



wwPDB EM Map/Model Validation Report ⓘ

Aug 10, 2016 – 09:11 PM EDT

PDB ID : 5KCR
EMDB ID: : EMD-8237
Title : Cryo-EM structure of the Escherichia coli 70S ribosome in complex with antibiotic Avilamycin C, mRNA and P-site tRNA at 3.6Å resolution
Authors : Arenz, S.; Juette, M.F.; Graf, M.; Nguyen, F.; Huter, P.; Polikanov, Y.S.; Blanchard, S.C.; Wilson, D.N.
Deposited on : 2016-06-06
Resolution : 3.60 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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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

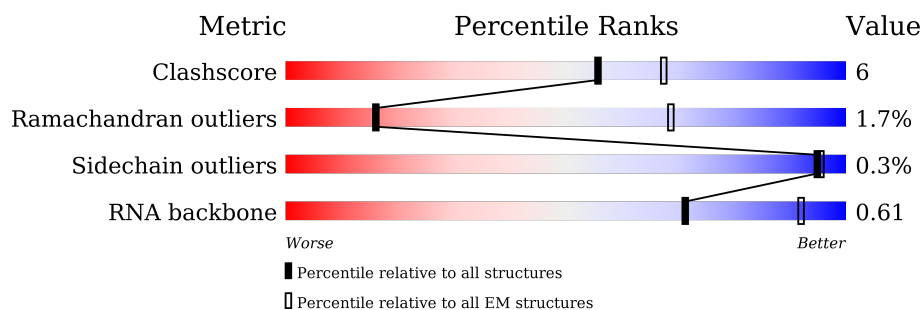
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




























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

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1A	2904	75% 22% .
2	1B	120	83% 16% .
3	1D	273	71% 28% .
4	1E	209	78% 22%
5	1F	201	79% 21%
6	1G	179	73% 25% ..
7	1H	177	77% 22% ..
8	1I	149	78% 22%



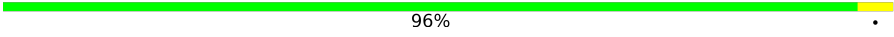



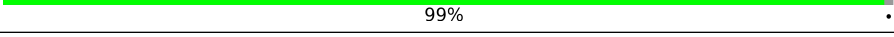
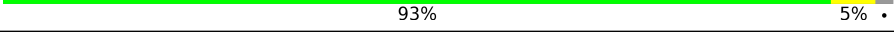
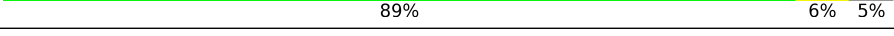

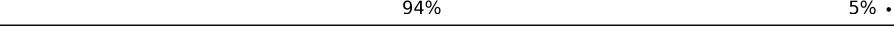
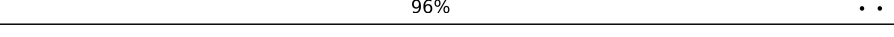

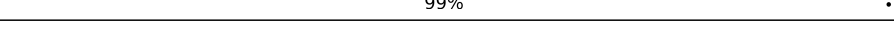
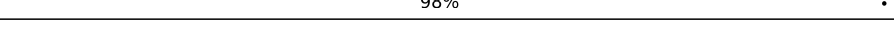

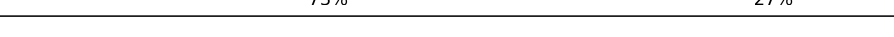

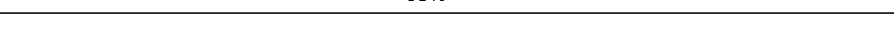



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Mol	Chain	Length	Quality of chain
9	1J	165	
10	1K	142	
11	1N	142	
12	1O	123	
13	1P	144	
14	1Q	136	
15	1R	127	
16	1S	117	
17	1T	115	
18	1U	118	
19	1V	103	
20	1W	110	
21	1X	100	
22	1Y	104	
23	1Z	94	
24	10	85	
25	11	78	
26	12	63	
27	13	59	
28	15	57	
29	16	55	
30	17	46	
31	18	65	
32	19	38	
33	1a	1539	

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Mol	Chain	Length	Quality of chain
34	1b	241	
35	1c	233	
36	1d	206	
37	1e	167	
38	1f	135	
39	1g	179	
40	1h	130	
41	1i	130	
42	1j	103	
43	1k	129	
44	1l	124	
45	1m	118	
46	1n	101	
47	1o	89	
48	1p	82	
49	1q	84	
50	1r	75	
51	1s	92	
52	1t	87	
53	1u	71	
54	1v	9	
55	1x	87	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 145689 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	2897	Total	C	N	O	P	8	0
			62361	27826	11476	20155	2904		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	1847	G	A	conflict	GB 802133627

