:G:H1'	45:S:57:ASN:OD1	2.04	0.57
31:E:148:ILE:O	31:E:169:VAL:HA	2.04	0.57
27:A:2554:U:H2'	27:A:2555:U:C6	2.39	0.57
27:A:2285:C:OP2	54:1:5:ARG:NH1	2.37	0.57
56:3:30:HIS:ND1	56:3:31:ILE:HG13	2.18	0.57
27:A:1614:A:N1	45:S:93:ALA:HB2	2.20	0.57
31:E:3:LEU:HD13	31:E:120:VAL:HG21	1.85	0.57
27:A:2867:G:O2'	27:A:2868:A:C8	2.57	0.57
27:A:281:C:N3	27:A:359:G:N2	2.53	0.57
27:A:2328:A:H2'	27:A:2329:U:C6	2.39	0.57
55:2:24:THR:HG23	55:2:27:GLY:H	1.70	0.57
58:5:56:ARG:HD3	58:5:81:LEU:HD21	1.87	0.57
27:A:1019:U:H2'	27:A:1020:A:C8	2.40	0.57
27:A:859:G:O2'	27:A:860:U:OP2	2.23	0.57
42:P:31:VAL:HG13	42:P:38:ARG:HB3	1.86	0.57
55:2:12:ARG:NE	55:2:44:VAL:HG21	2.19	0.57
43:Q:70:GLN:C	43:Q:71:ASN:HD22	2.08	0.57
27:A:861:A:H2'	27:A:862:G:O4'	2.05	0.57
37:K:40:LYS:NZ	37:K:89:ASN:OD1	2.38	0.56
35:I:135:MET:HB2	35:I:137:LEU:HG	1.85	0.56
33:G:41:GLU:HA	33:G:54:ARG:HH21	1.69	0.56
58:5:34:THR:O	58:5:37:LYS:HB3	2.05	0.56
58:5:27:VAL:HG13	58:5:83:ALA:HB3	1.87	0.56
27:A:394:C:H2'	27:A:395:U:O4'	2.05	0.56
48:V:42:LEU:HD13	48:V:47:VAL:HG21	1.86	0.56
51:Y:2:LYS:HB3	51:Y:52:ARG:HD3	1.87	0.56
35:I:74:PRO:HG2	35:I:77:VAL:HG22	1.87	0.56
36:J:102:GLU:HG3	36:J:119:PHE:HZ	1.69	0.56
32:F:116:LEU:HB2	32:F:175:PRO:HB2	1.87	0.56
27:A:2518:A:N3	27:A:2518:A:H2'	2.20	0.56
27:A:289:G:H2'	27:A:290:U:O4'	2.04	0.56
27:A:704:G:C2'	27:A:726:G:H22	2.14	0.56
27:A:630:G:N2	27:A:633:A:OP2	2.34	0.56
27:A:1869:G:H1'	27:A:1872:A:N6	2.20	0.56
27:A:1111:A:O2'	27:A:1112:G:OP1	2.22	0.56
27:A:505:A:HO2'	27:A:509:C:HO2'	1.53	0.56
38:L:14:LYS:O	38:L:16:GLY:N	2.39	0.56
27:A:2283:C:OP2	27:A:2390:U:H5	1.89	0.56
27:A:1283:G:H1'	27:A:1329:U:O2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:N:34:ILE:HG13	40:N:113:ILE:HG23	1.88	0.56
27:A:2644:G:H2'	27:A:2645:G:H5'	1.86	0.56
40:N:44:LEU:HD23	40:N:113:ILE:HD13	1.87	0.56
27:A:1315:C:H2'	27:A:1316:U:H6	1.71	0.56
27:A:2297:A:N1	27:A:2321:U:H5	2.03	0.56
27:A:1199:U:H1'	43:Q:3:VAL:HG22	1.88	0.56
36:J:36:LEU:O	36:J:51:GLY:HA3	2.05	0.56
27:A:290:U:H2'	27:A:291:G:C8	2.41	0.56
27:A:162:U:O2'	27:A:163:C:H5'	2.06	0.56
27:A:204:A:H4'	27:A:205:G:OP1	2.06	0.56
58:5:37:LYS:HG3	58:5:41:LEU:HD12	1.88	0.56
27:A:1422:G:H5'	37:K:48:PRO:HG3	99.24	0.56
29:C:154:ALA:HB2	29:C:161:VAL:HG23	1.88	0.56
45:S:56:ALA:HA	45:S:59:GLU:HG2	1.87	0.56
28:B:118:C:H2'	28:B:119:A:H8	1.70	0.55
27:A:2341:G:H2'	27:A:2342:C:O4'	2.07	0.55
27:A:1858:A:N6	27:A:1884:G:O2'	2.38	0.55
37:K:21:CYS:HA	37:K:41:ILE:HG22	1.87	0.55
27:A:1251:C:OP2	43:Q:5:ARG:HD2	2.06	0.55
27:A:2648:G:H2'	27:A:2649:C:O4'	2.06	0.55
57:4:37:GLN:HG3	57:4:38:GLY:H	1.71	0.55
27:A:1040:A:H2	27:A:1115:G:H22	1.54	0.55
27:A:468:G:H2'	27:A:469:G:H5'	1.88	0.55
27:A:1222:U:H2'	27:A:1223:G:C8	2.40	0.55
27:A:301:G:H4'	27:A:302:C:OP1	2.04	0.55
58:5:29:ASP:HB2	58:5:56:ARG:HH12	1.71	0.55
27:A:368:A:H2'	27:A:369:U:O4'	2.06	0.55
39:M:11:LYS:HD2	39:M:86:LYS:HG2	1.88	0.55
27:A:1689:A:H2'	27:A:1690:A:C8	2.41	0.55
27:A:1847:G:H21	27:A:1848:A:H62	1.54	0.55
27:A:493:G:H2'	27:A:494:G:O4'	2.07	0.55
27:A:1179:G:C4	27:A:1180:U:H1'	2.42	0.55
27:A:851:C:H2'	27:A:852:U:C6	2.42	0.55
27:A:2469:A:N6	27:A:2481:G:O2'	2.40	0.55
27:A:1396:U:H5''	27:A:1397:U:OP2	2.06	0.55
27:A:107:G:H2'	27:A:108:G:C8	2.41	0.55
27:A:1857:G:H2'	27:A:1884:G:N2	2.21	0.55
29:C:162:GLN:OE1	29:C:174:ARG:NH2	2.40	0.55
27:A:2345:G:H4'	27:A:2346:A:C5'	2.36	0.55
27:A:28:A:O2'	27:A:296:U:OP1	49.76	0.55
27:A:1434:A:H2'	27:A:1435:G:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1434:A:H2'	27:A:1435:G:H8	1.71	0.54
27:A:712:G:H2'	27:A:713:G:H5'	1.88	0.54
34:H:84:ALA:HA	34:H:91:PHE:H	1.73	0.54
27:A:1330:C:O2'	27:A:1331:G:H5'	2.07	0.54
27:A:2198:A:HO2'	27:A:2199:A:H8	1.56	0.54
27:A:542:C:H3'	27:A:543:G:H5''	1.89	0.54
35:I:33:ASN:HB2	35:I:64:ARG:HH12	1.72	0.54
32:F:39:VAL:HG12	32:F:85:GLY:HA2	1.89	0.54
27:A:1297:C:O2'	27:A:1302:A:N1	2.36	0.54
27:A:1930:G:O2'	27:A:1931:U:OP2	2.26	0.54
27:A:1028:A:H61	27:A:1125:G:H2'	1.71	0.54
27:A:2725:A:O2'	27:A:2726:A:O5'	2.16	0.54
27:A:956:G:HO2'	27:A:959:A:H62	1.54	0.54
47:U:14:THR:OG1	47:U:68:ASN:ND2	2.38	0.54
27:A:947:A:O2'	27:A:984:A:H2	1.91	0.54
27:A:841:G:H2'	27:A:842:U:H6	1.71	0.54
27:A:373:U:O2'	27:A:423:A:H1'	2.07	0.54
27:A:1405:U:H2'	27:A:1406:U:C6	2.42	0.54
27:A:969:G:H2'	27:A:970:U:C6	2.41	0.54
27:A:1548:A:H2'	27:A:1549:A:C8	2.42	0.54
27:A:277:G:H1'	27:A:361:G:H1	1.71	0.54
27:A:1794:A:H2'	27:A:1795:C:C6	2.42	0.54
59:6:56:ARG:O	59:6:59:ARG:HB3	2.08	0.54
30:D:49:GLN:HA	30:D:80:TRP:O	2.07	0.54
27:A:1565:C:O2'	27:A:1566:A:H2'	2.07	0.54
27:A:265:A:H1'	27:A:266:G:O4'	2.08	0.54
58:5:114:GLU:HA	58:5:123:ILE:HB	1.90	0.54
58:5:88:HIS:HB2	58:5:89:PRO:HD3	1.89	0.54
27:A:2576:G:H8	27:A:2581:G:O6	1.90	0.54
27:A:747:5MC:CM5	27:A:2612:C:H4'	2.38	0.54
27:A:1021:A:N3	27:A:1022:G:H5''	2.22	0.54
27:A:1565:C:O2'	27:A:1566:A:C8	2.60	0.54
58:5:37:LYS:O	58:5:41:LEU:HB2	2.08	0.54
30:D:1:MET:HG2	30:D:205:PRO:HG2	1.88	0.54
39:M:74:THR:HA	39:M:89:VAL:HA	1.89	0.54
27:A:743:A:OP1	30:D:135:GLY:HA2	2.08	0.53
27:A:468:G:N7	55:2:39:ARG:NH2	2.56	0.53
38:L:122:VAL:HB	38:L:142:ILE:HG23	1.89	0.53
35:I:11:GLN:NE2	35:I:54:ILE:O	2.41	0.53
27:A:1410:G:H2'	27:A:1411:U:C6	2.43	0.53
27:A:2832:U:H1'	27:A:2834:G:C4	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2852:G:H2'	27:A:2853:C:O4'	2.08	0.53
30:D:114:LYS:HE3	30:D:196:ALA:HB2	1.90	0.53
27:A:468:G:C2'	27:A:469:G:H5'	2.39	0.53
27:A:1177:G:H2'	27:A:1178:C:O4'	2.09	0.53
27:A:2884:U:H3	53:0:39:ARG:CZ	2.22	0.53
41:O:49:VAL:HG21	41:O:82:ALA:HA	1.91	0.53
58:5:57:ASN:HB2	58:5:62:ARG:HD2	1.91	0.53
39:M:28:PHE:HB2	39:M:104:GLU:OE1	2.08	0.53
51:Y:23:ARG:O	51:Y:25:GLN:N	2.41	0.53
27:A:760:G:H2'	27:A:761:A:O4'	2.09	0.53
27:A:1266:G:O2'	27:A:2012:G:N1	2.38	0.53
27:A:2746:U:H1'	33:G:138:GLN:HE22	1.72	0.53
27:A:2678:C:H2'	27:A:2679:A:O4'	2.09	0.53
41:O:51:ALA:HB3	41:O:78:VAL:HG22	1.91	0.53
58:5:57:ASN:HD22	58:5:63:ALA:HB2	1.74	0.53
27:A:1332:G:N3	27:A:1332:G:H5''	2.24	0.53
39:M:34:LYS:HE3	39:M:131:VAL:HG11	1.91	0.53
27:A:2114:A:N6	27:A:2117:A:H62	2.05	0.53
27:A:1203:U:H1'	38:L:4:ASN:HB3	1.90	0.53
27:A:2126:A:N1	27:A:2163:A:H1'	2.24	0.53
27:A:784:G:O2'	27:A:785:G:H5''	2.09	0.53
27:A:1475:G:O2'	27:A:1476:U:OP2	2.27	0.53
27:A:358:U:H2'	27:A:359:G:C8	2.88	0.53
27:A:2756:U:H5''	57:4:19:ARG:HA	1.90	0.53
27:A:2879:A:H8	27:A:2881:U:O4	1.92	0.53
27:A:2346:A:H3'	27:A:2347:C:H5'	1.91	0.52
27:A:390:U:H4'	27:A:391:A:O5'	2.08	0.52
27:A:844:A:H61	27:A:934:U:H3	1.56	0.52
27:A:2258:C:O2'	27:A:2426:A:H4'	2.09	0.52
45:S:14:ALA:O	45:S:18:ARG:HB2	2.08	0.52
27:A:2497:A:N3	27:A:2498:OMC:N4	2.55	0.52
27:A:321:U:H5''	31:E:131:THR:HG23	1.91	0.52
41:O:69:ASP:N	41:O:69:ASP:OD1	2.42	0.52
37:K:33:ALA:HB1	37:K:37:ASP:HB2	1.90	0.52
27:A:910:A:H2'	27:A:911:A:C8	2.44	0.52
28:B:41:G:H2'	28:B:41:G:N3	2.24	0.52
31:E:143:LEU:HB3	31:E:146:VAL:HG11	1.91	0.52
27:A:2514:U:H2'	27:A:2515:C:C6	2.45	0.52
27:A:715:A:H2'	27:A:716:A:C8	3.34	0.52
27:A:884:U:H2'	27:A:885:C:O4'	2.09	0.52
27:A:32:C:N4	27:A:446:G:O2'	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:P:48:ALA:HB3	42:P:59:THR:OG1	2.09	0.52
27:A:677:A:O2'	27:A:2071:A:H5'	2.10	0.52
32:F:110:ILE:O	32:F:113:PHE:HB2	2.10	0.52
30:D:49:GLN:NE2	30:D:67:HIS:NE2	2.52	0.52
48:V:30:ILE:HD11	48:V:63:ILE:HD12	1.92	0.52
27:A:1701:A:C2'	27:A:1702:G:H5'	2.40	0.52
32:F:134:GLN:H	32:F:134:GLN:CD	2.12	0.52
48:V:76:ASP:OD1	48:V:77:VAL:N	2.41	0.52
31:E:148:ILE:HB	31:E:169:VAL:HG22	1.92	0.52
27:A:1962:5MC:O2'	27:A:1964:G:OP2	2.28	0.52
27:A:1796:U:H2'	27:A:1797:G:C8	2.44	0.52
31:E:97:ASN:HB2	31:E:100:MET:HG3	1.92	0.52
49:W:33:ILE:HG22	49:W:34:VAL:HG23	1.92	0.52
27:A:2788:C:O2'	27:A:2809:A:N3	2.43	0.52
27:A:2809:A:H2'	27:A:2810:A:C8	2.45	0.52
27:A:1112:G:H2'	27:A:1113:U:C6	2.45	0.52
32:F:126:ASN:OD1	32:F:156:THR:HG23	2.10	0.52
27:A:1682:G:C4	27:A:1757:A:H1'	2.45	0.52
27:A:2296:U:H4'	27:A:2297:A:OP1	2.08	0.52
53:O:54:ILE:HG23	53:O:56:LYS:H	1.74	0.52
39:M:41:LEU:HD22	39:M:124:LEU:HD22	1.92	0.52
46:T:70:HIS:O	46:T:72:GLN:N	2.43	0.52
28:B:104:A:H2'	28:B:105:G:O4'	2.09	0.52
27:A:2406:A:H5'	27:A:2407:A:OP1	2.10	0.52
27:A:1088:A:H61	35:I:134:SER:HB3	1.75	0.52
27:A:542:C:C3'	27:A:543:G:H5''	2.40	0.52
41:O:89:ASP:HA	41:O:116:GLN:O	2.10	0.52
27:A:259:G:O2'	27:A:260:G:H5'	2.10	0.52
55:2:34:ARG:HH21	55:2:39:ARG:HD3	1.74	0.51
41:O:53:THR:HG23	41:O:74:VAL:HG21	1.92	0.51
27:A:2230:G:H5''	50:X:29:LEU:HD12	1.92	0.51
27:A:722:A:H2'	27:A:723:C:O4'	2.10	0.51
49:W:74:LYS:HD2	49:W:74:LYS:H	1.75	0.51
27:A:1645:G:H5''	27:A:1646:C:H5'	1.91	0.51
28:B:28:C:H2'	28:B:29:A:C8	2.45	0.51
27:A:192:C:OP1	66:A:3306:HOH:O	2.19	0.51
27:A:2808:G:HO2'	27:A:2809:A:H8	1.56	0.51
27:A:2591:C:H2'	27:A:2592:G:H8	1.75	0.51
45:S:4:ILE:HD12	45:S:6:LYS:HE3	1.92	0.51
27:A:1239:G:H2'	27:A:1240:U:O4'	2.10	0.51
27:A:405:U:H3'	27:A:406:G:H5'	2.96	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:6:58:ASP:O	59:6:62:LYS:HG3	2.11	0.51
27:A:413:C:H2'	27:A:414:C:C6	2.44	0.51
27:A:1509:A:H2'	27:A:1510:G:C8	2.45	0.51
27:A:2262:U:O2'	27:A:2263:C:H5'	2.10	0.51
36:J:36:LEU:HD22	36:J:121:LYS:HB2	1.92	0.51
35:I:25:PRO:O	35:I:29:GLN:HB2	2.11	0.51
31:E:31:VAL:HG21	31:E:104:ALA:HB2	1.91	0.51
27:A:2625:G:H2'	27:A:2626:C:O4'	2.10	0.51
27:A:642:U:H2'	27:A:644:A:OP2	2.10	0.51
32:F:141:ASP:O	32:F:143:ASP:N	2.44	0.51
27:A:2405:G:HO2'	27:A:2406:A:P	2.33	0.51
34:H:70:GLU:HB2	34:H:134:VAL:HG21	1.91	0.51
31:E:170:ARG:NH2	31:E:176:ASP:OD1	2.44	0.51
27:A:2303:G:H2'	27:A:2304:G:O4'	2.10	0.51
58:5:48:ALA:HB3	58:5:51:TYR:HE2	1.75	0.51
58:5:48:ALA:HB3	58:5:51:TYR:CE2	2.45	0.51
27:A:948:C:H2'	27:A:949:G:C8	2.46	0.51
39:M:102:LEU:HD11	39:M:126:ILE:HD11	1.91	0.51
32:F:39:VAL:O	32:F:41:GLU:HG2	2.11	0.51
30:D:133:THR:HG23	30:D:134:HIS:N	2.26	0.51
27:A:774:G:N2	27:A:787:C:O2'	2.41	0.51
27:A:28:A:H2'	27:A:29:U:O4'	2.63	0.51
43:Q:25:GLY:O	43:Q:29:ARG:NH1	2.44	0.51
57:4:27:CYS:SG	57:4:30:GLU:N	2.79	0.51
57:4:11:CYS:HB3	57:4:33:HIS:CE1	2.46	0.51
27:A:2101:A:H2'	27:A:2102:G:H8	1.76	0.51
27:A:833:A:H2'	27:A:834:G:C8	2.44	0.51
27:A:2298:A:H2'	27:A:2299:U:O4'	2.11	0.51
27:A:519:U:H5''	45:S:25:ARG:HH21	1.74	0.51
36:J:63:ALA:HA	36:J:69:ARG:HH22	1.75	0.51
31:E:76:PRO:HA	31:E:82:GLY:HA3	1.93	0.51
27:A:1210:G:O6	27:A:1237:A:H2'	2.11	0.51
27:A:2649:C:H2'	27:A:2650:U:C6	2.46	0.51
27:A:1815:A:H4'	27:A:1816:C:OP1	2.11	0.51
37:K:43:ILE:HD12	37:K:56:ASP:HB2	1.93	0.51
34:H:33:GLN:HB2	34:H:35:LYS:HG2	1.93	0.51
52:Z:40:THR:HG22	52:Z:43:ILE:HG12	1.92	0.51
27:A:479:A:O2'	27:A:481:G:H5''	2.11	0.50
47:U:36:GLU:HA	47:U:61:GLU:HG2	1.94	0.50
42:P:74:GLN:HB2	42:P:77:SER:HB2	1.93	0.50
33:G:23:ILE:HD11	33:G:42:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:792:A:H1'	27:A:794:A:N7	14.55	0.50
31:E:41:GLN:OE1	31:E:43:THR:OG1	2.29	0.50
30:D:55:LYS:HE2	30:D:77:ARG:HA	1.92	0.50
27:A:1243:C:H1'	38:L:4:ASN:O	2.11	0.50
46:T:22:THR:HA	46:T:25:GLU:HG2	1.94	0.50
40:N:56:LYS:NZ	40:N:87:PHE:O	2.44	0.50
27:A:123:G:O2'	27:A:124:G:H5'	2.11	0.50
27:A:2758:A:H2	33:G:34:ARG:HH21	1.59	0.50
27:A:175:G:H2'	27:A:176:A:O4'	2.11	0.50
27:A:2515:C:H2'	27:A:2516:A:C8	2.46	0.50
27:A:716:A:H2'	27:A:717:C:O4'	2.11	0.50
38:L:110:VAL:HG11	38:L:135:ILE:HD11	1.93	0.50
27:A:1877:A:H2'	27:A:1878:G:O4'	2.12	0.50
27:A:196:A:H5''	38:L:47:ARG:HH22	1.76	0.50
27:A:2572:A:H2'	30:D:149:ASN:HD22	1.76	0.50
37:K:92:GLU:O	37:K:93:GLN:O	2.29	0.50
27:A:1130:U:O2'	27:A:1131:G:OP1	2.26	0.50
27:A:2759:G:N2	33:G:138:GLN:NE2	2.59	0.50
27:A:2327:A:H2'	27:A:2328:A:C8	2.46	0.50
27:A:1689:A:H2'	27:A:1690:A:H8	1.76	0.50
27:A:969:G:H2'	27:A:970:U:H6	1.76	0.50
27:A:1266:G:O2'	27:A:1267:U:OP2	2.30	0.50
37:K:24:VAL:HG13	37:K:33:ALA:HB2	1.93	0.50
27:A:2845:U:H5''	42:P:51:ASN:O	2.11	0.50
27:A:2224:G:H4'	27:A:2226:C:C2	2.46	0.50
59:6:44:PHE:HD1	59:6:45:THR:HG23	1.76	0.50
27:A:948:C:H2'	27:A:949:G:H8	1.76	0.50
27:A:1019:U:O2'	27:A:1020:A:H5'	2.11	0.50
49:W:61:GLY:HA3	49:W:79:GLU:O	2.11	0.50
27:A:301:G:OP2	47:U:81:ARG:NH1	2.41	0.50
27:A:395:U:H2'	27:A:396:G:C8	2.47	0.50
27:A:1005:C:O2'	36:J:30:THR:HG21	2.11	0.50
27:A:2134:A:N6	27:A:2156:G:H2'	2.27	0.50
28:B:111:U:O2'	28:B:112:G:H5'	2.12	0.50
27:A:1142:A:H4'	27:A:1143:A:OP1	2.10	0.50
33:G:153:PRO:HA	33:G:159:LYS:O	2.12	0.50
27:A:589:U:H2'	27:A:590:A:C8	2.46	0.50
27:A:549:G:HO2'	27:A:550:C:P	2.35	0.50
27:A:1106:G:H3'	27:A:1107:G:H8	1.76	0.50
32:F:3:LEU:HD11	32:F:100:GLU:HB2	1.93	0.49
37:K:102:PRO:HB3	37:K:121:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:39:G:H1'	31:E:43:THR:HG21	1.93	0.49
27:A:2529:G:OP2	27:A:2530:A:H5''	2.12	0.49
44:R:61:ALA:HB2	44:R:98:ILE:HD13	1.94	0.49
27:A:1111:A:HO2'	27:A:1112:G:P	2.35	0.49
45:S:52:GLU:HA	45:S:55:ILE:HD12	1.95	0.49
27:A:2101:A:H2'	27:A:2102:G:C8	2.47	0.49
27:A:2020:A:H5'	53:0:8:THR:HG22	1.94	0.49
27:A:580:U:H2'	27:A:581:C:C6	2.47	0.49
28:B:79:G:H2'	28:B:80:U:O4'	2.13	0.49
27:A:52:A:H8	27:A:52:A:OP2	1.94	0.49
27:A:1201:U:H2'	27:A:1202:G:H8	1.77	0.49
33:G:94:ARG:HD2	33:G:127:GLN:HB3	1.94	0.49
58:5:5:LEU:O	58:5:9:GLN:HB2	2.13	0.49
27:A:1047:G:HO2'	27:A:1048:A:H8	1.54	0.49
27:A:549:G:O2'	27:A:550:C:OP1	2.26	0.49
53:0:24:VAL:HG22	53:0:26:SER:H	1.77	0.49
32:F:133:GLU:HB3	32:F:135:ILE:HG13	1.94	0.49
27:A:670:A:OP2	27:A:670:A:H8	1.95	0.49
27:A:2159:G:H2'	27:A:2160:C:O4'	2.13	0.49
27:A:2725:A:O2'	27:A:2726:A:C8	2.66	0.49
27:A:721:A:H2'	27:A:722:A:C8	2.47	0.49
28:B:1:U:H2'	28:B:2:G:C8	2.47	0.49
27:A:2861:U:H2'	27:A:2862:G:H8	1.77	0.49
27:A:1378:A:O2'	27:A:1380:G:OP2	2.31	0.49
27:A:2291:U:H2'	27:A:2292:U:H6	1.77	0.49
32:F:102:LEU:HD12	32:F:106:ALA:HB3	1.95	0.49
27:A:2529:G:H4'	33:G:174:LYS:HE3	1.94	0.49
27:A:873:C:H2'	27:A:874:G:H8	1.77	0.49
38:L:33:ARG:HD3	38:L:40:SER:HA	1.95	0.49
27:A:473:G:O2'	27:A:474:G:H5'	2.12	0.49
27:A:636:G:N7	38:L:109:LYS:HD3	2.28	0.49
28:B:13:G:C8	28:B:70:C:H4'	2.48	0.49
27:A:1900:A:H1'	27:A:1970:A:H2'	1.95	0.49
32:F:134:GLN:HE22	32:F:149:ARG:N	2.11	0.49
27:A:974:G:H2'	27:A:974:G:N3	2.28	0.49
34:H:47:PHE:HA	34:H:51:ARG:HB2	1.95	0.49
27:A:962:G:H21	27:A:2250:G:H1	1.59	0.49
27:A:1329:U:O5'	27:A:1330:C:H5	1.95	0.49
27:A:356:G:H2'	27:A:357:C:C6	2.48	0.49
27:A:213:A:H2'	27:A:214:G:C8	2.48	0.49
27:A:441:U:H2'	27:A:442:G:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:495:G:H5''	45:S:4:ILE:HG13	1.95	0.48
27:A:687:C:H1'	55:2:4:THR:HG22	1.95	0.48
27:A:2120:G:H2'	27:A:2121:G:C8	2.48	0.48
27:A:2698:U:H2'	27:A:2699:C:C6	2.48	0.48
50:X:39:VAL:HG12	50:X:42:GLU:H	1.78	0.48
32:F:67:THR:O	32:F:83:PRO:HA	2.12	0.48
27:A:1139:G:O2'	27:A:1140:C:H5'	2.13	0.48
27:A:270:A:N1	27:A:369:U:O2'	2.40	0.48
27:A:1266:G:N2	27:A:1269:A:OP2	13.16	0.48
34:H:113:SER:O	34:H:116:ARG:NH1	2.39	0.48
28:B:90:C:H2'	28:B:91:C:O4'	2.13	0.48
27:A:2205:A:H2'	27:A:2206:C:C6	2.48	0.48
27:A:322:A:OP2	31:E:163:ASN:HB2	2.13	0.48
27:A:1586:A:C2	27:A:1587:G:H1'	2.48	0.48
33:G:102:ILE:O	33:G:113:ASP:HA	2.12	0.48
27:A:2808:G:O2'	27:A:2809:A:H8	1.97	0.48
28:B:106:G:H2'	28:B:107:G:O4'	2.13	0.48
27:A:2516:A:O2'	27:A:2517:C:H5'	2.12	0.48
27:A:367:G:N2	27:A:368:A:H1'	2.28	0.48
27:A:1881:C:H2'	27:A:1882:U:O4'	2.13	0.48
38:L:128:THR:OG1	38:L:129:LYS:N	2.44	0.48
27:A:2808:G:H2'	27:A:2890:G:O6	2.14	0.48
27:A:562:U:H2'	27:A:572:A:O4'	2.13	0.48
27:A:635:C:O2'	27:A:639:U:H5''	2.13	0.48
27:A:543:G:O6	27:A:550:C:N3	2.46	0.48
27:A:454:A:H3'	27:A:455:C:C6	2.48	0.48
27:A:2103:C:H2'	27:A:2104:C:C6	2.48	0.48
48:V:80:HIS:CG	48:V:81:PRO:HD2	2.48	0.48
27:A:1900:A:O4'	27:A:1970:A:H5''	2.12	0.48
27:A:2065:C:H1'	27:A:2449:H2U:HN3	1.79	0.48
36:J:15:TRP:HB3	36:J:137:PRO:HB3	1.95	0.48
27:A:437:U:H2'	27:A:438:G:C8	2.48	0.48
27:A:2526:G:H2'	27:A:2527:C:C6	2.49	0.48
29:C:7:PRO:HB3	29:C:13:ARG:HB2	1.95	0.48
52:Z:3:THR:HB	52:Z:36:GLU:HG2	1.94	0.48
27:A:2405:G:O2'	27:A:2406:A:OP2	2.32	0.48
33:G:136:ASP:OD2	33:G:139:VAL:HG23	2.14	0.48
39:M:42:THR:HG22	39:M:93:VAL:HG12	1.96	0.48
27:A:420:C:H2'	27:A:421:C:O4'	2.13	0.48
45:S:28:LYS:HE3	45:S:70:LYS:NZ	2.28	0.48
35:I:38:CYS:SG	35:I:39:LYS:N	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2172:U:OP2	27:A:2173:A:H5'	2.14	0.48
27:A:1715:G:HO2'	27:A:1716:U:H6	1.57	0.48
27:A:1182:G:H2'	27:A:1183:U:O4'	2.12	0.48
27:A:127:A:H5''	27:A:128:C:C6	2.48	0.48
27:A:692:C:H5''	29:C:38:LYS:HB3	1.96	0.48
32:F:89:THR:HG21	32:F:91:ARG:HH11	1.79	0.48
27:A:1320:C:O2'	27:A:1321:A:H5''	2.14	0.48
29:C:15:VAL:HG22	29:C:205:GLY:HA3	1.96	0.48
59:6:28:VAL:HG11	59:6:32:LEU:HD13	1.95	0.48
27:A:1558:C:H4'	27:A:1559:U:O5'	2.13	0.48
27:A:1019:U:H3	27:A:1142:A:H62	1.62	0.48
30:D:179:ARG:HB3	30:D:188:LEU:HD12	1.95	0.48
27:A:2443:C:OP1	31:E:63:LYS:HD3	2.14	0.48
27:A:2071:A:H2'	27:A:2072:C:C6	2.49	0.48
27:A:2720:U:H5''	42:P:52:ARG:NH2	2.28	0.48
44:R:77:PHE:HD1	44:R:84:ARG:HB3	1.79	0.48
38:L:118:THR:O	38:L:120:VAL:N	2.44	0.47
27:A:831:G:H5''	38:L:37:GLY:HA2	1.95	0.47
27:A:322:A:H5'	27:A:340:A:H1'	1.97	0.47
27:A:1046:A:O2'	58:5:61:ARG:O	2.23	0.47
27:A:2655:G:O2'	27:A:2656:U:OP2	2.31	0.47
27:A:2305:U:C2	32:F:150:GLY:O	2.67	0.47
27:A:172:A:H2'	27:A:173:A:H8	1.78	0.47
58:5:41:LEU:O	58:5:44:ALA:HB3	2.15	0.47