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1D	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1E	209	Total	C	N	O	S	1	0
			1576	986	290	296	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1F	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1G	177	Total	C	N	O	S	0	0
			1404	896	246	256	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1H	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1I	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1J	135	Total	C	N	O	S	0	0
			1023	648	179	192	4		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1K	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1N	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1O	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1P	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1Q	136	Total	C	N	O	S	2	0
			1090	696	211	177	6		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1R	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1S	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1T	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	1U	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1V	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1W	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1X	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1Y	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1Z	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	10	76	Total	C	N	O	S	1	0
			591	365	121	104	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	11	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	12	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	13	58	Total	C	N	O	S	2	0
			463	290	90	81	2		

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	15	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	16	51	Total	C	N	O	S	0	0
			414	266	76	72			

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	17	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	18	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	19	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 33 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1a	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1e	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1k	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1n	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1o	88	Total	C	N	O	S	0	0
			710	437	143	129	1		

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	1r	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1u	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

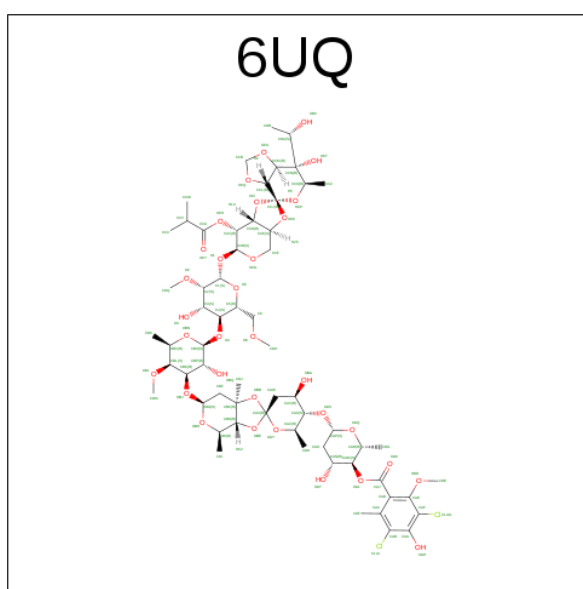
- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1v	3	Total	C	N	O	P	0	0
			60	27	7	23	3		

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	1x	87	Total	C	N	O	P	0	0
			1861	829	333	612	87		

- Molecule 56 is (2R,3S,4R,6S)-4-hydroxy-6-{{[(2R,3aR,4R,4'R,5'S,6S,6'R,7aR)-4'-hydroxy-6-{{[(2S,3R,4R,5S,6R)-3-hydroxy-2-{{[(2R,3S,4S,5S,6S)-4-hydroxy-6-{{(2R,3aS,3a'R,6S,6'R,7R,7'R,7aR,7a'R)-7'-hydroxy-7'-[(1S)-1-hydroxyethyl]-6'-methyl-7-[(2-methylpropanoyl)oxy]octahydro-4H-2,4'-spirobi[[1,3]dioxolo[4,5-c]pyran]-6-yl}oxy)-5-methoxy-2-(methoxymethyl)tetrahydro-2H-pyran-3-yl}oxy}-5-methoxy-6-methyltetrahydro-2H-pyran-4-yl}oxy}-4,6',7a-trimethyloctahydro-4H-spiro[1,3-dioxolo[4,5-c]pyran-2,2'-pyran]-5'-yl}oxy}-2-methyltetrahydro-2H-pyran-3-yl 3,5-dichloro-4-hydroxy-2-methoxy-6-methylbenzoate (non-preferred name) (three-letter code: 6UQ) (formula: C₆₁H₉₀Cl₂O₃₂).



Mol	Chain	Residues	Atoms				AltConf
56	1A	1	Total	C	Cl	O	0
			95	61	2	32	

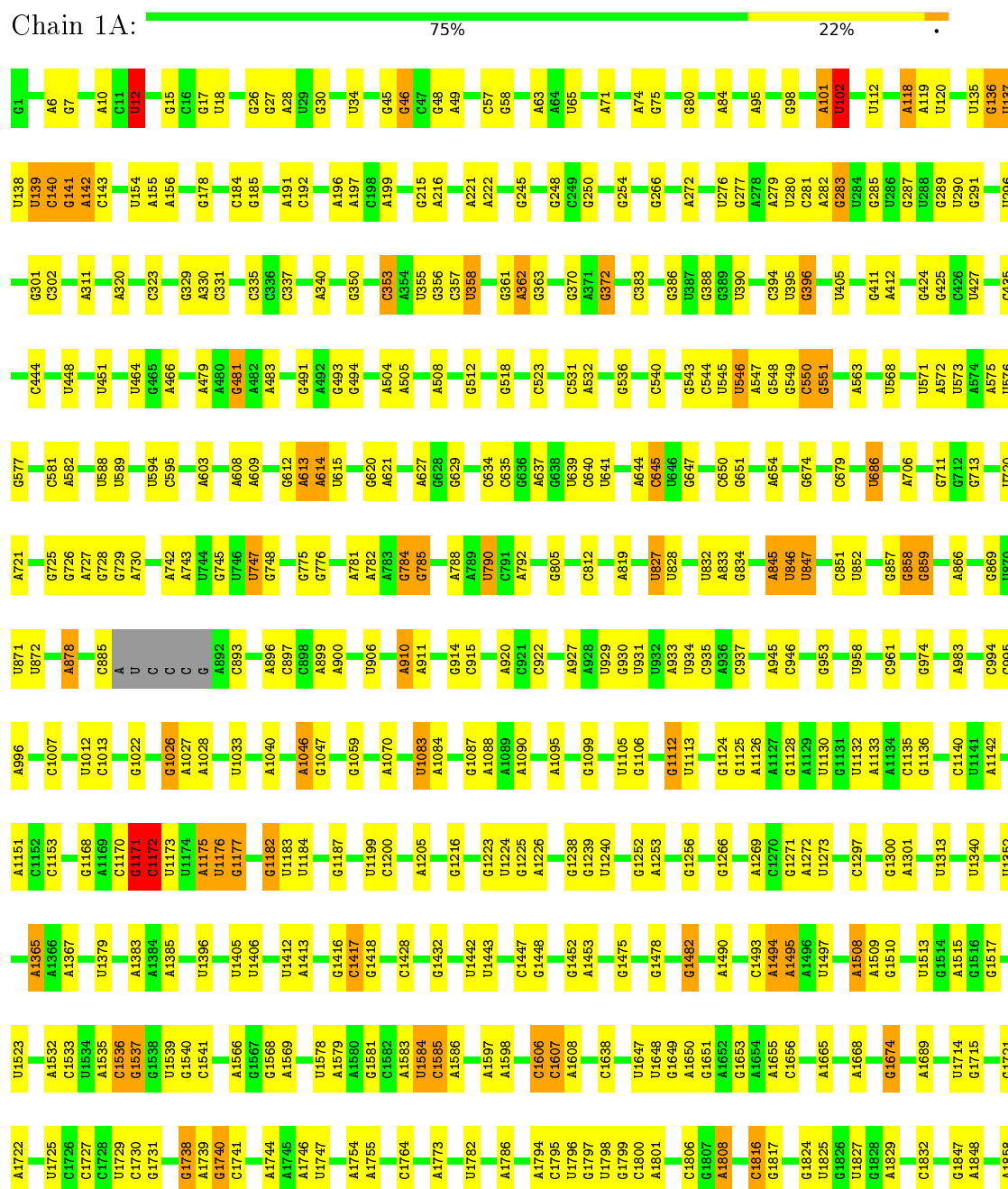
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