27:A:2405:G:H1'	27:A:2412:A:N6	2.29	0.47
27:A:39:G:H2'	27:A:40:U:C6	2.49	0.47
27:A:1183:U:H2'	27:A:1184:U:C6	2.49	0.47
27:A:2051:A:OP2	27:A:2051:A:H8	1.97	0.47
31:E:52:VAL:O	31:E:74:LYS:HE3	2.14	0.47
27:A:1590:A:H2'	27:A:1591:A:H8	1.79	0.47
32:F:73:VAL:HG22	32:F:78:ILE:HG12	1.95	0.47
27:A:528:A:C2	27:A:2042:A:H2'	2.48	0.47
32:F:165:GLY:O	32:F:168:LEU:HB3	2.14	0.47
27:A:934:U:H2'	27:A:935:C:C6	2.49	0.47
51:Y:44:LYS:HA	51:Y:47:ARG:HH22	1.79	0.47
27:A:1160:G:N7	27:A:1182:G:N2	20.72	0.47
38:L:24:GLY:C	38:L:26:GLY:H	2.17	0.47
27:A:1177:G:H2'	27:A:1178:C:C4'	2.45	0.47
38:L:77:ILE:O	38:L:110:VAL:O	2.32	0.47
42:P:24:THR:O	42:P:86:LYS:HB2	2.15	0.47
44:R:28:ALA:HB3	44:R:31:GLU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:160:A:H2'	27:A:161:A:O4'	2.74	0.47
27:A:1363:C:O2'	27:A:1809:A:N3	2.47	0.47
38:L:125:LEU:HB3	38:L:126:ARG:H	1.55	0.47
36:J:75:TYR:HB3	36:J:84:ILE:HD11	1.95	0.47
38:L:122:VAL:HG21	38:L:135:ILE:HD13	1.97	0.47
27:A:244:A:H2'	27:A:245:G:O4'	2.15	0.47
43:Q:71:ASN:N	43:Q:71:ASN:HD22	2.12	0.47
27:A:2297:A:N1	27:A:2321:U:C5	2.83	0.47
32:F:9:ASP:N	32:F:9:ASP:OD1	2.47	0.47
27:A:2756:U:H4'	27:A:2757:A:OP1	2.15	0.47
40:N:79:LEU:C	40:N:81:ASN:H	2.16	0.47
27:A:2178:C:H2'	27:A:2179:C:C6	2.49	0.47
27:A:20:C:H2'	27:A:21:A:C8	2.49	0.47
36:J:35:ARG:HA	36:J:40:HIS:HD2	1.79	0.47
27:A:120:U:H4'	27:A:121:G:H5'	1.96	0.47
27:A:1454:C:H5'	40:N:63:ARG:CZ	2.45	0.47
42:P:29:VAL:HG13	42:P:79:VAL:HG22	1.96	0.47
27:A:1340:U:H3'	46:T:61:LEU:HD22	1.97	0.47
30:D:32:ASN:HA	30:D:51:THR:O	2.13	0.47
27:A:2771:C:H2'	27:A:2772:C:C6	2.50	0.47
46:T:80:TRP:CZ3	46:T:82:LYS:HB3	2.50	0.47
27:A:108:G:H2'	27:A:109:C:O4'	2.15	0.47
27:A:404:A:H1'	27:A:406:G:N9	2.30	0.47
27:A:121:G:H4'	27:A:149:A:H5'	1.95	0.47
27:A:2286:G:H4'	27:A:2287:A:O5'	2.14	0.47
27:A:1052:C:H2'	27:A:1053:C:C5	2.50	0.47
30:D:48:ILE:O	30:D:81:GLU:HA	2.15	0.47
27:A:2266:A:OP1	27:A:2266:A:H8	1.98	0.47
28:B:75:G:H2'	28:B:76:G:O4'	2.14	0.47
37:K:34:GLY:O	37:K:36:GLY:N	2.47	0.47
50:X:48:LEU:HB3	50:X:50:VAL:HG13	1.96	0.47
27:A:2014:A:H2'	27:A:2015:A:C8	2.50	0.47
27:A:1430:G:H2'	27:A:1431:A:O4'	2.15	0.47
27:A:181:A:H2'	27:A:182:A:C8	2.49	0.47
35:I:133:ARG:HA	35:I:137:LEU:O	2.15	0.47
35:I:33:ASN:HB2	35:I:64:ARG:NH2	2.29	0.47
27:A:2391:G:OP2	56:3:34:LYS:HD2	2.14	0.47
27:A:1857:G:H1'	27:A:1885:A:N6	2.29	0.47
27:A:1287:A:H5'	40:N:103:ARG:HH11	1.80	0.47
27:A:2408:U:H2'	27:A:2409:G:H8	1.80	0.47
27:A:635:C:H2'	27:A:636:G:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1692:U:O2'	27:A:1693:U:H2'	2.15	0.47
27:A:2467:C:H2'	27:A:2468:A:O4'	2.14	0.47
47:U:85:ARG:NH1	47:U:99:SER:OG	2.47	0.47
27:A:1636:U:H2'	27:A:1637:A:C8	2.50	0.47
27:A:2875:C:O2'	27:A:2876:G:H5'	2.14	0.47
41:O:26:LEU:HD13	41:O:39:VAL:HG22	1.97	0.47
27:A:321:U:H4'	27:A:322:A:OP2	2.14	0.47
27:A:2584:U:C3'	27:A:2585:U:H5''	2.44	0.47
40:N:49:GLU:HB2	40:N:50:PRO:HD3	1.96	0.47
27:A:1477:A:H2'	27:A:1478:G:O4'	2.15	0.47
27:A:1530:G:H22	27:A:1542:U:H1'	1.79	0.47
41:O:34:HIS:CB	41:O:53:THR:HG1	2.28	0.47
27:A:2287:A:C2'	27:A:2288:A:O5'	2.63	0.47
33:G:70:LEU:O	33:G:74:MET:HG3	2.15	0.47
33:G:41:GLU:HB3	33:G:52:GLY:O	2.15	0.47
27:A:974:G:H1'	27:A:975:A:H8	1.80	0.47
32:F:138:PRO:HB3	59:6:32:LEU:HD11	1.97	0.47
27:A:2823:A:OP1	30:D:118:PHE:HB2	2.15	0.47
27:A:1728:C:O2'	27:A:1729:U:C6	2.68	0.47
34:H:64:ALA:O	34:H:67:ALA:HB3	2.15	0.47
27:A:2552:OMU:H5	27:A:2556:C:H41	1.79	0.46
32:F:12:VAL:O	32:F:16:MET:HG2	2.15	0.46
27:A:251:A:H2'	27:A:252:G:O4'	2.15	0.46
43:Q:85:ALA:HB2	43:Q:115:ALA:HB2	1.97	0.46
27:A:1538:G:H2'	27:A:1539:U:C6	2.50	0.46
27:A:2777:G:H1'	27:A:2779:U:H5	1.80	0.46
27:A:1315:C:H2'	27:A:1316:U:C6	2.50	0.46
52:Z:40:THR:HG23	52:Z:42:ALA:H	1.80	0.46
47:U:96:LYS:O	47:U:97:SER:O	2.34	0.46
28:B:50:A:H2'	28:B:51:G:O4'	2.15	0.46
27:A:1109:C:N3	27:A:1110:G:N2	2.63	0.46
27:A:435:C:H2'	27:A:436:C:H5'	1.96	0.46
27:A:1038:G:H2'	27:A:1039:A:C8	2.49	0.46
27:A:1085:A:H61	58:5:34:THR:HG22	1.81	0.46
27:A:2862:G:H2'	27:A:2863:C:C6	2.51	0.46
27:A:554:U:H2'	27:A:555:G:O4'	2.15	0.46
27:A:1751:U:H2'	27:A:1752:C:C6	2.51	0.46
27:A:674:G:H5''	31:E:71:GLY:H	1.81	0.46
27:A:685:A:H5''	27:A:788:A:H62	1.80	0.46
27:A:2721:A:H1'	27:A:2873:A:O2'	2.16	0.46
27:A:1980:G:O2'	27:A:1982:U:OP2	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:336:C:O2'	27:A:337:C:H5'	2.15	0.46
27:A:1684:G:H2'	27:A:1685:C:C6	2.51	0.46
27:A:2139:U:H2'	27:A:2140:G:C8	2.51	0.46
27:A:1418:G:H2'	27:A:1579:A:H62	1.80	0.46
27:A:2645:G:H4'	27:A:2732:G:H1'	1.97	0.46
27:A:2714:G:O2'	27:A:2715:C:H5'	2.14	0.46
27:A:1028:A:N3	27:A:2486:C:O2'	2.42	0.46
27:A:772:C:O2'	27:A:773:U:H5'	2.16	0.46
38:L:30:THR:O	38:L:32:GLY:N	2.48	0.46
27:A:2444:G:OP2	31:E:63:LYS:HD2	2.16	0.46
27:A:2705:A:O2'	27:A:2852:G:OP1	2.26	0.46
27:A:2688:G:H1'	27:A:2721:A:N6	2.31	0.46
52:Z:47:ILE:HD13	52:Z:56:VAL:HG21	1.97	0.46
37:K:35:VAL:HG22	37:K:69:VAL:HG12	1.98	0.46
27:A:1212:G:H1'	27:A:1237:A:N6	2.30	0.46
27:A:185:G:H4'	27:A:218:A:H4'	1.98	0.46
27:A:923:G:H2'	27:A:924:G:C8	2.48	0.46
27:A:1343:G:H1'	27:A:1597:A:C4	2.51	0.46
36:J:99:ARG:NH1	36:J:102:GLU:OE2	2.49	0.46
27:A:1152:C:H2'	27:A:1153:C:C6	2.51	0.46
27:A:259:G:C2'	27:A:260:G:H5'	2.46	0.46
27:A:2515:C:H2'	27:A:2516:A:H8	1.81	0.46
27:A:1310:G:H1'	27:A:1611:C:H5''	1.96	0.46
27:A:807:U:H1'	27:A:2445:2MG:OP1	2.15	0.46
33:G:126:THR:HG22	33:G:128:THR:H	1.81	0.46
27:A:1088:A:H61	35:I:134:SER:CB	2.29	0.46
27:A:2629:U:O2'	27:A:2630:G:H5''	2.15	0.46
32:F:4:HIS:CD2	32:F:8:LYS:HE3	2.51	0.46
47:U:17:ASP:HB3	47:U:20:LYS:HD2	1.98	0.46
40:N:38:LEU:HB3	40:N:39:PRO:HD3	1.97	0.46
32:F:129:MET:HG3	32:F:153:ILE:HB	1.98	0.46
27:A:1401:G:H8	27:A:1401:G:OP2	3.43	0.46
27:A:1306:C:N4	27:A:1606:C:H2'	2.30	0.46
28:B:13:G:N7	28:B:70:C:H4'	2.31	0.46
27:A:2331:G:O2'	27:A:2336:A:N1	2.46	0.46
27:A:1318:U:H2'	27:A:1319:C:C6	2.51	0.46
41:O:37:ALA:HB3	41:O:78:VAL:HG21	1.98	0.46
35:I:42:ASN:HA	35:I:45:THR:HB	1.97	0.46
27:A:1951:U:H2'	27:A:1953:A:OP2	2.15	0.46
27:A:2100:G:H1	27:A:2189:U:H3	1.64	0.46
27:A:1819:A:H3'	29:C:176:ARG:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:287:G:H2'	27:A:288:U:C6	2.51	0.46
27:A:1744:A:H3'	27:A:1745:A:H8	1.81	0.46
39:M:5:LYS:O	39:M:6:ARG:HG2	2.16	0.46
27:A:1188:U:O2'	27:A:1189:A:H5'	2.16	0.46
27:A:1045:C:H1'	27:A:1047:G:C2	2.51	0.46
37:K:41:ILE:HG13	37:K:58:LEU:O	2.15	0.46
27:A:1715:G:O2'	27:A:1716:U:H6	1.98	0.46
27:A:1:G:H2'	27:A:2:G:H8	1.80	0.45
27:A:2742:G:OP1	57:4:36:ARG:HD3	2.16	0.45
59:6:58:ASP:OD1	59:6:58:ASP:N	2.49	0.45
27:A:2329:U:H2'	27:A:2330:G:C8	2.51	0.45
27:A:974:G:H1'	27:A:975:A:C8	2.52	0.45
27:A:871:U:H2'	27:A:872:U:C6	2.50	0.45
45:S:28:LYS:HE3	45:S:70:LYS:HZ3	1.81	0.45
27:A:2183:A:H2'	27:A:2184:A:C8	2.51	0.45
27:A:1533:C:O2	27:A:1538:G:N2	2.47	0.45
27:A:973:A:H5'	27:A:1188:U:H1'	1.98	0.45
27:A:2808:G:H2'	27:A:2890:G:C6	2.51	0.45
59:6:37:CYS:SG	59:6:39:LYS:O	2.73	0.45
27:A:811:U:N3	38:L:21:ARG:NH2	2.64	0.45
27:A:930:G:H1'	52:Z:24:LEU:HD21	1.97	0.45
58:5:118:ILE:H	58:5:119:PRO:CD	2.29	0.45
27:A:1604:C:H2'	27:A:1605:C:C6	2.51	0.45
50:X:30:PRO:O	50:X:32:LEU:N	2.48	0.45
57:4:1:MET:HE3	57:4:34:LYS:HG2	1.99	0.45
27:A:2840:C:H2'	27:A:2841:C:C6	2.52	0.45
27:A:1361:G:H2'	27:A:1362:C:C6	2.52	0.45
27:A:1916:A:H2'	27:A:1917:PSU:O4'	2.16	0.45
38:L:95:LEU:HD22	38:L:100:ILE:HD11	1.98	0.45
27:A:1297:C:OP1	27:A:2710:C:H4'	2.16	0.45
35:I:48:ILE:HG13	35:I:49:GLU:H	1.80	0.45
33:G:95:ALA:HB1	33:G:130:ILE:HD11	1.97	0.45
30:D:40:LEU:HA	30:D:44:GLY:H	1.82	0.45
27:A:2379:G:H4'	41:O:21:LEU:HD11	1.98	0.45
27:A:1069:A:N6	27:A:1073:A:C4	2.84	0.45
27:A:1528:A:H2'	27:A:1529:G:O4'	2.17	0.45
27:A:465:G:H2'	27:A:466:A:C8	2.51	0.45
27:A:2712:C:OP1	27:A:2714:G:H4'	2.17	0.45
27:A:1328:A:H2'	27:A:1330:C:C4	2.52	0.45
27:A:357:C:H2'	27:A:358:U:C6	2.51	0.45
35:I:20:SER:HB3	35:I:21:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:5:26:VAL:HG21	58:5:114:GLU:HG2	1.98	0.45
27:A:1182:G:H4'	27:A:1183:U:O5'	4.94	0.45
27:A:136:G:H1	27:A:143:C:H42	1.63	0.45
28:B:87:U:H5''	28:B:88:C:OP2	2.16	0.45
38:L:51:GLU:OE1	38:L:56:PRO:HA	2.17	0.45
27:A:780:G:OP1	29:C:216:ARG:NH2	2.49	0.45
47:U:42:LYS:HG2	47:U:59:GLU:OE1	2.16	0.45
27:A:2638:G:H1'	27:A:2778:A:N6	2.32	0.45
28:B:114:C:H2'	28:B:115:A:C8	2.51	0.45
27:A:2528:U:H2'	27:A:2530:A:O5'	2.16	0.45
30:D:35:THR:HG22	30:D:73:VAL:HG21	1.98	0.45
30:D:31:ALA:O	30:D:33:ARG:HG2	2.17	0.45
27:A:89:A:H2'	27:A:90:U:C6	2.51	0.45
27:A:2208:C:H2'	27:A:2209:G:C8	2.52	0.45
27:A:1932:A:H2'	27:A:1933:G:O4'	2.17	0.45
27:A:2783:U:H2'	27:A:2784:U:C6	2.52	0.45
27:A:128:C:H2'	27:A:129:C:H6	1.81	0.45
36:J:35:ARG:HB2	36:J:54:ILE:HD11	1.98	0.45
38:L:62:PRO:HG2	56:3:24:LYS:HB3	1.99	0.45
27:A:2012:G:H8	27:A:2012:G:O5'	1.98	0.45
31:E:49:ARG:O	31:E:74:LYS:HE2	2.17	0.45
44:R:24:LYS:HD3	44:R:92:TRP:HB3	1.99	0.45
31:E:18:THR:HA	31:E:106:LYS:HE3	1.99	0.45
36:J:56:VAL:HB	36:J:124:VAL:HG12	1.99	0.45
32:F:24:VAL:O	32:F:27:VAL:HG12	2.17	0.45
32:F:97:GLU:HG2	59:6:25:ARG:HB2	1.99	0.45
27:A:2869:G:H2'	27:A:2870:C:O4'	2.17	0.45
27:A:2313:C:H5''	32:F:87:LYS:HD2	1.98	0.45
27:A:751:A:HO2'	27:A:752:A:H2	1.65	0.45
27:A:424:G:H2'	27:A:425:G:O4'	2.36	0.45
35:I:18:ASN:HB2	35:I:38:CYS:HB3	1.99	0.45
27:A:1858:A:C2	27:A:1885:A:H1'	2.51	0.45
51:Y:39:GLN:HB2	51:Y:41:HIS:CE1	2.52	0.45
27:A:2146:C:H4'	27:A:2147:A:C4	2.52	0.45
27:A:500:G:N1	27:A:503:A:OP2	2.49	0.45
38:L:57:LEU:HD22	56:3:53:ASP:HB3	1.98	0.45
27:A:2514:U:H5''	36:J:81:ILE:HD11	1.99	0.45
27:A:2512:C:H2'	27:A:2513:A:O4'	2.17	0.45
35:I:4:VAL:HA	35:I:7:TYR:CE2	2.51	0.45
27:A:2846:G:H2'	27:A:2847:U:O4'	2.17	0.45
27:A:2489:U:C4	27:A:2490:G:C6	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2221:G:H2'	27:A:2222:C:C6	2.52	0.45
27:A:1204:A:H4'	27:A:1205:A:H5''	1.99	0.45
27:A:1637:A:H5'	27:A:1760:C:O2'	2.17	0.45
27:A:2793:C:H2'	27:A:2794:C:C6	2.52	0.44
27:A:529:A:OP2	36:J:113:PRO:HD3	2.17	0.44
33:G:37:ASN:OD1	33:G:38:ASP:N	2.50	0.44
27:A:1014:A:H2'	27:A:1015:U:C6	2.52	0.44
30:D:36:GLN:HB3	30:D:49:GLN:HB3	1.97	0.44
32:F:153:ILE:H	32:F:153:ILE:HD12	1.82	0.44
27:A:955:PSU:H5'	39:M:86:LYS:HD3	1.99	0.44
34:H:2:GLN:HB3	34:H:39:ALA:HB3	1.98	0.44
27:A:1525:A:H2'	27:A:1526:C:O4'	2.17	0.44
34:H:30:LEU:HB3	34:H:36:ALA:HB3	2.00	0.44
27:A:651:G:H5'	56:3:18:LYS:HG3	1.99	0.44
58:5:87:GLU:OE2	58:5:95:LEU:HB2	2.17	0.44
27:A:2022:U:O4	53:0:5:ASN:ND2	2.50	0.44
27:A:973:A:H5''	44:R:81:LYS:HD2	1.99	0.44
57:4:22:VAL:HG11	57:4:36:ARG:HH11	1.82	0.44
27:A:1386:C:H2'	27:A:1387:A:H8	1.81	0.44
27:A:600:G:H2'	27:A:601:C:O4'	2.17	0.44
27:A:1682:G:H2'	27:A:1683:U:C6	2.52	0.44
39:M:69:PRO:HA	39:M:94:ALA:HB2	2.00	0.44
50:X:17:ARG:HE	50:X:23:ALA:CB	2.15	0.44
27:A:568:U:H2'	27:A:570:G:OP2	2.17	0.44
35:I:104:GLN:O	35:I:108:ILE:HG13	2.17	0.44
27:A:286:U:H2'	27:A:287:G:C8	2.52	0.44
27:A:2141:G:N2	27:A:2151:U:H1'	2.31	0.44
56:3:29:ARG:HA	56:3:29:ARG:HD3	1.76	0.44
45:S:72:THR:HG21	45:S:108:SER:HB3	1.98	0.44
40:N:28:LEU:HD13	40:N:34:ILE:HG12	2.00	0.44
27:A:414:C:H2'	27:A:415:A:C8	2.52	0.44
27:A:1107:G:H1'	58:5:81:LEU:HD12	1.97	0.44
36:J:63:ALA:HA	36:J:69:ARG:NH2	2.32	0.44
30:D:149:ASN:CG	30:D:150:GLN:H	2.20	0.44
32:F:137:PHE:HA	32:F:138:PRO:HD3	1.77	0.44
27:A:1610:A:OP1	27:A:1611:C:H5	2.00	0.44
27:A:1820:U:C2	29:C:200:MET:HB2	2.53	0.44
27:A:278:A:N3	27:A:278:A:H2'	2.32	0.44
27:A:458:G:O2'	27:A:459:U:P	2.76	0.44
27:A:19:A:H5''	43:Q:21:LYS:HG2	2.00	0.44
35:I:104:GLN:O	35:I:107:GLU:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:598:U:H2'	27:A:599:A:C8	2.52	0.44
27:A:2861:U:H2'	27:A:2862:G:C8	2.52	0.44
27:A:278:A:C2	27:A:362:A:H1'	2.53	0.44
27:A:938:G:H2'	27:A:939:G:H8	1.83	0.44
27:A:2682:A:H61	27:A:2728:U:C1'	2.27	0.44
27:A:789:A:N1	55:2:3:ARG:NH1	2.55	0.44
32:F:56:LEU:HD13	32:F:88:VAL:HG23	1.99	0.44
27:A:1783:A:N1	27:A:2587:A:H2'	2.33	0.44
27:A:2466:C:OP1	57:4:4:ARG:HB3	2.18	0.44
27:A:1278:C:H2'	27:A:1279:G:C8	2.53	0.44
27:A:2204:G:H4'	29:C:149:LYS:HD3	1.99	0.44
42:P:77:SER:O	42:P:80:VAL:HG22	2.18	0.44
27:A:2851:A:H2'	27:A:2852:G:O4'	2.17	0.44
38:L:36:LYS:HB3	38:L:37:GLY:H	1.68	0.44
27:A:2121:G:H2'	27:A:2122:U:O4'	2.18	0.44
27:A:18:U:O2'	27:A:554:U:OP1	2.35	0.44
27:A:232:G:OP2	27:A:232:G:H8	2.01	0.44
27:A:1328:A:H2'	27:A:1330:C:C5	2.53	0.44
32:F:3:LEU:HD13	32:F:96:TRP:HE3	1.83	0.44
27:A:117:G:C6	27:A:119:A:C6	3.05	0.44
27:A:1198:U:H2'	27:A:1199:U:C6	2.52	0.44
47:U:88:ASP:CG	47:U:89:GLY:H	2.21	0.44
27:A:563:A:OP2	44:R:79:ARG:NH2	2.50	0.44
27:A:1563:U:H2'	27:A:1564:C:C6	2.53	0.44
27:A:2427:C:C5'	27:A:2429:G:H5'	2.46	0.44
27:A:1103:A:H3'	27:A:1104:C:C5'	2.42	0.44
36:J:7:LYS:HB2	36:J:10:THR:OG1	2.17	0.44
52:Z:23:LEU:HD11	52:Z:53:MET:SD	2.58	0.44
27:A:2065:C:H2'	27:A:2066:C:C6	2.52	0.44
27:A:2112:G:H5'	27:A:2113:U:C5	2.53	0.44
27:A:909:A:OP1	38:L:17:LYS:HD3	63.52	0.44
43:Q:57:ARG:HA	43:Q:60:TRP:CE3	2.52	0.44
37:K:71:ARG:HH11	37:K:77:ILE:HD11	1.83	0.44
27:A:63:A:H2'	27:A:64:A:C8	2.53	0.44
27:A:2271:G:OP1	49:W:14:ALA:HB1	2.17	0.43
27:A:249:C:O2	56:3:11:LYS:NZ	2.51	0.43
27:A:2093:G:OP1	34:H:24:GLY:HA3	2.18	0.43
27:A:2730:C:O2'	27:A:2731:G:H5'	2.18	0.43
27:A:1806:C:H1'	29:C:43:ASN:HD21	1.83	0.43
27:A:1094:U:H2'	27:A:1096:A:N7	2.33	0.43
27:A:1746:A:H2'	27:A:1747:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:V:30:ILE:HG12	48:V:91:PHE:HB2	2.00	0.43
55:2:30:VAL:O	55:2:34:ARG:HG2	2.17	0.43
36:J:110:PRO:O	36:J:115:GLY:HA3	2.17	0.43
27:A:2233:U:H2'	27:A:2234:G:H8	1.80	0.43
27:A:1614:A:C2	45:S:93:ALA:HB2	2.53	0.43
27:A:2848:G:O2'	27:A:2849:U:H5'	2.18	0.43
30:D:85:ALA:C	30:D:87:GLY:H	2.22	0.43
46:T:5:GLU:HA	46:T:8:LEU:HD12	1.98	0.43
27:A:971:G:H2'	27:A:972:A:O4'	2.18	0.43
52:Z:44:ARG:HD2	52:Z:47:ILE:HD12	2.00	0.43
50:X:32:LEU:HD22	50:X:49:ARG:HG2	1.98	0.43
56:3:27:ASN:O	56:3:35:LYS:HE2	2.18	0.43
27:A:155:A:H2'	27:A:156:A:C8	2.52	0.43
27:A:2019:A:H2	27:A:2035:G:H22	1.64	0.43
28:B:79:G:N7	48:V:14:LYS:NZ	2.66	0.43
45:S:23:LEU:HD22	53:0:23:ALA:HB2	2.00	0.43
48:V:2:PHE:HA	48:V:50:MET:HE1	2.01	0.43
32:F:134:GLN:OE1	32:F:147:ARG:O	2.36	0.43
27:A:1789:A:OP2	29:C:220:ARG:NH2	2.45	0.43
27:A:2859:G:H2'	27:A:2860:A:C8	2.53	0.43
27:A:1143:A:N7	36:J:27:ARG:NH1	2.67	0.43
27:A:307:G:N1	27:A:310:A:OP2	2.50	0.43
27:A:2286:G:H5''	27:A:2287:A:OP1	2.18	0.43
35:I:56:VAL:HG13	35:I:58:ILE:HD11	2.00	0.43
27:A:182:A:H2'	27:A:183:C:O4'	2.18	0.43
56:3:32:LEU:HD23	56:3:35:LYS:HD2	2.00	0.43
31:E:102:ARG:NH1	31:E:200:LEU:O	2.51	0.43
27:A:2712:C:H3'	27:A:2714:G:H5''	1.99	0.43
27:A:1590:A:H2'	27:A:1591:A:C8	2.53	0.43
27:A:900:A:H2'	27:A:901:C:O4'	2.19	0.43
29:C:149:LYS:HG3	29:C:149:LYS:O	2.91	0.43
27:A:17:G:H4'	43:Q:24:TYR:HE1	1.83	0.43
39:M:60:GLN:NE2	39:M:108:VAL:HG12	2.33	0.43
32:F:120:SER:HB2	32:F:127:TYR:CE1	2.53	0.43
27:A:1235:G:C6	27:A:1236:G:N2	2.87	0.43
27:A:1213:A:H62	27:A:1236:G:H1'	1.84	0.43
28:B:53:A:N3	28:B:53:A:H2'	2.33	0.43
27:A:1469:A:H2'	27:A:1470:A:C8	2.54	0.43
36:J:37:ARG:NH2	36:J:110:PRO:HG3	2.33	0.43
27:A:310:A:C2'	27:A:311:A:H5''	2.48	0.43
27:A:2325:G:C6	27:A:2326:C:N4	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:G:82:PHE:O	33:G:133:LYS:HA	2.19	0.43
27:A:1421:G:C2	27:A:1422:G:C8	3.07	0.43
45:S:20:VAL:HG11	45:S:44:ALA:HA	2.00	0.43
27:A:2066:C:O2'	27:A:2067:G:H5'	2.18	0.43
27:A:490:C:H2'	27:A:491:G:C8	9.34	0.43
27:A:993:G:N3	27:A:993:G:H2'	3.04	0.43
27:A:2307:G:H8	27:A:2307:G:OP1	2.00	0.43
47:U:83:GLY:O	47:U:93:ARG:HA	2.19	0.43
27:A:1807:G:H2'	27:A:1808:A:H5'	1.99	0.43
27:A:1679:A:H2'	27:A:1680:U:C6	2.54	0.43
27:A:1432:G:O2'	27:A:1433:A:H5'	2.18	0.43
29:C:179:GLU:HG3	29:C:269:ARG:HA	2.00	0.43
38:L:135:ILE:HB	38:L:142:ILE:HD11	2.01	0.43
46:T:64:LYS:HD2	46:T:64:LYS:N	2.34	0.43
27:A:1127:A:H2'	27:A:1128:G:H5''	2.00	0.43
27:A:1788:C:O2'	27:A:1789:A:H5'	2.19	0.43
27:A:2128:G:H2'	27:A:2129:C:O4'	2.18	0.43
27:A:756:A:H2'	27:A:757:G:O4'	2.18	0.43
27:A:2347:C:H2'	27:A:2348:U:C6	2.54	0.43
27:A:1022:G:N2	27:A:1142:A:C2	2.87	0.43
27:A:2747:G:O6	27:A:2755:C:H5''	2.19	0.43
27:A:1527:G:N1	27:A:1544:A:OP2	2.49	0.43
27:A:2494:G:O2'	39:M:79:ALA:HA	2.18	0.43
27:A:2197:U:O2'	27:A:2198:A:H2'	2.17	0.43
27:A:2572:A:C8	30:D:149:ASN:ND2	2.86	0.43
40:N:79:LEU:O	40:N:81:ASN:N	2.42	0.43
27:A:571:U:OP1	27:A:819:A:O2'	20.54	0.43
27:A:682:G:H5'	55:2:26:ASN:CG	2.39	0.43
29:C:86:ARG:HD3	29:C:104:LEU:HD21	2.01	0.43
31:E:178:VAL:O	31:E:182:ALA:HB2	2.19	0.43
54:1:32:LYS:HB3	54:1:50:GLU:HB3	2.01	0.43
27:A:2646:C:H2'	27:A:2647:U:O4'	2.19	0.43
27:A:242:G:N7	56:3:4:LYS:HG2	2.34	0.43
27:A:2298:A:OP1	32:F:70:ARG:NH2	2.52	0.43
58:5:57:ASN:ND2	58:5:63:ALA:HB2	2.33	0.43
46:T:8:LEU:HA	46:T:50:LEU:HD21	2.01	0.43
27:A:17:G:H4'	43:Q:24:TYR:CE1	2.54	0.43
27:A:207:A:H2'	27:A:208:C:O4'	2.19	0.43
27:A:678:C:H2'	27:A:679:C:C6	2.53	0.43
27:A:1798:U:OP2	29:C:270:ARG:NH2	2.49	0.43
27:A:816:C:H2'	27:A:817:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2398:U:H2'	27:A:2399:G:C8	2.54	0.43
27:A:494:G:H4'	45:S:6:LYS:O	2.18	0.43
38:L:21:ARG:HA	38:L:21:ARG:HD3	1.85	0.43
41:O:31:THR:HG22	41:O:33:ARG:H	1.84	0.43
40:N:69:ARG:C	40:N:71:ARG:H	2.17	0.43