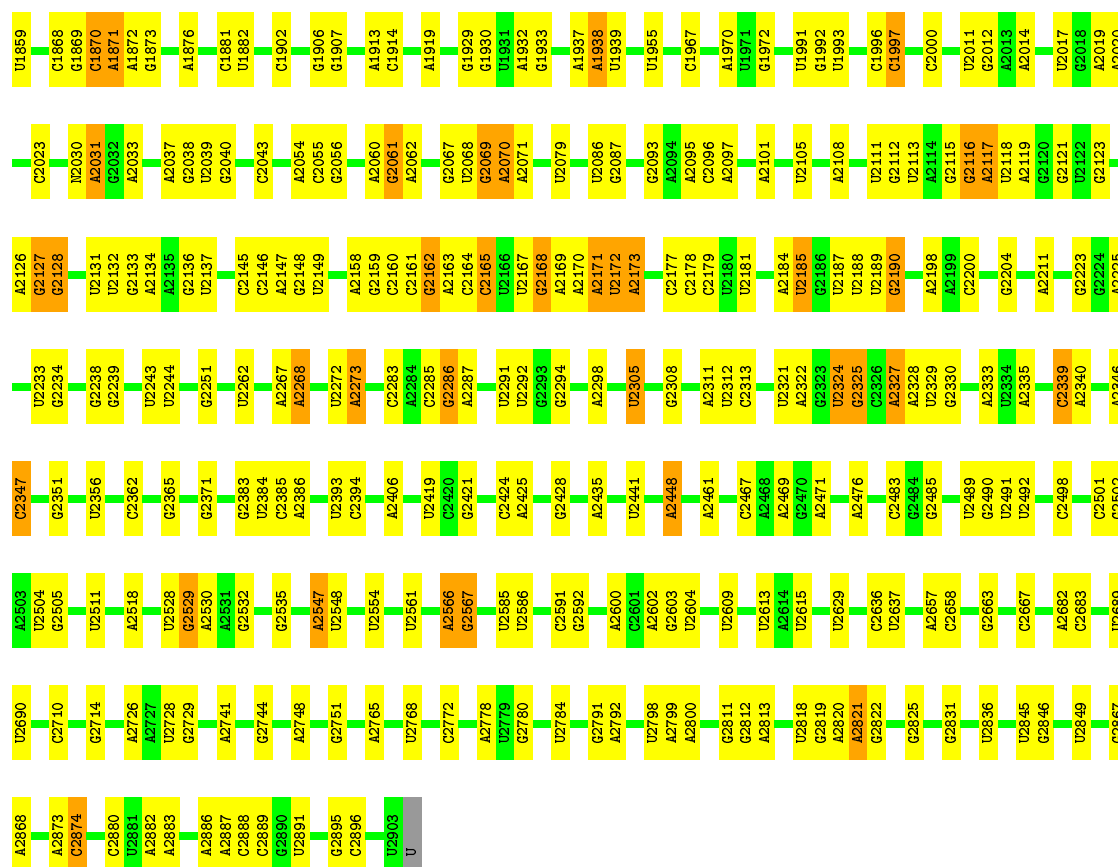
Mol	Chain	Residues	Atoms		AltConf
57	19	1	Total	Zn	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