27:A:1872:A:H2'	27:A:1873:G:O4'	2.18	0.43
38:L:23:ILE:H	38:L:23:ILE:HD12	1.84	0.43
27:A:2884:U:C6	53:O:49:ARG:HG2	2.54	0.43
35:I:112:LYS:O	35:I:116:MET:HG2	2.19	0.43
53:O:28:SER:O	53:O:36:LYS:HA	2.18	0.43
27:A:278:A:H2	27:A:362:A:H1'	1.83	0.43
27:A:364:C:H2'	27:A:365:U:C6	2.54	0.43
27:A:1956:U:C2'	27:A:1957:C:H5'	2.48	0.43
36:J:102:GLU:HG3	36:J:119:PHE:CZ	2.52	0.43
27:A:2773:C:H2'	27:A:2774:C:C6	2.53	0.43
27:A:2530:A:N6	33:G:155:PRO:HG3	2.34	0.43
36:J:4:PHE:HE2	36:J:43:GLU:HB2	1.84	0.42
58:5:18:VAL:HG11	58:5:70:GLU:HB3	2.01	0.42
27:A:1866:A:H2'	27:A:1867:G:O4'	2.18	0.42
36:J:80:HIS:C	36:J:82:GLY:H	2.13	0.42
27:A:2682:A:N6	27:A:2728:U:H1'	2.30	0.42
27:A:811:U:C4	38:L:21:ARG:NH2	2.87	0.42
58:5:40:GLU:O	58:5:43:LYS:HB3	2.18	0.42
44:R:33:VAL:HG23	44:R:61:ALA:HB3	2.01	0.42
34:H:114:GLU:OE1	34:H:114:GLU:N	2.51	0.42
35:I:11:GLN:NE2	35:I:56:VAL:HG12	2.34	0.42
27:A:1796:U:H2'	27:A:1797:G:H8	1.84	0.42
27:A:191:A:H2'	27:A:192:C:C6	2.54	0.42
46:T:38:ALA:HA	46:T:42:GLU:OE1	2.19	0.42
56:3:26:ALA:O	56:3:27:ASN:CG	2.57	0.42
27:A:2362:C:P	56:3:27:ASN:ND2	2.92	0.42
27:A:2728:U:H2'	27:A:2729:G:H8	1.84	0.42
27:A:189:G:H2'	27:A:205:G:N2	2.34	0.42
27:A:2637:U:H2'	27:A:2638:G:O4'	2.19	0.42
27:A:118:A:H2'	27:A:120:U:O4	2.19	0.42
27:A:2391:G:H5''	56:3:31:ILE:HD12	2.02	0.42
58:5:24:SER:HA	58:5:85:SER:O	2.19	0.42
27:A:2572:A:H2'	30:D:149:ASN:ND2	2.34	0.42
27:A:1378:A:C4	27:A:1380:G:N7	2.87	0.42
59:6:39:LYS:O	59:6:40:CYS:CB	2.67	0.42
27:A:2684:U:O4'	37:K:70:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:K:64:ARG:HB2	37:K:83:ALA:HB3	2.00	0.42
27:A:2287:A:O2'	27:A:2288:A:H2'	2.20	0.42
27:A:1509:A:H2'	27:A:1510:G:H8	1.83	0.42
27:A:2261:C:C6	49:W:12:SER:OG	2.71	0.42
27:A:1996:C:H4'	27:A:1997:C:OP1	2.19	0.42
46:T:33:LYS:HG2	46:T:80:TRP:CZ3	2.55	0.42
27:A:476:G:H4'	27:A:502:A:N1	2.34	0.42
28:B:13:G:O2'	28:B:15:A:H2'	2.19	0.42
27:A:789:A:C6	55:2:3:ARG:NH1	2.88	0.42
27:A:2285:C:O2'	27:A:2287:A:H1'	2.20	0.42
43:Q:57:ARG:NH1	43:Q:61:ILE:HD11	2.34	0.42
27:A:1816:C:H3'	29:C:61:TYR:CE1	2.54	0.42
40:N:67:PHE:O	40:N:71:ARG:HD2	2.19	0.42
27:A:1447:C:H2'	27:A:1448:G:C8	2.55	0.42
32:F:39:VAL:C	32:F:41:GLU:H	2.22	0.42
27:A:2572:A:H5''	27:A:2574:G:H4'	2.02	0.42
32:F:48:LEU:HA	32:F:51:ASN:ND2	2.34	0.42
40:N:81:ASN:N	40:N:81:ASN:OD1	2.52	0.42
27:A:156:A:H2'	27:A:157:C:O4'	2.20	0.42
27:A:1649:G:O2'	40:N:106:ASP:OD2	2.37	0.42
27:A:2358:A:H2'	27:A:2359:C:O4'	2.19	0.42
43:Q:107:ALA:O	44:R:48:LYS:HE3	2.19	0.42
53:0:6:LYS:HA	53:0:7:PRO:HD3	1.87	0.42
27:A:2415:G:H2'	27:A:2416:C:C6	2.55	0.42
27:A:822:G:OP2	27:A:946:C:H5''	2.20	0.42
27:A:2837:A:H2'	27:A:2838:G:C8	2.54	0.42
47:U:40:LEU:HD23	47:U:61:GLU:HG3	2.01	0.42
27:A:2590:A:H2'	27:A:2591:C:C6	2.54	0.42
27:A:2287:A:C6	27:A:2289:G:C5	3.07	0.42
33:G:41:GLU:HB2	33:G:54:ARG:HE	1.85	0.42
27:A:1857:G:H2'	27:A:1884:G:H22	1.82	0.42
27:A:366:C:H2'	27:A:367:G:O4'	2.20	0.42
27:A:723:C:H2'	27:A:724:U:O4'	2.19	0.42
27:A:2526:G:H2'	27:A:2527:C:H6	1.83	0.42
32:F:139:GLU:HA	59:6:28:VAL:HG22	2.01	0.42
27:A:1747:U:H2'	27:A:1748:C:C6	2.55	0.42
47:U:52:ASN:OD1	47:U:54:PRO:HD3	2.19	0.42
32:F:7:TYR:OH	32:F:29:ARG:HB3	2.20	0.42
36:J:35:ARG:HD3	36:J:40:HIS:CD2	2.54	0.42
27:A:687:C:H5''	55:2:2:LYS:NZ	2.35	0.42
38:L:17:LYS:HE3	38:L:27:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:J:31:GLU:HG2	36:J:142:ILE:HG12	2.01	0.42
27:A:546:U:H1'	27:A:548:G:C2	2.53	0.42
27:A:779:U:P	29:C:48:ILE:HG22	2.60	0.42
29:C:16:VAL:H	29:C:203:VAL:HG22	1.84	0.42
58:5:117:LEU:HD22	58:5:120:ALA:HA	2.02	0.42
32:F:132:ARG:O	32:F:150:GLY:HA3	2.19	0.42
28:B:16:G:C6	28:B:17:C:C4	3.08	0.42
58:5:71:CYS:HB3	58:5:117:LEU:HD12	2.02	0.42
45:S:84:ARG:HB2	45:S:96:ILE:HG13	2.00	0.42
27:A:698:C:O2'	27:A:734:A:N6	2.50	0.42
27:A:1070:A:H4'	27:A:1071:G:OP2	2.19	0.42
27:A:1923:U:H2'	27:A:1924:C:C6	2.55	0.42
27:A:1486:U:O2'	27:A:1487:U:H5'	2.19	0.42
32:F:92:GLY:N	32:F:95:MET:HG2	2.34	0.42
27:A:1319:C:H2'	27:A:1320:C:O4'	2.20	0.42
43:Q:5:ARG:HB2	43:Q:8:ILE:HD11	2.00	0.42
27:A:1736:U:H2'	27:A:1737:G:O4'	2.20	0.42
27:A:919:U:H2'	27:A:920:A:O4'	2.19	0.42
34:H:132:PHE:HB2	34:H:140:ALA:HB3	2.02	0.42
27:A:2567:G:H2'	27:A:2568:U:C6	2.54	0.42
33:G:51:PHE:CE1	33:G:71:LEU:HD22	2.54	0.42
40:N:54:LEU:HD21	40:N:65:LEU:HB3	2.02	0.42
34:H:84:ALA:HB2	34:H:90:LEU:HD12	2.02	0.42
27:A:310:A:O2'	27:A:311:A:H5''	2.20	0.42
27:A:935:C:O2'	27:A:936:A:H5'	2.19	0.42
36:J:99:ARG:HA	36:J:102:GLU:HB3	2.01	0.42
27:A:158:U:O2	27:A:169:G:N2	2.52	0.42
27:A:2141:G:H2'	27:A:2142:A:H8	1.84	0.42
27:A:97:C:H2'	27:A:98:G:O4'	2.19	0.42
27:A:1843:C:O2'	29:C:253:GLY:O	2.32	0.42
27:A:594:U:H2'	27:A:595:C:C6	2.54	0.42
27:A:2648:G:N2	27:A:2673:G:H1'	2.35	0.42
28:B:43:C:O2'	32:F:91:ARG:HG2	2.20	0.42
29:C:2:VAL:HG21	29:C:201:LEU:HD12	2.02	0.42
40:N:31:HIS:O	40:N:32:GLU:HB2	2.20	0.42
27:A:255:A:H2'	27:A:256:A:O4'	2.19	0.42
37:K:108:ARG:NH1	37:K:116:ILE:HD13	2.34	0.42
27:A:706:A:H2'	27:A:707:G:O4'	2.20	0.42
28:B:85:G:H2'	28:B:86:G:H8	1.84	0.42
27:A:2016:U:H1'	53:0:2:VAL:HG13	2.02	0.42
27:A:460:A:H2'	27:A:461:C:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1943:U:H1'	27:A:1945:G:OP2	2.20	0.42
36:J:17:VAL:HG22	36:J:55:ILE:HB	2.02	0.42
27:A:218:A:C8	27:A:218:A:OP2	2.67	0.42
27:A:2884:U:C5	53:O:49:ARG:HG2	2.54	0.42
57:4:30:GLU:HA	57:4:31:PRO:HD3	1.89	0.42
27:A:2064:C:H2'	27:A:2065:C:C6	2.55	0.42
27:A:1366:A:H2'	27:A:1367:A:O4'	2.20	0.42
50:X:4:CYS:HA	50:X:32:LEU:HD21	2.01	0.41
30:D:33:ARG:H	30:D:33:ARG:HG2	1.58	0.41
27:A:2146:C:O2'	27:A:2147:A:N7	2.52	0.41
27:A:1078:U:H4'	27:A:1079:C:H5''	2.02	0.41
27:A:2619:C:O2'	27:A:2620:C:H5'	2.19	0.41
27:A:137:U:H3	27:A:142:A:H61	1.68	0.41
27:A:1717:A:H2'	27:A:1718:G:O4'	2.20	0.41
27:A:2896:C:H2'	27:A:2897:U:C6	2.54	0.41
31:E:128:ALA:O	31:E:130:LYS:N	2.51	0.41
34:H:3:VAL:HA	34:H:38:PRO:HA	2.02	0.41
27:A:358:U:H2'	27:A:359:G:H8	2.06	0.41
48:V:6:ALA:HB2	48:V:42:LEU:HB3	2.01	0.41
49:W:21:ARG:HB2	49:W:33:ILE:HG23	2.02	0.41
27:A:1884:G:H5'	27:A:1885:A:OP1	2.20	0.41
54:1:10:LEU:HD23	54:1:50:GLU:HA	2.02	0.41
27:A:2545:G:H2'	27:A:2546:U:O4'	2.20	0.41
27:A:2572:A:OP1	27:A:2574:G:H4'	2.20	0.41
27:A:745:1MG:HM11	27:A:745:1MG:HN21	1.67	0.41
27:A:1204:A:H4'	27:A:1205:A:C5'	2.49	0.41
27:A:1726:C:H2'	27:A:1727:C:C6	2.54	0.41
29:C:259:ASN:O	29:C:261:ARG:N	2.47	0.41
27:A:2038:G:H2'	27:A:2039:U:O4'	2.19	0.41
27:A:848:C:H2'	27:A:849:A:C8	2.55	0.41
35:I:20:SER:HA	35:I:24:GLY:HA3	2.02	0.41
27:A:1222:U:H2'	27:A:1223:G:H8	1.86	0.41
27:A:832:U:H2'	27:A:833:A:C8	2.55	0.41
27:A:1880:U:H2'	27:A:1881:C:C6	2.55	0.41
37:K:36:GLY:HA2	37:K:62:VAL:O	2.19	0.41
43:Q:106:THR:O	43:Q:110:GLU:HG2	2.21	0.41
27:A:1801:A:H5'	27:A:2203:U:O2'	2.20	0.41
27:A:736:C:H2'	27:A:737:C:C6	2.82	0.41
28:B:78:A:H2'	28:B:79:G:O4'	2.20	0.41
44:R:16:GLU:HB2	44:R:101:ILE:HG12	2.01	0.41
27:A:1511:G:H2'	27:A:1512:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1432:G:O2'	27:A:1433:A:H8	3.82	0.41
27:A:1201:U:H2'	27:A:1202:G:C8	2.55	0.41
27:A:783:A:H2'	27:A:784:G:H4'	2.02	0.41
27:A:2756:U:H1'	27:A:2757:A:H5''	2.02	0.41
27:A:591:U:H2'	27:A:592:A:C8	2.55	0.41
32:F:135:ILE:HG13	32:F:135:ILE:H	1.64	0.41
27:A:1418:G:N1	27:A:1579:A:OP2	2.44	0.41
29:C:132:ARG:NH1	34:H:93:SER:OG	2.54	0.41
30:D:151:THR:HB	30:D:152:PRO:HD3	2.01	0.41
50:X:31:ASN:O	50:X:51:SER:HA	2.19	0.41
27:A:2556:C:H2'	27:A:2557:G:O4'	2.20	0.41
34:H:66:ASN:HB3	34:H:134:VAL:O	2.20	0.41
46:T:8:LEU:HD13	51:Y:21:LEU:HB3	2.02	0.41
35:I:72:THR:HG21	35:I:112:LYS:HB3	2.02	0.41
48:V:83:LYS:HA	48:V:84:PRO:HD3	1.91	0.41
27:A:249:C:O2'	38:L:63:LYS:NZ	2.30	0.41
27:A:813:U:H2'	27:A:814:C:C6	2.55	0.41
43:Q:34:ALA:O	43:Q:38:VAL:HG23	2.21	0.41
27:A:1235:G:N1	27:A:1236:G:N2	2.68	0.41
38:L:123:ARG:HA	38:L:143:GLU:O	2.20	0.41
27:A:1045:C:H5'	27:A:1046:A:C5'	2.50	0.41
27:A:463:G:N2	27:A:466:A:OP2	2.36	0.41
41:O:33:ARG:HG2	41:O:34:HIS:CD2	2.55	0.41
57:4:5:ALA:O	57:4:38:GLY:HA2	2.21	0.41
30:D:110:THR:HG21	30:D:169:ARG:HH11	1.85	0.41
27:A:2709:G:H2'	27:A:2710:C:C6	2.55	0.41
27:A:2803:G:H2'	27:A:2804:U:C6	2.56	0.41
30:D:43:ASP:HB3	30:D:45:TYR:CE2	2.55	0.41
27:A:1562:U:H2'	27:A:1563:U:O4'	2.20	0.41
27:A:609:A:H2'	27:A:610:C:O4'	2.21	0.41
43:Q:109:VAL:HG12	43:Q:113:LYS:HE2	2.02	0.41
27:A:2108:A:H2'	27:A:2109:U:O4'	2.21	0.41
27:A:1826:G:OP1	29:C:222:THR:HG23	2.19	0.41
27:A:2746:U:H5''	33:G:137:LYS:HG2	2.01	0.41
27:A:911:A:H2'	39:M:9:PHE:CZ	2.56	0.41
43:Q:75:TYR:CZ	43:Q:79:ILE:HG13	2.55	0.41
35:I:33:ASN:HB3	35:I:36:GLU:HG2	2.01	0.41
27:A:1067:A:H4'	27:A:1068:G:O5'	4.70	0.41
33:G:88:LEU:HG	33:G:161:VAL:HG22	2.03	0.41
27:A:974:G:C8	27:A:990:A:N6	2.76	0.41
27:A:1754:A:N1	27:A:2716:C:O2'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:M:34:LYS:HA	39:M:101:VAL:HA	2.01	0.41
27:A:1287:A:H5'	40:N:103:ARG:NH1	2.36	0.41
29:C:24:HIS:HB3	29:C:81:GLU:OE1	2.20	0.41
27:A:869:G:H1'	39:M:8:LYS:HD2	2.02	0.41
27:A:340:A:H2'	27:A:341:C:O4'	2.21	0.41
27:A:1132:U:H3'	27:A:1132:U:OP2	2.21	0.41
27:A:1495:A:O5'	27:A:1495:A:H8	2.04	0.41
27:A:1529:G:H2'	27:A:1530:G:O4'	2.20	0.41
27:A:2674:G:H5'	37:K:30:ARG:HH21	1.85	0.41
27:A:1454:C:H5'	40:N:63:ARG:NH2	2.36	0.41
27:A:1957:C:H2'	27:A:1958:C:C6	2.56	0.41
42:P:27:VAL:HG12	42:P:29:VAL:HG23	2.01	0.41
27:A:2230:G:H2'	27:A:2231:U:C6	2.56	0.41
27:A:833:A:H2'	27:A:834:G:H8	1.85	0.41
27:A:1413:A:H2'	27:A:1414:C:O4'	2.20	0.41
27:A:2837:A:H2'	27:A:2838:G:H8	1.86	0.41
27:A:1292:G:H2'	27:A:1293:C:C6	2.56	0.41
30:D:38:LYS:O	30:D:46:ARG:HA	2.21	0.41
40:N:82:GLU:O	40:N:86:ARG:HB2	2.21	0.41
41:O:92:PHE:HB2	41:O:117:PHE:CE1	2.56	0.41
27:A:2599:G:C8	29:C:235:GLU:HG2	2.56	0.41
47:U:40:LEU:HB3	47:U:59:GLU:HG3	2.03	0.41
39:M:33:LEU:HD12	39:M:129:THR:O	2.20	0.41
27:A:1275:A:C3'	27:A:1645:G:HO2'	2.33	0.41
27:A:192:C:H2'	27:A:193:U:H5'	2.03	0.41
58:5:49:GLY:H	58:5:51:TYR:HE2	1.68	0.41
27:A:329:G:OP2	47:U:68:ASN:ND2	2.54	0.41
29:C:252:LYS:HE3	29:C:252:LYS:HB2	1.83	0.41
50:X:12:VAL:HG23	50:X:28:PHE:HB2	2.03	0.41
27:A:1739:A:H2'	27:A:1740:G:O4'	2.21	0.41
27:A:1741:C:H2'	27:A:1742:U:C6	2.56	0.41
31:E:47:LYS:HB3	31:E:47:LYS:HE2	1.87	0.41
27:A:2368:C:H2'	27:A:2369:A:H8	1.86	0.41
29:C:209:ALA:HA	29:C:212:TRP:CE2	2.56	0.41
27:A:995:C:O2'	43:Q:92:LYS:HE2	2.20	0.41
27:A:2045:C:H5''	53:0:14:MET:SD	2.61	0.41
30:D:14:ILE:HA	42:P:11:GLN:OE1	2.21	0.41
55:2:34:ARG:HE	55:2:39:ARG:HD2	1.86	0.41
27:A:779:U:OP1	29:C:48:ILE:HG22	2.21	0.41
28:B:45:A:O4'	32:F:91:ARG:NH2	2.54	0.41
27:A:859:G:H1'	27:A:860:U:H5	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:306:U:H2'	27:A:307:G:O4'	2.21	0.41
32:F:175:PRO:HB2	32:F:176:PHE:H	1.71	0.41
27:A:507:A:H5''	27:A:508:A:H3'	2.02	0.41
27:A:1847:G:O2'	27:A:1848:A:H8	2.03	0.41
31:E:97:ASN:O	31:E:100:MET:N	2.51	0.41
27:A:1993:U:H4'	30:D:133:THR:HG22	2.02	0.41
30:D:80:TRP:NE1	30:D:202:ILE:HD11	2.36	0.41
27:A:737:C:H2'	27:A:738:G:O4'	2.21	0.41
44:R:11:GLN:N	44:R:11:GLN:OE1	2.53	0.41
56:3:36:ALA:O	56:3:39:ARG:HB2	2.20	0.41
43:Q:35:PHE:CZ	43:Q:39:ILE:HD11	2.56	0.41
35:I:12:VAL:HB	35:I:13:ALA:H	1.68	0.41
27:A:1565:C:HO2'	27:A:1566:A:H2'	1.85	0.41
53:0:27:LEU:HD23	53:0:36:LYS:HB3	2.03	0.41
27:A:84:A:N7	27:A:101:A:H2	2.18	0.41
27:A:413:C:H2'	27:A:414:C:H6	1.85	0.41
27:A:162:U:HO2'	27:A:163:C:H6	1.66	0.41
46:T:8:LEU:HD11	51:Y:22:LEU:HD12	2.03	0.41
27:A:2825:G:N3	27:A:2825:G:H5''	2.36	0.41
27:A:22:C:H2'	27:A:23:G:O4'	2.21	0.41
56:3:51:LYS:HB2	56:3:51:LYS:HE3	1.87	0.41
45:S:34:ASP:HB3	53:0:27:LEU:HD22	2.03	0.40
27:A:1278:C:H2'	27:A:1279:G:H8	1.86	0.40
39:M:109:PRO:HD2	39:M:112:LEU:HD23	2.03	0.40
27:A:1071:G:N2	27:A:1089:A:O2'	2.54	0.40
27:A:2039:U:H2'	27:A:2040:G:C8	2.55	0.40
27:A:2040:G:H2'	27:A:2041:U:O4'	2.20	0.40
27:A:2804:U:H2'	27:A:2805:C:C6	2.56	0.40
43:Q:78:PHE:HE1	43:Q:109:VAL:HA	1.85	0.40
27:A:2475:C:O5'	27:A:2475:C:H6	2.04	0.40
35:I:33:ASN:HB2	35:I:64:ARG:NH1	2.34	0.40
45:S:14:ALA:HB1	45:S:18:ARG:HH21	1.85	0.40
27:A:2092:U:H4'	27:A:2093:G:O5'	2.20	0.40
27:A:608:A:H2'	27:A:609:A:O4'	2.41	0.40
28:B:54:G:H2'	28:B:55:U:C6	2.56	0.40
27:A:456:C:C2	46:T:73:ARG:NH2	2.87	0.40
36:J:40:HIS:CE1	36:J:41:LYS:HG3	2.56	0.40
27:A:190:A:OP2	50:X:25:LYS:NZ	2.53	0.40
29:C:70:LYS:HD2	29:C:73:ILE:HD12	2.03	0.40
57:4:7:VAL:HG22	57:4:38:GLY:HA3	2.03	0.40
55:2:21:ARG:O	55:2:27:GLY:HA3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2405:G:H1'	27:A:2412:A:H61	1.87	0.40
27:A:2844:G:H2'	27:A:2845:U:O4'	2.20	0.40
27:A:1443:U:H2'	27:A:1444:G:H8	1.87	0.40
27:A:1824:G:O3'	29:C:246:PRO:HD3	2.21	0.40
27:A:739:A:H1'	27:A:740:C:H5	1.86	0.40
48:V:32:GLY:O	48:V:93:ARG:NH1	2.52	0.40
30:D:14:ILE:HD11	30:D:188:LEU:HD13	2.03	0.40
34:H:9:VAL:HG12	34:H:11:ASN:H	1.85	0.40
36:J:37:ARG:HD3	36:J:37:ARG:HA	4.48	0.40
27:A:78:U:OP2	51:Y:2:LYS:HD2	2.21	0.40
42:P:77:SER:HA	42:P:78:PRO:HD3	1.89	0.40
35:I:37:PHE:CZ	35:I:58:ILE:HD12	2.56	0.40
27:A:376:G:H2'	27:A:377:G:H8	1.86	0.40
27:A:1591:A:H2'	27:A:1592:C:O4'	2.21	0.40
27:A:758:C:O2	27:A:758:C:H2'	2.20	0.40
27:A:1072:C:N3	27:A:1092:C:N4	2.70	0.40
27:A:1023:U:H4'	27:A:1123:C:OP1	2.21	0.40
27:A:1988:G:H2'	27:A:1989:G:O4'	2.22	0.40
59:6:2:LYS:O	59:6:5:ILE:HG12	2.21	0.40
27:A:2106:U:H2'	27:A:2107:G:C8	2.56	0.40
27:A:1730:C:O2	27:A:1731:G:N1	2.54	0.40
48:V:30:ILE:HG21	48:V:70:ILE:HG21	2.02	0.40
27:A:1180:U:H2'	27:A:1181:U:H5'	2.03	0.40
46:T:44:LYS:HG3	46:T:55:VAL:HG11	2.04	0.40
30:D:101:PHE:HA	30:D:104:VAL:HG22	2.02	0.40
43:Q:71:ASN:N	43:Q:71:ASN:ND2	2.69	0.40
28:B:17:C:H2'	28:B:18:G:O4'	2.22	0.40
27:A:981:A:OP2	27:A:982:C:N4	2.43	0.40
39:M:41:LEU:HG	39:M:96:ILE:HG13	2.03	0.40
42:P:51:ASN:O	42:P:52:ARG:HD3	2.21	0.40
27:A:20:C:H2'	27:A:21:A:H8	1.87	0.40
27:A:1752:C:H2'	27:A:1753:G:C8	2.56	0.40
27:A:1078:U:O2'	27:A:1088:A:H5''	2.22	0.40
30:D:20:VAL:HG22	37:K:72:PRO:HB2	2.03	0.40
27:A:1045:C:H1'	27:A:1047:G:N3	2.36	0.40
27:A:753:A:H2'	27:A:754:U:C6	2.56	0.40
27:A:2060:A:H1'	27:A:2502:G:O4'	2.21	0.40
51:Y:28:LEU:HD13	51:Y:42:LEU:HB3	2.03	0.40
27:A:974:G:H4'	27:A:975:A:OP1	2.19	0.40
27:A:1275:A:H4'	27:A:1276:A:O5'	2.20	0.40
30:D:6:GLY:O	30:D:201:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2697:G:H2'	27:A:2698:U:O4'	2.21	0.40
51:Y:44:LYS:HA	51:Y:47:ARG:NH2	2.37	0.40
27:A:21:A:H2'	27:A:22:C:O4'	2.21	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	
2	b	216/240 (90%)	183 (85%)	23 (11%)	10 (5%)	3	11
3	c	204/233 (88%)	184 (90%)	18 (9%)	2 (1%)	19	54
4	d	203/206 (98%)	172 (85%)	21 (10%)	10 (5%)	3	10
5	e	155/167 (93%)	130 (84%)	16 (10%)	9 (6%)	2	6
6	f	98/135 (73%)	81 (83%)	11 (11%)	6 (6%)	2	5
7	g	149/179 (83%)	124 (83%)	15 (10%)	10 (7%)	1	4
8	h	127/130 (98%)	110 (87%)	14 (11%)	3 (2%)	7	29
9	i	125/130 (96%)	98 (78%)	19 (15%)	8 (6%)	2	5
10	j	96/103 (93%)	74 (77%)	16 (17%)	6 (6%)	2	5
11	k	114/129 (88%)	92 (81%)	16 (14%)	6 (5%)	2	8
12	l	121/124 (98%)	96 (79%)	20 (16%)	5 (4%)	3	14
13	m	112/118 (95%)	99 (88%)	8 (7%)	5 (4%)	3	12
14	n	99/102 (97%)	82 (83%)	12 (12%)	5 (5%)	2	9
15	o	86/89 (97%)	71 (83%)	10 (12%)	5 (6%)	2	6
16	p	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	7	27
17	q	78/84 (93%)	65 (83%)	8 (10%)	5 (6%)	2	5
18	r	63/75 (84%)	53 (84%)	5 (8%)	5 (8%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	s	77/92 (84%)	66 (86%)	11 (14%)	0	100	100
20	t	83/87 (95%)	77 (93%)	4 (5%)	2 (2%)	7	29
21	u	63/71 (89%)	44 (70%)	14 (22%)	5 (8%)	1	3
26	z	368/393 (94%)	327 (89%)	35 (10%)	6 (2%)	12	40
29	C	269/273 (98%)	243 (90%)	21 (8%)	5 (2%)	10	35
30	D	207/209 (99%)	185 (89%)	20 (10%)	2 (1%)	19	54
31	E	199/201 (99%)	172 (86%)	20 (10%)	7 (4%)	4	18
32	F	175/179 (98%)	149 (85%)	20 (11%)	6 (3%)	5	19
33	G	174/177 (98%)	148 (85%)	21 (12%)	5 (3%)	6	23
34	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	6	25
35	I	139/142 (98%)	110 (79%)	20 (14%)	9 (6%)	1	4
36	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	14	44
37	K	120/123 (98%)	103 (86%)	14 (12%)	3 (2%)	7	27
38	L	141/144 (98%)	110 (78%)	20 (14%)	11 (8%)	1	3
39	M	134/136 (98%)	117 (87%)	14 (10%)	3 (2%)	8	31
40	N	118/127 (93%)	103 (87%)	12 (10%)	3 (2%)	7	27
41	O	114/117 (97%)	102 (90%)	11 (10%)	1 (1%)	21	57
42	P	112/115 (97%)	93 (83%)	18 (16%)	1 (1%)	21	57
43	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
44	R	101/103 (98%)	82 (81%)	17 (17%)	2 (2%)	9	33
45	S	108/110 (98%)	90 (83%)	12 (11%)	6 (6%)	2	7
46	T	91/100 (91%)	77 (85%)	11 (12%)	3 (3%)	5	20
47	U	100/104 (96%)	80 (80%)	17 (17%)	3 (3%)	5	22
48	V	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	8	31
49	W	73/85 (86%)	66 (90%)	6 (8%)	1 (1%)	14	44
50	X	75/78 (96%)	69 (92%)	5 (7%)	1 (1%)	15	46
51	Y	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	12	40
52	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
53	0	54/57 (95%)	49 (91%)	4 (7%)	1 (2%)	10	35
54	1	48/55 (87%)	43 (90%)	5 (10%)	0	100	100
55	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	3	62/65 (95%)	54 (87%)	7 (11%)	1 (2%)	12	40
57	4	36/38 (95%)	28 (78%)	8 (22%)	0	100	100
58	5	129/165 (78%)	100 (78%)	22 (17%)	7 (5%)	2	7
59	6	64/70 (91%)	53 (83%)	10 (16%)	1 (2%)	12	40
All	All	6215/6613 (94%)	5318 (86%)	691 (11%)	206 (3%)	8	20

All (206) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	c	156	LEU
5	e	122	VAL
6	f	63	ASN
9	i	12	LYS
9	i	71	ILE
10	j	57	VAL
10	j	75	ASP
10	j	89	ARG
16	p	8	ARG
17	q	79	GLU
18	r	17	VAL
29	C	204	LEU
32	F	175	PRO
33	G	108	PHE
36	J	81	ILE
37	K	93	GLN
38	L	15	ALA
38	L	85	VAL
38	L	128	THR
45	S	67	ASP
47	U	6	ARG
47	U	97	SER
50	X	31	ASN
56	3	27	ASN
2	b	17	HIS
2	b	19	THR
2	b	179	GLY
3	c	13	ILE
4	d	26	ALA
4	d	108	ALA
5	e	23	THR
5	e	93	VAL

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Mol	Chain	Res	Type
7	g	16	LYS
7	g	56	SER
7	g	63	VAL
7	g	112	ASP
7	g	145	GLU
8	h	66	GLN
9	i	57	VAL
10	j	29	ALA
10	j	77	VAL
11	k	76	TYR
11	k	77	GLY
11	k	88	PRO
12	l	75	GLU
13	m	104	ASN
14	n	54	ASP
15	o	21	THR
15	o	45	HIS
17	q	17	GLU
17	q	49	ASN
18	r	46	THR
20	t	68	LYS
21	u	12	ASP
29	C	195	GLY
29	C	231	HIS
34	H	9	VAL
35	I	64	ARG
35	I	89	SER
35	I	92	PRO
37	K	35	VAL
37	K	110	GLU
38	L	29	LYS
38	L	31	GLY
38	L	111	ILE
39	M	70	ASP
41	O	66	GLY
42	P	65	ASN
44	R	43	ASN
44	R	54	VAL
45	S	2	GLU
45	S	3	THR
46	T	37	ASP
46	T	38	ALA

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Mol	Chain	Res	Type
46	T	71	GLY
51	Y	24	GLU
58	5	55	VAL
2	b	73	ARG
2	b	87	ASP
2	b	153	MET
4	d	7	LYS
4	d	31	CYS
4	d	152	SER
4	d	166	LYS
4	d	174	ALA
5	e	98	ALA
5	e	99	SER
5	e	121	ASN
6	f	54	LEU
6	f	92	THR
7	g	64	ALA
7	g	95	ARG
8	h	74	ILE
9	i	90	ASP
9	i	107	ALA
9	i	125	GLN
10	j	35	GLN
11	k	14	GLN
12	l	2	THR
12	l	46	SER
13	m	6	ILE
13	m	7	ASN
13	m	113	LYS
14	n	22	LYS
14	n	38	ASP
14	n	55	SER
15	o	2	LEU
15	o	13	GLU
16	p	49	GLY
17	q	16	MET
20	t	76	ALA
21	u	29	ALA
21	u	32	ARG
21	u	34	ARG
29	C	239	PHE
31	E	89	PRO

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Mol	Chain	Res	Type
31	E	122	GLU
33	G	44	HIS
33	G	45	ALA
34	H	15	LEU
35	I	12	VAL
38	L	88	GLY
39	M	6	ARG
40	N	59	SER
45	S	62	ASP
58	5	88	HIS
58	5	118	ILE
59	6	40	CYS
2	b	11	ALA
2	b	88	GLN
2	b	126	ASP
5	e	100	GLU
5	e	102	THR
6	f	56	LYS
6	f	86	ARG
6	f	99	ALA
7	g	29	LEU
8	h	22	ALA
9	i	99	LYS
11	k	92	ARG
12	l	23	LEU
14	n	2	LYS
15	o	75	ALA
18	r	18	GLN
18	r	71	ASP
26	z	9	LYS
30	D	32	ASN
31	E	80	SER
31	E	160	ALA
32	F	20	ASN
32	F	142	TYR
32	F	173	ASP
32	F	176	PHE
34	H	2	GLN
35	I	6	ALA
35	I	20	SER
38	L	25	SER
40	N	117	ASP

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Mol	Chain	Res	Type
45	S	65	ASP
48	V	58	SER
49	W	8	ASN
53	0	2	VAL
58	5	22	ALA
58	5	90	GLY
58	5	130	PRO
2	b	14	HIS
4	d	34	GLU
18	r	70	THR
26	z	164	GLY
26	z	207	ASP
26	z	249	GLU
31	E	84	THR
32	F	174	PHE
33	G	70	LEU
34	H	3	VAL
35	I	22	PRO
35	I	100	ILE
36	J	82	GLY
38	L	94	THR
4	d	6	PRO
4	d	28	ASP
9	i	13	SER
26	z	14	VAL
30	D	148	GLN
31	E	83	VAL
35	I	38	CYS
38	L	119	PRO
45	S	101	SER
11	k	119	GLY
12	l	44	PRO
29	C	168	GLY
38	L	26	GLY
39	M	69	PRO
40	N	116	VAL
17	q	20	ILE
21	u	9	GLU
47	U	38	ILE
7	g	5	VAL
26	z	286	ILE
48	V	15	GLY

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Mol	Chain	Res	Type
58	5	108	VAL
7	g	28	ILE
31	E	129	PRO
5	e	26	GLY
13	m	9	PRO
33	G	155	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/198 (91%)	175 (97%)	5 (3%)	51	84
3	c	170/190 (90%)	163 (96%)	7 (4%)	37	73
4	d	172/173 (99%)	166 (96%)	6 (4%)	43	78
5	e	114/126 (90%)	105 (92%)	9 (8%)	15	41
6	f	87/116 (75%)	83 (95%)	4 (5%)	33	69
7	g	124/147 (84%)	122 (98%)	2 (2%)	70	91
8	h	104/105 (99%)	103 (99%)	1 (1%)	82	95
9	i	105/107 (98%)	100 (95%)	5 (5%)	31	67
10	j	86/90 (96%)	84 (98%)	2 (2%)	58	87
11	k	89/99 (90%)	87 (98%)	2 (2%)	60	88
12	l	103/104 (99%)	100 (97%)	3 (3%)	50	83
13	m	92/96 (96%)	90 (98%)	2 (2%)	60	88
14	n	79/84 (94%)	75 (95%)	4 (5%)	29	65
15	o	76/77 (99%)	74 (97%)	2 (3%)	54	85
16	p	65/65 (100%)	61 (94%)	4 (6%)	23	55
17	q	74/78 (95%)	71 (96%)	3 (4%)	37	73
18	r	48/65 (74%)	47 (98%)	1 (2%)	61	88
19	s	70/79 (89%)	69 (99%)	1 (1%)	74	93
20	t	65/66 (98%)	63 (97%)	2 (3%)	47	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	u	44/61 (72%)	42 (96%)	2 (4%)	34	70
26	z	311/326 (95%)	304 (98%)	7 (2%)	58	87
29	C	216/218 (99%)	208 (96%)	8 (4%)	41	77
30	D	164/164 (100%)	161 (98%)	3 (2%)	66	90
31	E	165/165 (100%)	160 (97%)	5 (3%)	48	83
32	F	148/150 (99%)	141 (95%)	7 (5%)	32	68
33	G	137/138 (99%)	137 (100%)	0	100	100
34	H	114/114 (100%)	114 (100%)	0	100	100
35	I	109/110 (99%)	106 (97%)	3 (3%)	51	84
36	J	116/116 (100%)	114 (98%)	2 (2%)	68	91
37	K	103/104 (99%)	98 (95%)	5 (5%)	31	67
38	L	102/103 (99%)	100 (98%)	2 (2%)	63	88
39	M	109/109 (100%)	108 (99%)	1 (1%)	84	96
40	N	100/103 (97%)	98 (98%)	2 (2%)	63	88
41	O	86/87 (99%)	84 (98%)	2 (2%)	58	87
42	P	99/100 (99%)	96 (97%)	3 (3%)	48	83
43	Q	89/90 (99%)	87 (98%)	2 (2%)	60	88
44	R	84/84 (100%)	83 (99%)	1 (1%)	78	94
45	S	93/93 (100%)	90 (97%)	3 (3%)	46	81
46	T	80/84 (95%)	76 (95%)	4 (5%)	30	65
47	U	83/85 (98%)	82 (99%)	1 (1%)	78	94
48	V	78/78 (100%)	77 (99%)	1 (1%)	76	94
49	W	57/63 (90%)	56 (98%)	1 (2%)	66	90
50	X	67/68 (98%)	67 (100%)	0	100	100
51	Y	55/55 (100%)	54 (98%)	1 (2%)	66	90
52	Z	48/49 (98%)	48 (100%)	0	100	100
53	0	47/48 (98%)	45 (96%)	2 (4%)	35	71
54	1	45/49 (92%)	44 (98%)	1 (2%)	60	88
55	2	38/38 (100%)	38 (100%)	0	100	100
56	3	51/52 (98%)	50 (98%)	1 (2%)	63	88
57	4	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
58	5	100/123 (81%)	97 (97%)	3 (3%)	48 83
59	6	59/62 (95%)	58 (98%)	1 (2%)	68 91
All	All	5134/5388 (95%)	4995 (97%)	139 (3%)	56 84

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	9	LEU
2	b	35	ASN
2	b	71	THR
2	b	185	ILE
2	b	202	ASN
3	c	3	LYS
3	c	40	GLN
3	c	96	VAL
3	c	127	VAL
3	c	133	MET
3	c	149	LYS
3	c	156	LEU
4	d	16	THR
4	d	52	VAL
4	d	115	GLN
4	d	119	HIS
4	d	141	VAL
4	d	196	GLU
5	e	10	LEU
5	e	11	GLN
5	e	45	VAL
5	e	51	LYS
5	e	75	LEU
5	e	122	VAL
5	e	140	ILE
5	e	156	ARG
5	e	158	LYS
6	f	54	LEU
6	f	74	LEU
6	f	86	ARG
6	f	89	VAL
7	g	58	LEU
7	g	83	THR
8	h	58	LEU

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Mol	Chain	Res	Type
9	i	38	PHE
9	i	54	VAL
9	i	60	LEU
9	i	88	GLU
9	i	108	ARG
10	j	10	LEU
10	j	64	GLN
11	k	30	ILE
11	k	39	ASN
12	l	20	VAL
12	l	28	GLN
12	l	63	THR
13	m	15	VAL
13	m	99	GLN
14	n	26	LEU
14	n	33	VAL
14	n	49	GLN
14	n	60	GLN
15	o	44	GLU
15	o	86	LEU
16	p	19	VAL
16	p	26	ASN
16	p	34	GLU
16	p	70	ARG
17	q	51	GLU
17	q	61	ARG
17	q	69	THR
18	r	24	ASP
19	s	62	THR
20	t	22	SER
20	t	26	MET
21	u	19	LYS
21	u	23	GLU
26	z	68	GLU
26	z	73	THR
26	z	143	GLU
26	z	190	GLU
26	z	323	PHE
26	z	329	GLN
26	z	362	LEU
29	C	12	ARG
29	C	13	ARG

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Mol	Chain	Res	Type
29	C	45	ASN
29	C	129	LEU
29	C	181	ARG
29	C	206	LYS
29	C	212	TRP
29	C	257	ARG
30	D	33	ARG
30	D	52	THR
30	D	88	GLU
31	E	7	ASP
31	E	19	PHE
31	E	40	ARG
31	E	41	GLN
31	E	96	VAL
32	F	3	LEU
32	F	5	ASP
32	F	9	ASP
32	F	55	ASP
32	F	95	MET
32	F	129	MET
32	F	134	GLN
35	I	10	LEU
35	I	95	ASP
35	I	134	SER
36	J	57	LEU
36	J	64	VAL
37	K	8	LEU
37	K	30	ARG
37	K	32	TYR
37	K	58	LEU
37	K	73	ASP
38	L	27	LEU
38	L	41	ARG
39	M	46	ILE
40	N	15	SER
40	N	113	ILE
41	O	69	ASP
41	O	100	HIS
42	P	7	LEU
42	P	31	VAL
42	P	99	LEU
43	Q	48	ASP

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Mol	Chain	Res	Type
43	Q	94	LEU
44	R	22	LEU
45	S	25	ARG
45	S	62	ASP
45	S	77	ASP
46	T	32	LEU
46	T	37	ASP
46	T	59	ASN
46	T	60	THR
47	U	82	VAL
48	V	42	LEU
49	W	67	VAL
51	Y	40	SER
53	0	22	THR
53	0	24	VAL
54	1	46	VAL
56	3	61	LEU
58	5	3	LEU
58	5	57	ASN
58	5	122	GLN
59	6	16	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	202	ASN
3	c	40	GLN
4	d	70	GLN
4	d	119	HIS
4	d	135	GLN
6	f	11	HIS
7	g	141	HIS
10	j	70	HIS
11	k	39	ASN
13	m	90	HIS
14	n	49	GLN
15	o	45	HIS
16	p	26	ASN
17	q	30	HIS
18	r	51	GLN
19	s	51	HIS
19	s	56	HIS

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Mol	Chain	Res	Type
26	z	19	HIS
26	z	78	HIS
26	z	135	ASN
26	z	329	GLN
29	C	196	ASN
30	D	49	GLN
30	D	149	ASN
32	F	134	GLN
33	G	103	ASN
33	G	138	GLN
35	I	11	GLN
36	J	40	HIS
43	Q	71	ASN
45	S	61	ASN
47	U	65	GLN
51	Y	41	HIS
53	0	5	ASN
59	6	65	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	242 (15%)	0
22	v	76/78 (97%)	17 (22%)	0
23	w	76/77 (98%)	43 (56%)	0
24	x	10/11 (90%)	1 (10%)	0
25	y	74/77 (96%)	19 (25%)	0
27	A	2894/2903 (99%)	542 (18%)	90 (3%)
28	B	119/120 (99%)	17 (14%)	4 (3%)
All	All	4784/4805 (99%)	881 (18%)	94 (1%)

All (881) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	9	G
1	a	14	U
1	a	22	G
1	a	30	U
1	a	32	A
1	a	39	G
1	a	47	C

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Mol	Chain	Res	Type
1	a	49	U
1	a	51	A
1	a	71	A
1	a	85	U
1	a	86	G
1	a	87	C
1	a	94	G
1	a	95	C
1	a	120	A
1	a	121	U
1	a	130	A
1	a	174	A
1	a	175	C
1	a	181	A
1	a	183	C
1	a	184	G
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	226	G
1	a	246	A
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	281	G
1	a	283	U
1	a	289	G
1	a	306	A
1	a	321	A
1	a	328	C
1	a	345	C
1	a	346	G
1	a	351	G
1	a	352	C
1	a	354	G
1	a	355	C
1	a	367	U
1	a	368	U
1	a	372	C
1	a	373	A

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Mol	Chain	Res	Type
1	a	387	U
1	a	392	C
1	a	398	U
1	a	406	G
1	a	412	A
1	a	413	G
1	a	414	A
1	a	422	C
1	a	423	G
1	a	424	G
1	a	429	U
1	a	430	A
1	a	439	U
1	a	467	U
1	a	468	A
1	a	482	A
1	a	484	G
1	a	485	U
1	a	486	U
1	a	496	A
1	a	497	G
1	a	500	G
1	a	511	C
1	a	527	7MG
1	a	531	U
1	a	532	A
1	a	536	C
1	a	547	A
1	a	559	A
1	a	561	U
1	a	562	U
1	a	564	C
1	a	572	A
1	a	573	A
1	a	574	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	579	A
1	a	597	G
1	a	618	C
1	a	626	G

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Mol	Chain	Res	Type
1	a	633	G
1	a	641	U
1	a	642	A
1	a	654	G
1	a	661	G
1	a	665	A
1	a	671	G
1	a	687	A
1	a	688	G
1	a	701	U
1	a	702	A
1	a	703	G
1	a	724	G
1	a	731	G
1	a	755	G
1	a	777	A
1	a	792	A
1	a	793	U
1	a	794	A
1	a	814	A
1	a	815	A
1	a	817	C
1	a	818	G
1	a	819	A
1	a	820	U
1	a	832	G
1	a	843	U
1	a	844	G
1	a	846	G
1	a	871	U
1	a	874	G
1	a	884	U
1	a	890	G
1	a	902	G
1	a	914	A
1	a	934	C
1	a	935	A
1	a	960	U
1	a	961	U
1	a	966	2MG
1	a	969	A
1	a	975	A

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Mol	Chain	Res	Type
1	a	976	G
1	a	977	A
1	a	979	C
1	a	981	U
1	a	991	U
1	a	992	U
1	a	993	G
1	a	994	A
1	a	1004	A
1	a	1026	G
1	a	1028	C
1	a	1029	U
1	a	1030	U
1	a	1031	C
1	a	1033	G
1	a	1034	G
1	a	1035	A
1	a	1053	G
1	a	1056	U
1	a	1065	U
1	a	1067	A
1	a	1085	U
1	a	1086	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1127	G
1	a	1129	C
1	a	1130	A
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1140	C
1	a	1152	A
1	a	1159	U
1	a	1160	G
1	a	1168	U
1	a	1182	G
1	a	1183	U
1	a	1184	G
1	a	1191	A
1	a	1196	A

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Mol	Chain	Res	Type
1	a	1197	A
1	a	1198	G
1	a	1200	C
1	a	1201	A
1	a	1202	U
1	a	1207	2MG
1	a	1212	U
1	a	1213	A
1	a	1224	U
1	a	1225	A
1	a	1226	C
1	a	1227	A
1	a	1228	C
1	a	1236	A
1	a	1238	A
1	a	1240	U
1	a	1241	G
1	a	1256	A
1	a	1258	G
1	a	1260	G
1	a	1278	G
1	a	1279	G
1	a	1280	A
1	a	1281	C
1	a	1282	C
1	a	1286	U
1	a	1287	A
1	a	1297	G
1	a	1298	U
1	a	1300	G
1	a	1301	U
1	a	1302	C
1	a	1306	A
1	a	1312	G
1	a	1317	C
1	a	1320	C
1	a	1323	G
1	a	1331	G
1	a	1332	A
1	a	1346	A
1	a	1347	G
1	a	1348	U

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Mol	Chain	Res	Type
1	a	1353	G
1	a	1363	A
1	a	1381	U
1	a	1395	C
1	a	1400	C
1	a	1401	G
1	a	1418	A
1	a	1429	A
1	a	1433	A
1	a	1446	A
1	a	1448	C
1	a	1451	U
1	a	1452	C
1	a	1492	A
1	a	1502	A
1	a	1503	A
1	a	1506	U
1	a	1517	G
1	a	1529	G
1	a	1530	G
1	a	1533	C
1	a	1534	A
1	a	1535	C
1	a	1536	C
1	a	1539	C
22	v	7	G
22	v	8	4SU
22	v	9	G
22	v	14	A
22	v	16	C
22	v	17	C
22	v	17(A)	U
22	v	18	G
22	v	19	G
22	v	20	H2U
22	v	21	A
22	v	22	G
22	v	59	A
22	v	60	U
22	v	67	C
22	v	75	C
22	v	76	A

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Mol	Chain	Res	Type
23	w	2	G
23	w	3	C
23	w	5	G
23	w	7	G
23	w	8	4SU
23	w	9	G
23	w	10	G
23	w	13	C
23	w	14	A
23	w	15	G
23	w	16	C
23	w	17	C
23	w	117	U
23	w	18	G
23	w	19	G
23	w	20	H2U
23	w	21	A
23	w	22	G
23	w	25	C
23	w	26	G
23	w	28	C
23	w	32	C
23	w	33	U
23	w	34	C
23	w	37	A
23	w	38	A
23	w	40	C
23	w	43	A
23	w	44	A
23	w	48	C
23	w	49	G
23	w	53	G
23	w	59	A
23	w	60	U
23	w	64	G
23	w	66	C
23	w	67	C
23	w	69	C
23	w	70	G
23	w	71	C
23	w	73	A
23	w	75	C

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Mol	Chain	Res	Type
23	w	76	A
24	x	13	A
25	y	7	A
25	y	8	4SU
25	y	9	A
25	y	10	G
25	y	16	H2U
25	y	17	C
25	y	18	G
25	y	19	G
25	y	20	H2U
25	y	21	A
25	y	22	G
25	y	44	G
25	y	45	U
25	y	46	7MG
25	y	48	C
25	y	59	U
25	y	61	C
25	y	75	C
25	y	76	A
27	A	10	A
27	A	12	U
27	A	23	G
27	A	27	G
27	A	28	A
27	A	34	U
27	A	35	G
27	A	42	A
27	A	46	G
27	A	49	A
27	A	51	G
27	A	52	A
27	A	60	G
27	A	63	A
27	A	71	A
27	A	73	A
27	A	74	A
27	A	75	G
27	A	91	A
27	A	92	U
27	A	103	A

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Mol	Chain	Res	Type
27	A	110	G
27	A	118	A
27	A	119	A
27	A	120	U
27	A	127	A
27	A	138	U
27	A	139	U
27	A	140	C
27	A	141	G
27	A	142	A
27	A	158	U
27	A	162	U
27	A	163	C
27	A	181	A
27	A	196	A
27	A	199	A
27	A	204	A
27	A	205	G
27	A	215	G
27	A	216	A
27	A	218	A
27	A	219	A
27	A	221	A
27	A	222	A
27	A	227	A
27	A	228	C
27	A	242	G
27	A	243	U
27	A	248	G
27	A	249	C
27	A	255	A
27	A	265	A
27	A	266	G
27	A	267	C
27	A	272	A
27	A	276	U
27	A	278	A
27	A	281	C
27	A	294	A
27	A	301	G
27	A	302	C
27	A	311	A

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Mol	Chain	Res	Type
27	A	321	U
27	A	322	A
27	A	323	C
27	A	324	A
27	A	329	G
27	A	330	A
27	A	333	G
27	A	334	C
27	A	346	A
27	A	353	C
27	A	361	G
27	A	362	A
27	A	370	G
27	A	371	A
27	A	372	G
27	A	373	U
27	A	386	G
27	A	387	U
27	A	390	U
27	A	391	A
27	A	404	A
27	A	405	U
27	A	406	G
27	A	411	G
27	A	422	A
27	A	424	G
27	A	442	G
27	A	446	G
27	A	454	A
27	A	455	C
27	A	457	A
27	A	458	G
27	A	459	U
27	A	467	G
27	A	480	A
27	A	481	G
27	A	490	C
27	A	491	G
27	A	504	A
27	A	505	A
27	A	506	G
27	A	508	A

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Mol	Chain	Res	Type
27	A	518	G
27	A	527	C
27	A	529	A
27	A	530	G
27	A	532	A
27	A	533	G
27	A	542	C
27	A	543	G
27	A	545	U
27	A	547	A
27	A	550	C
27	A	555	G
27	A	563	A
27	A	572	A
27	A	573	U
27	A	575	A
27	A	603	A
27	A	614	A
27	A	616	A
27	A	627	A
27	A	637	A
27	A	645	C
27	A	646	U
27	A	654	A
27	A	655	A
27	A	659	G
27	A	668	A
27	A	669	G
27	A	670	A
27	A	677	A
27	A	685	A
27	A	686	U
27	A	687	C
27	A	694	U
27	A	695	G
27	A	717	C
27	A	726	G
27	A	730	A
27	A	740	C
27	A	747	5MC
27	A	748	G
27	A	752	A

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Mol	Chain	Res	Type
27	A	753	A
27	A	765	C
27	A	772	C
27	A	775	G
27	A	776	G
27	A	777	G
27	A	782	A
27	A	784	G
27	A	785	G
27	A	789	A
27	A	791	C
27	A	801	G
27	A	802	A
27	A	805	G
27	A	806	C
27	A	812	C
27	A	819	A
27	A	822	G
27	A	827	U
27	A	828	U
27	A	830	G
27	A	831	G
27	A	845	A
27	A	846	U
27	A	847	U
27	A	858	G
27	A	859	G
27	A	860	U
27	A	878	A
27	A	896	A
27	A	897	C
27	A	907	G
27	A	910	A
27	A	932	U
27	A	941	A
27	A	946	C
27	A	953	G
27	A	958	U
27	A	961	C
27	A	974	G
27	A	975	A
27	A	982	C

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Mol	Chain	Res	Type
27	A	983	A
27	A	985	C
27	A	989	G
27	A	990	A
27	A	995	C
27	A	996	A
27	A	999	U
27	A	1011	G
27	A	1012	U
27	A	1013	C
27	A	1021	A
27	A	1022	G
27	A	1023	U
27	A	1026	G
27	A	1033	U
27	A	1046	A
27	A	1053	C
27	A	1054	A
27	A	1057	A
27	A	1060	U
27	A	1061	U
27	A	1062	G
27	A	1064	C
27	A	1065	U
27	A	1066	U
27	A	1068	G
27	A	1069	A
27	A	1070	A
27	A	1071	G
27	A	1072	C
27	A	1075	C
27	A	1076	C
27	A	1079	C
27	A	1084	A
27	A	1088	A
27	A	1089	A
27	A	1090	A
27	A	1104	C
27	A	1111	A
27	A	1112	G
27	A	1119	U
27	A	1130	U

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Mol	Chain	Res	Type
27	A	1131	G
27	A	1132	U
27	A	1134	A
27	A	1135	C
27	A	1142	A
27	A	1143	A
27	A	1151	A
27	A	1174	U
27	A	1175	A
27	A	1176	U
27	A	1179	G
27	A	1180	U
27	A	1206	G
27	A	1212	G
27	A	1213	A
27	A	1218	G
27	A	1237	A
27	A	1238	G
27	A	1247	A
27	A	1248	G
27	A	1250	G
27	A	1251	C
27	A	1253	A
27	A	1256	G
27	A	1271	G
27	A	1272	A
27	A	1273	U
27	A	1276	A
27	A	1289	C
27	A	1298	C
27	A	1300	G
27	A	1301	A
27	A	1302	A
27	A	1311	G
27	A	1315	C
27	A	1321	A
27	A	1329	U
27	A	1330	C
27	A	1332	G
27	A	1341	G
27	A	1345	C
27	A	1352	U

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Mol	Chain	Res	Type
27	A	1365	A
27	A	1368	G
27	A	1378	A
27	A	1379	U
27	A	1380	G
27	A	1383	A
27	A	1385	A
27	A	1395	A
27	A	1397	U
27	A	1416	G
27	A	1419	A
27	A	1420	A
27	A	1428	C
27	A	1454	C
27	A	1458	U
27	A	1461	C
27	A	1482	G
27	A	1483	G
27	A	1490	A
27	A	1491	G
27	A	1493	C
27	A	1504	A
27	A	1515	A
27	A	1524	G
27	A	1533	C
27	A	1535	A
27	A	1536	C
27	A	1537	G
27	A	1555	G
27	A	1559	U
27	A	1560	G
27	A	1567	G
27	A	1569	A
27	A	1578	U
27	A	1581	G
27	A	1585	C
27	A	1607	C
27	A	1611	C
27	A	1616	A
27	A	1627	G
27	A	1647	U
27	A	1648	U

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Mol	Chain	Res	Type
27	A	1651	G
27	A	1654	A
27	A	1664	A
27	A	1665	A
27	A	1667	G
27	A	1674	G
27	A	1694	C
27	A	1695	G
27	A	1715	G
27	A	1729	U
27	A	1730	C
27	A	1738	G
27	A	1756	G
27	A	1758	U
27	A	1764	C
27	A	1773	A
27	A	1780	A
27	A	1781	U
27	A	1782	U
27	A	1784	A
27	A	1787	A
27	A	1800	C
27	A	1801	A
27	A	1808	A
27	A	1816	C
27	A	1818	U
27	A	1829	A
27	A	1833	C
27	A	1847	G
27	A	1858	A
27	A	1865	U
27	A	1871	A
27	A	1885	A
27	A	1896	G
27	A	1900	A
27	A	1901	A
27	A	1906	G
27	A	1907	G
27	A	1913	A
27	A	1914	C
27	A	1927	A
27	A	1929	G

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Mol	Chain	Res	Type
27	A	1930	G
27	A	1931	U
27	A	1937	A
27	A	1938	A
27	A	1940	U
27	A	1941	C
27	A	1955	U
27	A	1960	A
27	A	1962	5MC
27	A	1963	U
27	A	1967	C
27	A	1970	A
27	A	1971	U
27	A	1972	G
27	A	1981	A
27	A	1991	U
27	A	1992	G
27	A	1993	U
27	A	1997	C
27	A	2022	U
27	A	2023	C
27	A	2031	A
27	A	2033	A
27	A	2043	C
27	A	2049	G
27	A	2052	A
27	A	2055	C
27	A	2056	G
27	A	2060	A
27	A	2061	G
27	A	2062	A
27	A	2069	7MG
27	A	2093	G
27	A	2095	A
27	A	2096	C
27	A	2098	U
27	A	2108	A
27	A	2110	G
27	A	2111	U
27	A	2112	G
27	A	2113	U
27	A	2118	U

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Mol	Chain	Res	Type
27	A	2119	A
27	A	2127	G
27	A	2131	U
27	A	2132	U
27	A	2133	G
27	A	2145	C
27	A	2146	C
27	A	2157	G
27	A	2162	G
27	A	2164	C
27	A	2172	U
27	A	2173	A
27	A	2189	U
27	A	2192	U
27	A	2198	A
27	A	2199	A
27	A	2204	G
27	A	2211	A
27	A	2212	A
27	A	2213	U
27	A	2225	A
27	A	2238	G
27	A	2239	G
27	A	2250	G
27	A	2268	A
27	A	2273	A
27	A	2278	A
27	A	2283	C
27	A	2287	A
27	A	2288	A
27	A	2297	A
27	A	2305	U
27	A	2309	A
27	A	2311	A
27	A	2312	U
27	A	2320	U
27	A	2325	G
27	A	2327	A
27	A	2334	U
27	A	2336	A
27	A	2337	G
27	A	2345	G

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Mol	Chain	Res	Type
27	A	2347	C
27	A	2350	C
27	A	2382	G
27	A	2383	G
27	A	2385	C
27	A	2391	G
27	A	2392	A
27	A	2402	U
27	A	2406	A
27	A	2407	A
27	A	2423	U
27	A	2424	C
27	A	2426	A
27	A	2427	C
27	A	2428	G
27	A	2429	G
27	A	2430	A
27	A	2435	A
27	A	2441	U
27	A	2445	2MG
27	A	2447	G
27	A	2448	A
27	A	2449	H2U
27	A	2459	A
27	A	2468	A
27	A	2476	A
27	A	2478	A
27	A	2484	G
27	A	2494	G
27	A	2497	A
27	A	2498	OMC
27	A	2502	G
27	A	2504	PSU
27	A	2505	G
27	A	2506	U
27	A	2517	C
27	A	2518	A
27	A	2519	U
27	A	2529	G
27	A	2547	A
27	A	2554	U
27	A	2567	G

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Mol	Chain	Res	Type
27	A	2572	A
27	A	2573	C
27	A	2585	U
27	A	2602	A
27	A	2603	G
27	A	2608	G
27	A	2609	U
27	A	2613	U
27	A	2614	A
27	A	2636	C
27	A	2645	G
27	A	2646	C
27	A	2655	G
27	A	2656	U
27	A	2682	A
27	A	2689	U
27	A	2690	U
27	A	2707	U
27	A	2712	C
27	A	2713	U
27	A	2714	G
27	A	2718	G
27	A	2722	G
27	A	2726	A
27	A	2731	G
27	A	2732	G
27	A	2733	A
27	A	2739	U
27	A	2744	G
27	A	2748	A
27	A	2757	A
27	A	2764	A
27	A	2765	A
27	A	2769	U
27	A	2778	A
27	A	2779	U
27	A	2791	G
27	A	2794	C
27	A	2797	U
27	A	2799	A
27	A	2800	A
27	A	2801	G

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Mol	Chain	Res	Type
27	A	2808	G
27	A	2809	A
27	A	2818	U
27	A	2820	A
27	A	2821	A
27	A	2823	A
27	A	2833	U
27	A	2834	G
27	A	2835	A
27	A	2848	G
27	A	2849	U
27	A	2867	G
27	A	2868	A
27	A	2872	A
27	A	2873	A
27	A	2880	C
27	A	2884	U
28	B	4	C
28	B	12	C
28	B	13	G
28	B	24	G
28	B	25	U
28	B	35	C
28	B	40	U
28	B	44	G
28	B	45	A
28	B	56	G
28	B	67	G
28	B	88	C
28	B	89	U
28	B	91	C
28	B	108	A
28	B	109	A
28	B	116	G

All (94) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	A	51	G
27	A	86	G
27	A	204	A
27	A	227	A

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Mol	Chain	Res	Type
27	A	242	G
27	A	265	A
27	A	271	G
27	A	301	G
27	A	311	A
27	A	321	U
27	A	332	A
27	A	345	A
27	A	372	G
27	A	386	G
27	A	390	U
27	A	446	G
27	A	454	A
27	A	458	G
27	A	479	A
27	A	480	A
27	A	490	C
27	A	503	A
27	A	549	G
27	A	571	U
27	A	637	A
27	A	685	A
27	A	686	U
27	A	747	5MC
27	A	752	A
27	A	774	G
27	A	776	G
27	A	800	A
27	A	830	G
27	A	858	G
27	A	859	G
27	A	974	G
27	A	1012	U
27	A	1020	A
27	A	1022	G
27	A	1070	A
27	A	1089	A
27	A	1111	A
27	A	1124	G
27	A	1130	U
27	A	1133	A
27	A	1134	A

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Mol	Chain	Res	Type
27	A	1141	U
27	A	1142	A
27	A	1182	G
27	A	1190	G
27	A	1210	G
27	A	1212	G
27	A	1275	A
27	A	1288	G
27	A	1300	G
27	A	1331	G
27	A	1378	A
27	A	1399	C
27	A	1432	G
27	A	1626	A
27	A	1693	U
27	A	1713	A
27	A	1783	A
27	A	1799	G
27	A	1857	G
27	A	1930	G
27	A	1940	U
27	A	2060	A
27	A	2092	U
27	A	2197	U
27	A	2210	U
27	A	2282	G
27	A	2286	G
27	A	2296	U
27	A	2326	C
27	A	2333	A
27	A	2391	G
27	A	2405	G
27	A	2406	A
27	A	2517	C
27	A	2518	A
27	A	2566	A
27	A	2614	A
27	A	2655	G
27	A	2712	C
27	A	2756	U
27	A	2798	U
27	A	2808	G

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Mol	Chain	Res	Type
27	A	2820	A
27	A	2866	U
28	B	24	G
28	B	56	G
28	B	66	A
28	B	88	C

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

53 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$
27	6MZ	A	1618	27	17,25,26	1.11	1 (5%)	15,36,39	2.55	2 (13%)
27	2MG	A	1835	27	18,26,27	0.91	2 (11%)	21,38,41	2.08	6 (28%)
27	PSU	A	1911	27	15,21,22	1.45	1 (6%)	16,30,33	2.11	4 (25%)
27	3TD	A	1915	27	15,22,23	1.29	3 (20%)	17,32,35	1.57	3 (17%)
27	PSU	A	1917	27	15,21,22	1.43	1 (6%)	16,30,33	2.31	4 (25%)
27	5MU	A	1939	27	13,22,23	0.71	1 (7%)	16,32,35	2.31	2 (12%)
27	5MC	A	1962	27	14,22,23	1.32	1 (7%)	17,32,35	0.99	1 (5%)
27	6MZ	A	2030	27	17,25,26	1.02	1 (5%)	15,36,39	2.87	3 (20%)
27	7MG	A	2069	27	20,26,27	1.17	2 (10%)	23,39,42	3.18	6 (26%)
27	OMG	A	2251	27,22	18,26,27	0.94	2 (11%)	21,38,41	2.10	4 (19%)
27	2MG	A	2445	27	18,26,27	0.88	2 (11%)	21,38,41	2.34	7 (33%)
27	H2U	A	2449	27	17,21,22	0.96	2 (11%)	23,30,33	2.05	5 (21%)
27	PSU	A	2457	27	15,21,22	1.80	1 (6%)	16,30,33	2.20	4 (25%)
27	OMC	A	2498	60,27	15,22,23	0.79	1 (6%)	20,31,34	1.45	1 (5%)
27	2MA	A	2503	60,27	17,25,26	1.58	3 (17%)	18,37,40	2.70	1 (5%)
27	PSU	A	2504	27	15,21,22	1.51	1 (6%)	16,30,33	2.40	4 (25%)
27	OMU	A	2552	27	14,22,23	0.70	0	19,31,34	1.49	1 (5%)
27	PSU	A	2580	27	15,21,22	1.70	2 (13%)	16,30,33	2.21	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	PSU	A	2604	27	15,21,22	1.61	2 (13%)	16,30,33	2.47	4 (25%)
27	PSU	A	2605	27	15,21,22	1.26	2 (13%)	16,30,33	2.39	4 (25%)
27	1MG	A	745	27	17,26,27	1.49	3 (17%)	19,39,42	0.84	0
27	PSU	A	746	60,27	15,21,22	1.37	1 (6%)	16,30,33	2.11	3 (18%)
27	5MC	A	747	27	14,22,23	1.36	1 (7%)	17,32,35	1.36	3 (17%)
27	PSU	A	955	27	15,21,22	1.62	4 (26%)	16,30,33	2.28	4 (25%)
1	2MG	a	1207	1	18,26,27	1.20	2 (11%)	21,38,41	2.22	6 (28%)
1	4OC	a	1402	1	15,23,24	0.59	0	21,32,35	1.66	3 (14%)
1	5MC	a	1407	1	14,22,23	1.26	1 (7%)	17,32,35	1.00	1 (5%)
1	UR3	a	1498	1	13,22,23	0.69	0	18,32,35	0.75	0
1	2MG	a	1516	1	18,26,27	1.21	2 (11%)	21,38,41	2.28	6 (28%)
1	MA6	a	1518	1	18,26,27	1.12	1 (5%)	15,38,41	2.43	2 (13%)
1	MA6	a	1519	1	18,26,27	0.91	1 (5%)	15,38,41	2.67	4 (26%)
1	PSU	a	516	1,60	15,21,22	1.50	3 (20%)	16,30,33	2.07	3 (18%)
1	7MG	a	527	1	20,26,27	1.26	2 (10%)	23,39,42	3.12	6 (26%)
1	2MG	a	966	1	18,26,27	1.14	2 (11%)	21,38,41	2.22	6 (28%)
1	5MC	a	967	1	14,22,23	1.20	1 (7%)	17,32,35	1.08	1 (5%)
22	H2U	v	20	22	17,21,22	0.95	2 (11%)	23,30,33	1.91	4 (17%)
22	5MU	v	54	22	13,22,23	0.56	0	16,32,35	2.39	2 (12%)
22	PSU	v	55	22	15,21,22	1.18	1 (6%)	16,30,33	2.25	4 (25%)
22	FME	v	77	-	8,9,10	0.93	1 (12%)	5,9,11	1.60	1 (20%)
22	4SU	v	8	22	12,21,22	0.69	0	15,30,33	1.07	1 (6%)
23	H2U	w	20	23	17,21,22	1.37	4 (23%)	23,30,33	3.36	5 (21%)
23	5MU	w	54	23	13,22,23	0.61	0	16,32,35	2.69	3 (18%)
23	PSU	w	55	23	15,21,22	1.54	3 (20%)	16,30,33	2.28	4 (25%)
23	4SU	w	8	23	12,21,22	0.78	1 (8%)	15,30,33	1.09	1 (6%)
25	H2U	y	16	25	17,21,22	1.00	2 (11%)	23,30,33	1.81	2 (8%)
25	H2U	y	20	25	17,21,22	0.98	2 (11%)	23,30,33	2.36	4 (17%)
25	PSU	y	32	25	15,21,22	1.38	1 (6%)	16,30,33	2.24	4 (25%)
25	MIA	y	37	25	22,31,32	1.75	2 (9%)	26,44,47	1.67	6 (23%)
25	PSU	y	39	25	15,21,22	1.45	1 (6%)	16,30,33	2.39	4 (25%)
25	7MG	y	46	25	20,26,27	1.51	2 (10%)	23,39,42	3.22	5 (21%)
25	5MU	y	54	25	13,22,23	0.66	1 (7%)	16,32,35	2.30	2 (12%)
25	PSU	y	55	25	15,21,22	1.31	1 (6%)	16,30,33	2.32	4 (25%)
25	4SU	y	8	25	12,21,22	0.78	0	15,30,33	0.86	1 (6%)

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
27	6MZ	A	1618	27	-	0/5/27/28	0/3/3/3
27	2MG	A	1835	27	-	0/5/27/28	0/3/3/3
27	PSU	A	1911	27	-	0/7/25/26	0/2/2/2
27	3TD	A	1915	27	-	0/7/25/26	0/2/2/2
27	PSU	A	1917	27	-	0/7/25/26	0/2/2/2
27	5MU	A	1939	27	-	0/3/25/26	0/2/2/2
27	5MC	A	1962	27	-	0/3/25/26	0/2/2/2
27	6MZ	A	2030	27	-	0/5/27/28	0/3/3/3
27	7MG	A	2069	27	-	0/7/37/38	0/3/3/3
27	OMG	A	2251	27,22	-	0/5/27/28	0/3/3/3
27	2MG	A	2445	27	-	0/5/27/28	0/3/3/3
27	H2U	A	2449	27	-	0/7/38/39	0/2/2/2
27	PSU	A	2457	27	-	0/7/25/26	0/2/2/2
27	OMC	A	2498	60,27	-	0/5/27/28	0/2/2/2
27	2MA	A	2503	60,27	-	0/3/25/26	0/3/3/3
27	PSU	A	2504	27	-	0/7/25/26	0/2/2/2
27	OMU	A	2552	27	-	0/5/27/28	0/2/2/2
27	PSU	A	2580	27	-	0/7/25/26	0/2/2/2
27	PSU	A	2604	27	-	0/7/25/26	0/2/2/2
27	PSU	A	2605	27	-	0/7/25/26	0/2/2/2
27	1MG	A	745	27	-	0/3/25/26	0/3/3/3
27	PSU	A	746	60,27	-	0/7/25/26	0/2/2/2
27	5MC	A	747	27	-	0/3/25/26	0/2/2/2
27	PSU	A	955	27	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	a	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	a	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	a	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	a	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	a	516	1,60	-	0/7/25/26	0/2/2/2
1	7MG	a	527	1	-	0/7/37/38	0/3/3/3
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3
1	5MC	a	967	1	-	0/3/25/26	0/2/2/2
22	H2U	v	20	22	-	0/7/38/39	0/2/2/2
22	5MU	v	54	22	-	0/3/25/26	0/2/2/2
22	PSU	v	55	22	-	0/7/25/26	0/2/2/2
22	FME	v	77	-	-	1/6/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	4SU	v	8	22	-	0/3/25/26	0/2/2/2
23	H2U	w	20	23	-	0/7/38/39	0/2/2/2
23	5MU	w	54	23	-	0/3/25/26	0/2/2/2
23	PSU	w	55	23	-	0/7/25/26	0/2/2/2
23	4SU	w	8	23	-	0/3/25/26	0/2/2/2
25	H2U	y	16	25	-	0/7/38/39	0/2/2/2
25	H2U	y	20	25	-	0/7/38/39	0/2/2/2
25	PSU	y	32	25	-	0/7/25/26	0/2/2/2
25	MIA	y	37	25	-	0/11/33/34	0/3/3/3
25	PSU	y	39	25	-	0/7/25/26	0/2/2/2
25	7MG	y	46	25	-	0/7/37/38	0/3/3/3
25	5MU	y	54	25	-	0/3/25/26	0/2/2/2
25	PSU	y	55	25	-	0/7/25/26	0/2/2/2
25	4SU	y	8	25	-	0/3/25/26	0/2/2/2

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	37	MIA	C2-S10	-7.15	1.69	1.75
27	A	2457	PSU	C5-C1'	-6.03	1.47	1.52
27	A	2580	PSU	C5-C1'	-5.43	1.47	1.52
27	A	2604	PSU	C5-C1'	-5.18	1.47	1.52
27	A	955	PSU	C5-C1'	-4.88	1.48	1.52
27	A	2504	PSU	C5-C1'	-4.79	1.48	1.52
25	y	39	PSU	C5-C1'	-4.66	1.48	1.52
27	A	1911	PSU	C5-C1'	-4.50	1.48	1.52
23	w	55	PSU	C5-C1'	-4.46	1.48	1.52
27	A	1917	PSU	C5-C1'	-4.40	1.48	1.52
1	a	516	PSU	C5-C1'	-4.39	1.48	1.52
25	y	32	PSU	C5-C1'	-4.30	1.48	1.52
27	A	746	PSU	C5-C1'	-4.12	1.48	1.52
25	y	55	PSU	C5-C1'	-3.94	1.48	1.52
27	A	2605	PSU	C5-C1'	-3.39	1.49	1.52
23	w	20	H2U	C2-N3	-3.26	1.31	1.38
22	v	55	PSU	C5-C1'	-3.25	1.49	1.52
23	w	20	H2U	C2-N1	-2.54	1.31	1.35
23	w	20	H2U	C4-N3	-2.54	1.33	1.37
23	w	55	PSU	C2-N1	-2.52	1.32	1.38
27	A	2605	PSU	C2-N3	-2.43	1.33	1.38
22	v	20	H2U	C4-N3	-2.41	1.33	1.37
27	A	2604	PSU	C2-N3	-2.41	1.33	1.38
27	A	2449	H2U	C4-N3	-2.40	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	20	H2U	C2-N3	-2.37	1.33	1.38
27	A	2449	H2U	C2-N3	-2.36	1.33	1.38
25	y	20	H2U	C4-N3	-2.35	1.33	1.37
25	y	16	H2U	C4-N3	-2.34	1.33	1.37
1	a	516	PSU	O4'-C1'	-2.34	1.40	1.44
25	y	16	H2U	C2-N3	-2.33	1.33	1.38
22	v	20	H2U	C2-N3	-2.33	1.33	1.38
1	a	516	PSU	C2-N3	-2.24	1.33	1.38
27	A	955	PSU	C2-N3	-2.24	1.33	1.38
27	A	2498	OMC	C6-N1	-2.19	1.33	1.35
27	A	1939	5MU	C2-N3	-2.19	1.33	1.38
27	A	955	PSU	C2-N1	-2.17	1.33	1.38
27	A	2580	PSU	O4'-C1'	-2.17	1.41	1.44
25	y	54	5MU	C2-N3	-2.14	1.33	1.38
27	A	1915	3TD	C6-C5	-2.12	1.35	1.38
23	w	8	4SU	C2-N3	-2.11	1.33	1.38
23	w	20	H2U	C6-N1	-2.09	1.44	1.47
27	A	1915	3TD	C4-N3	-2.09	1.35	1.38
23	w	55	PSU	O4'-C1'	-2.07	1.41	1.44
27	A	955	PSU	O4'-C1'	-2.04	1.41	1.44
27	A	2445	2MG	C6-C5	2.04	1.45	1.41
27	A	745	1MG	C6-N1	2.17	1.41	1.38
22	v	77	FME	CA-N	2.21	1.49	1.46
27	A	2445	2MG	C5-C4	2.24	1.45	1.40
27	A	1835	2MG	C5-C4	2.51	1.46	1.40
27	A	2251	OMG	C6-C5	2.59	1.46	1.41
27	A	2251	OMG	C5-C4	2.64	1.46	1.40
27	A	1835	2MG	C6-C5	2.65	1.46	1.41
27	A	1915	3TD	C10-N3	2.67	1.53	1.47
27	A	2069	7MG	C5-C4	2.69	1.46	1.39
1	a	1519	MA6	C5-C4	2.77	1.46	1.40
27	A	2503	2MA	C5-C4	2.79	1.46	1.40
25	y	37	MIA	C5-C4	2.87	1.47	1.40
1	a	527	7MG	C5-C4	2.97	1.47	1.39
1	a	966	2MG	C5-C4	3.01	1.47	1.40
27	A	745	1MG	C5-C4	3.17	1.47	1.40
1	a	1207	2MG	C5-C4	3.22	1.47	1.40
1	a	1516	2MG	C5-C4	3.26	1.47	1.40
25	y	46	7MG	C5-C4	3.26	1.47	1.39
1	a	1516	2MG	C6-C5	3.39	1.48	1.41
1	a	1518	MA6	C5-C4	3.43	1.48	1.40
1	a	1207	2MG	C6-C5	3.50	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	2069	7MG	C6-C5	3.51	1.46	1.41
1	a	966	2MG	C6-C5	3.53	1.48	1.41
27	A	2030	6MZ	C5-C4	3.57	1.48	1.40
1	a	527	7MG	C6-C5	3.69	1.46	1.41
27	A	2503	2MA	C6-N6	3.85	1.36	1.29
27	A	1618	6MZ	C5-C4	3.91	1.49	1.40
27	A	2503	2MA	C6-C5	4.01	1.48	1.40
1	a	967	5MC	C5-C4	4.27	1.48	1.41
27	A	747	5MC	C5-C4	4.32	1.48	1.41
1	a	1407	5MC	C5-C4	4.37	1.48	1.41
27	A	745	1MG	C6-C5	4.41	1.49	1.40
27	A	1962	5MC	C5-C4	4.44	1.48	1.41
25	y	46	7MG	C6-C5	4.96	1.48	1.41

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	w	20	H2U	C5-C6-N1	-11.65	98.00	110.76
25	y	46	7MG	C5-C4-N3	-8.74	117.84	126.74
25	y	20	H2U	C4-N3-C2	-8.68	117.91	125.77
1	a	1519	MA6	N3-C2-N1	-8.18	122.45	128.87
1	a	527	7MG	C5-C4-N3	-7.86	118.73	126.74
23	w	20	H2U	C4-N3-C2	-7.84	118.66	125.77
27	A	2069	7MG	C5-C4-N3	-7.75	118.85	126.74
23	w	54	5MU	C5-C4-N3	-7.51	119.05	125.35
1	a	1518	MA6	N3-C2-N1	-7.27	123.16	128.87
27	A	1939	5MU	C5-C4-N3	-6.88	119.57	125.35
22	v	54	5MU	C5-C4-N3	-6.82	119.62	125.35
25	y	54	5MU	C5-C4-N3	-6.72	119.70	125.35
27	A	1618	6MZ	N3-C2-N1	-6.30	123.92	128.87
27	A	2030	6MZ	N3-C2-N1	-6.00	124.16	128.87
27	A	2449	H2U	C5-C6-N1	-5.94	104.26	110.76
25	y	16	H2U	C5-C6-N1	-5.72	104.49	110.76
27	A	2604	PSU	C5-C1'-C2'	-5.69	105.78	115.44
27	A	2069	7MG	C5-C6-N1	-5.64	115.00	123.39
25	y	37	MIA	C11-S10-C2	-5.52	98.42	102.31
27	A	2449	H2U	C4-N3-C2	-5.48	120.80	125.77
1	a	527	7MG	C5-C6-N1	-5.36	115.42	123.39
22	v	20	H2U	C4-N3-C2	-5.19	121.06	125.77
22	v	20	H2U	C5-C6-N1	-5.07	105.21	110.76
27	A	2251	OMG	C5-C6-N1	-5.06	116.90	123.52
25	y	46	7MG	C5-C6-N1	-5.01	115.94	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	955	PSU	C5-C1'-C2'	-4.90	107.12	115.44
25	y	16	H2U	C4-N3-C2	-4.73	121.48	125.77
25	y	20	H2U	C5-C6-N1	-4.73	105.58	110.76
25	y	39	PSU	C5-C1'-C2'	-4.61	107.61	115.44
27	A	2445	2MG	C5-C6-N1	-4.47	117.68	123.52
27	A	2604	PSU	C5-C6-N1	-4.38	118.28	124.38
1	a	1516	2MG	C5-C6-N1	-4.37	117.81	123.52
27	A	2580	PSU	C5-C6-N1	-4.28	118.41	124.38
23	w	20	H2U	N3-C2-N1	-4.28	112.68	116.64
27	A	2605	PSU	C5-C1'-C2'	-4.24	108.23	115.44
27	A	2504	PSU	C5-C1'-C2'	-4.19	108.32	115.44
27	A	2457	PSU	C5-C6-N1	-4.17	118.57	124.38
1	a	1207	2MG	C5-C6-N1	-4.10	118.16	123.52
25	y	39	PSU	C5-C6-N1	-4.06	118.72	124.38
27	A	1915	3TD	C5-C1'-C2'	-4.01	108.62	115.44
27	A	746	PSU	C5-C6-N1	-3.98	118.83	124.38
25	y	55	PSU	C5-C1'-C2'	-3.98	108.68	115.44
1	a	516	PSU	C5-C6-N1	-3.98	118.83	124.38
23	w	55	PSU	C5-C6-N1	-3.92	118.91	124.38
27	A	955	PSU	C5-C6-N1	-3.89	118.95	124.38
1	a	966	2MG	C5-C6-N1	-3.88	118.44	123.52
27	A	1911	PSU	C5-C6-N1	-3.87	118.98	124.38
25	y	32	PSU	C5-C6-N1	-3.68	119.25	124.38
25	y	32	PSU	C5-C1'-C2'	-3.66	109.21	115.44
27	A	1835	2MG	C5-C6-N1	-3.58	118.84	123.52
27	A	2504	PSU	C5-C6-N1	-3.55	119.43	124.38
25	y	55	PSU	C5-C6-N1	-3.53	119.46	124.38
27	A	2445	2MG	C6-C5-C4	-3.53	116.83	120.86
1	a	1402	4OC	CM4-N4-C4	-3.44	119.97	122.87
27	A	1917	PSU	C5-C6-N1	-3.41	119.62	124.38
27	A	2457	PSU	C5-C1'-C2'	-3.41	109.65	115.44
27	A	1917	PSU	C5-C1'-C2'	-3.35	109.74	115.44
22	v	8	4SU	C5-C4-N3	-3.34	120.02	123.56
22	v	55	PSU	C5-C6-N1	-3.31	119.76	124.38
27	A	746	PSU	C5-C1'-C2'	-3.29	109.84	115.44
27	A	2251	OMG	N3-C2-N1	-3.26	123.11	127.56
23	w	55	PSU	C5-C1'-C2'	-3.24	109.93	115.44
27	A	2605	PSU	C5-C6-N1	-3.21	119.90	124.38
25	y	37	MIA	C5-C6-N1	-3.19	117.34	120.58
1	a	1516	2MG	C6-C5-C4	-3.15	117.26	120.86
27	A	1915	3TD	C5-C6-N1	-3.12	120.03	124.38
23	w	8	4SU	C5-C4-N3	-3.11	120.27	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	966	2MG	C6-C5-C4	-3.08	117.34	120.86
27	A	1835	2MG	CM2-N2-C2	-3.06	119.60	123.03
22	v	77	FME	O1-CN-N	-3.04	120.15	124.80
27	A	2030	6MZ	C1'-N9-C4	-3.01	123.44	126.81
27	A	2445	2MG	N3-C2-N1	-2.97	121.74	126.19
25	y	46	7MG	C8-N9-C1'	-2.91	113.70	122.43
27	A	1835	2MG	C6-C5-C4	-2.90	117.54	120.86
22	v	55	PSU	C5-C1'-C2'	-2.90	110.51	115.44
27	A	2445	2MG	CM2-N2-C2	-2.89	119.79	123.03
1	a	1207	2MG	C6-C5-C4	-2.87	117.58	120.86
1	a	966	2MG	CM2-N2-C2	-2.87	119.81	123.03
1	a	1516	2MG	CM2-N2-C2	-2.84	119.83	123.03
1	a	527	7MG	C8-N9-C1'	-2.83	113.94	122.43
1	a	1519	MA6	C10-N6-C9	-2.79	106.86	115.96
27	A	2251	OMG	C6-C5-C4	-2.75	117.71	120.86
1	a	1207	2MG	CM2-N2-C2	-2.66	120.04	123.03
1	a	1519	MA6	C1'-N9-C4	-2.63	123.87	126.81
27	A	2069	7MG	C8-N9-C1'	-2.62	114.55	122.43
27	A	1911	PSU	C5-C1'-C2'	-2.59	111.04	115.44
25	y	8	4SU	C5-C4-N3	-2.55	120.86	123.56
1	a	1516	2MG	N3-C2-N1	-2.44	122.54	126.19
25	y	37	MIA	C12-N6-C6	-2.30	120.80	123.46
1	a	966	2MG	N3-C2-N1	-2.27	122.79	126.19
1	a	1207	2MG	N3-C2-N1	-2.20	122.90	126.19
27	A	2069	7MG	C5-C4-N9	-2.12	102.81	106.25
27	A	1835	2MG	N3-C2-N1	-2.05	123.12	126.19
25	y	20	H2U	N3-C2-N1	-2.04	114.76	116.64
25	y	37	MIA	N3-C2-N1	-2.02	123.11	126.84
1	a	527	7MG	C5-C4-N9	-2.01	103.00	106.25
27	A	2445	2MG	N2-C2-N3	2.02	119.29	116.94
27	A	747	5MC	C4'-O4'-C1'	2.07	111.84	109.64
27	A	2449	H2U	N3-C2-N1	2.17	118.65	116.64
25	y	37	MIA	N6-C6-N1	2.21	121.18	118.55
27	A	2449	H2U	O4-C4-N3	2.22	123.94	120.46
27	A	955	PSU	O4'-C1'-C2'	2.26	107.13	104.69
27	A	747	5MC	O4'-C1'-N1	2.29	112.46	108.10
22	v	20	H2U	N3-C2-N1	2.38	118.85	116.64
27	A	2605	PSU	O4'-C1'-C2'	2.46	107.35	104.69
27	A	2457	PSU	O4'-C1'-C2'	2.47	107.36	104.69
25	y	55	PSU	O4'-C1'-C2'	2.49	107.39	104.69
27	A	2504	PSU	O4'-C1'-C2'	2.50	107.39	104.69
27	A	2604	PSU	O4'-C1'-C2'	2.51	107.41	104.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1407	5MC	N4-C4-N3	2.67	120.84	116.92
27	A	1917	PSU	O4'-C1'-C2'	2.70	107.61	104.69
27	A	1911	PSU	O4'-C1'-C2'	2.73	107.64	104.69
25	y	39	PSU	O4'-C1'-C2'	2.74	107.65	104.69
27	A	1915	3TD	O4'-C1'-C2'	2.78	107.69	104.69
23	w	54	5MU	C5M-C5-C4	2.78	123.05	119.97
25	y	32	PSU	O4'-C1'-C2'	2.81	107.73	104.69
27	A	747	5MC	N4-C4-N3	2.83	121.06	116.92
22	v	55	PSU	O4'-C1'-C2'	2.83	107.75	104.69
27	A	1962	5MC	N4-C4-N3	2.92	121.20	116.92
27	A	2580	PSU	O4'-C1'-C2'	2.95	107.88	104.69
27	A	2449	H2U	C6-N1-C2	3.27	127.21	122.16
1	a	967	5MC	N4-C4-N3	3.27	121.72	116.92
25	y	37	MIA	C2-N1-C6	3.29	122.18	113.13
22	v	20	H2U	C6-N1-C2	3.32	127.30	122.16
1	a	516	PSU	O4'-C1'-C2'	3.41	108.38	104.69
23	w	55	PSU	O4'-C1'-C2'	3.41	108.38	104.69
23	w	20	H2U	C1'-N1-C2	3.49	123.08	118.19
1	a	1402	4OC	C2-N3-C4	3.62	120.03	115.43
25	y	20	H2U	C1'-N1-C2	4.20	124.08	118.19
27	A	1835	2MG	C6-N1-C2	4.36	121.48	115.24
27	A	2445	2MG	C2-N3-C4	4.42	119.84	114.99
1	a	966	2MG	C6-N1-C2	4.67	121.94	115.24
1	a	1519	MA6	C2-N1-C6	4.68	122.67	111.64
23	w	20	H2U	C5-C4-N3	4.70	121.59	116.62
1	a	1207	2MG	C6-N1-C2	4.78	122.09	115.24
1	a	1518	MA6	C2-N1-C6	4.81	122.97	111.64
1	a	1402	4OC	C6-C5-C4	4.99	119.38	117.42
1	a	1516	2MG	C6-N1-C2	5.18	122.66	115.24
27	A	2552	OMU	C4-N3-C2	5.32	119.81	114.21
1	a	1516	2MG	C2-N3-C4	5.37	120.88	114.99
27	A	1835	2MG	C2-N3-C4	5.44	120.95	114.99
27	A	2498	OMC	C6-C5-C4	5.44	119.57	117.44
1	a	516	PSU	C4-N3-C2	5.65	119.87	115.16
27	A	1939	5MU	C4-N3-C2	5.73	119.94	115.16
25	y	46	7MG	C6-N1-C2	5.77	122.64	115.88
27	A	2445	2MG	C6-N1-C2	5.83	123.58	115.24
1	a	1207	2MG	C2-N3-C4	5.84	121.39	114.99
27	A	955	PSU	C4-N3-C2	5.86	120.05	115.16
25	y	54	5MU	C4-N3-C2	5.91	120.09	115.16
27	A	2604	PSU	C4-N3-C2	5.92	120.10	115.16
1	a	966	2MG	C2-N3-C4	5.94	121.50	114.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	2457	PSU	C4-N3-C2	6.07	120.22	115.16
27	A	1911	PSU	C4-N3-C2	6.11	120.26	115.16
1	a	527	7MG	C6-N1-C2	6.20	123.14	115.88
22	v	54	5MU	C4-N3-C2	6.21	120.34	115.16
27	A	746	PSU	C4-N3-C2	6.37	120.47	115.16
23	w	55	PSU	C4-N3-C2	6.37	120.47	115.16
27	A	2251	OMG	C6-N1-C2	6.37	123.35	115.88
25	y	39	PSU	C4-N3-C2	6.38	120.48	115.16
25	y	32	PSU	C4-N3-C2	6.42	120.51	115.16
27	A	2069	7MG	C6-N1-C2	6.57	123.58	115.88
27	A	2580	PSU	C4-N3-C2	6.84	120.86	115.16
25	y	55	PSU	C4-N3-C2	6.85	120.87	115.16
22	v	55	PSU	C4-N3-C2	6.86	120.88	115.16
23	w	54	5MU	C4-N3-C2	6.89	120.90	115.16
27	A	1917	PSU	C4-N3-C2	7.06	121.05	115.16
27	A	2504	PSU	C4-N3-C2	7.14	121.11	115.16
27	A	2605	PSU	C4-N3-C2	7.16	121.13	115.16
27	A	1618	6MZ	C2-N1-C6	7.35	121.75	116.47
1	a	527	7MG	N3-C4-N9	8.72	138.26	126.98
27	A	2030	6MZ	C2-N1-C6	8.73	122.75	116.47
27	A	2069	7MG	N3-C4-N9	8.77	138.32	126.98
25	y	46	7MG	N3-C4-N9	9.05	138.69	126.98
27	A	2503	2MA	C2-N3-C4	10.94	120.56	115.29

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	v	77	FME	O1-CN-N-CA

There are no ring outliers.

10 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	1917	PSU	1	0
27	A	1962	5MC	1	0
27	A	2030	6MZ	1	0
27	A	2445	2MG	1	0
27	A	2449	H2U	1	0
27	A	2498	OMC	1	0
27	A	2552	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	745	1MG	1	0
27	A	747	5MC	1	0
27	A	955	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 341 ligands modelled in this entry, 339 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	KIR	z	401	-	54,59,59	0.63	1 (1%)	52,84,84	1.97	12 (23%)
63	GDP	z	402	60	24,30,30	1.12	2 (8%)	26,47,47	1.93	5 (19%)

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	KIR	z	401	-	-	0/54/98/98	0/3/3/3
63	GDP	z	402	60	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	z	401	KIR	C2-C3	2.28	1.49	1.44
63	z	402	GDP	C5-C4	2.91	1.47	1.40
63	z	402	GDP	C6-C5	3.61	1.48	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	z	401	KIR	C23-C22-C21	-7.49	118.50	127.69
62	z	401	KIR	C15-C14-C13	-4.53	107.29	114.52
62	z	401	KIR	C5-C4-C3	-4.42	117.84	120.63
63	z	402	GDP	C5-C6-N1	-4.04	118.25	123.52
62	z	401	KIR	C39-C38-C37	-3.91	118.60	125.83
63	z	402	GDP	N3-C2-N1	-3.61	122.65	127.56
63	z	402	GDP	C6-C5-C4	-3.44	116.93	120.86
62	z	401	KIR	C36-C37-C38	-2.94	119.39	125.07
62	z	401	KIR	C10-C9-C8	-2.51	119.90	127.02
62	z	401	KIR	O27-C27-C28	-2.16	118.76	121.97
62	z	401	KIR	C12-C11-C10	-2.05	120.29	124.96
63	z	402	GDP	O3B-PB-O1B	2.06	117.34	110.63
62	z	401	KIR	C15-C16-C17	2.10	105.45	102.46
62	z	401	KIR	C6-N1-C2	2.23	122.25	116.54
62	z	401	KIR	C44-C21-C20	2.89	120.70	115.61
62	z	401	KIR	C16-C15-C14	3.62	106.04	101.63
63	z	402	GDP	C6-N1-C2	5.50	122.33	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.