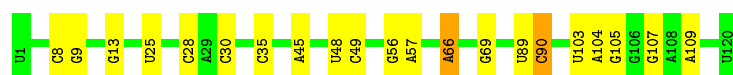
- Molecule 1: 23S Ribosomal RNA





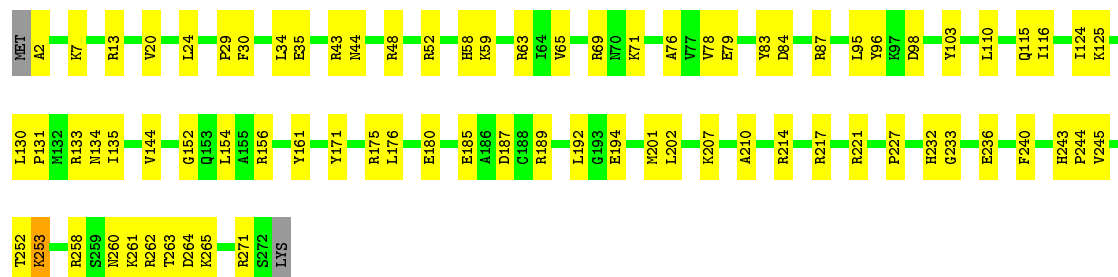
- Molecule 2: 5S Ribosomal RNA

Chain 1B: 83% 16%



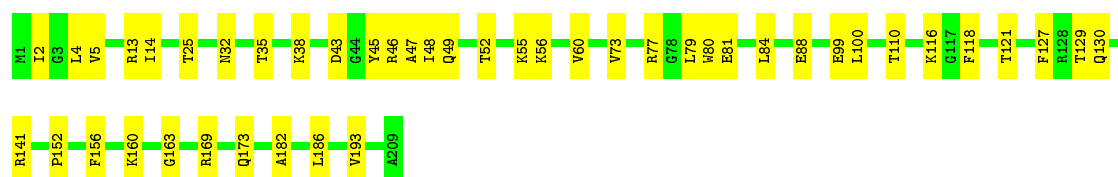
- Molecule 3: 50S ribosomal protein L2

Chain 1D: 71% 28%

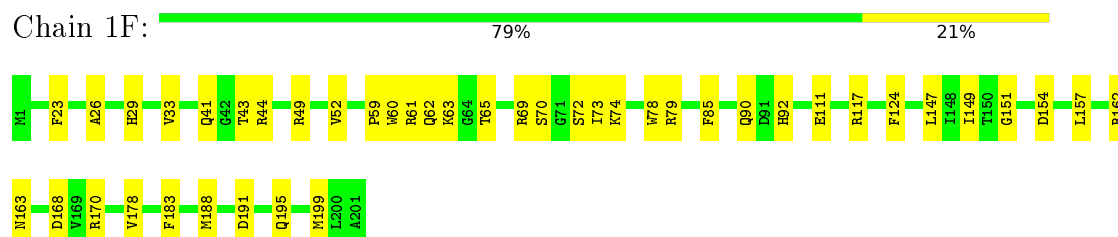


- Molecule 4: 50S ribosomal protein L3

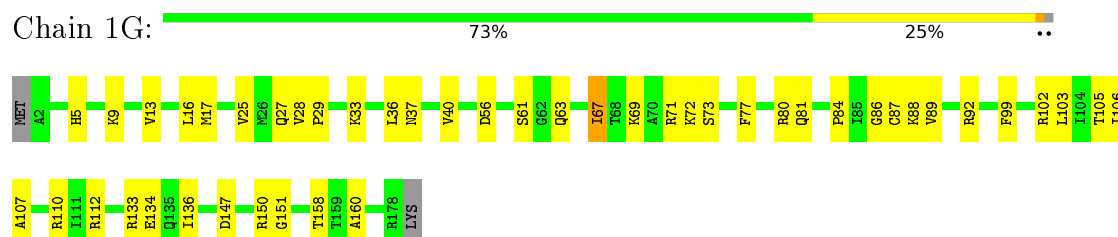
Chain 1E: 78% 22%



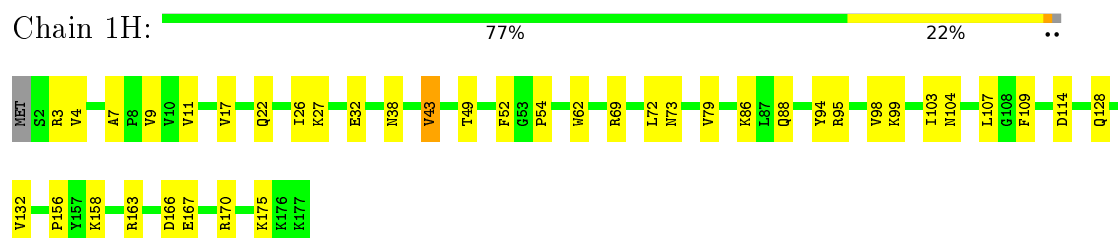
- Molecule 5: 50S ribosomal protein L4



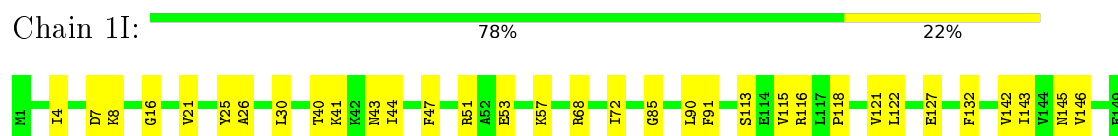
- Molecule 6: 50S ribosomal protein L5



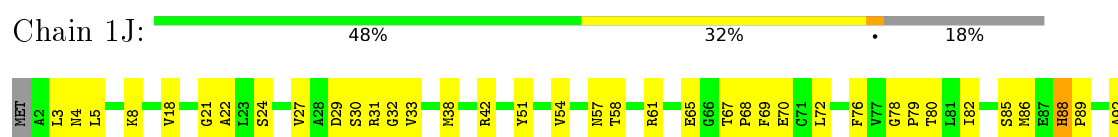
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L10





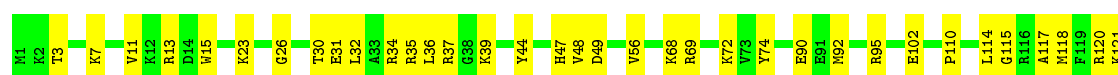
- Molecule 10: 50S ribosomal protein L11

Chain 1K: 63% 30% 6%



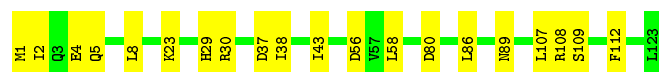
- Molecule 11: 50S ribosomal protein L13

Chain 1N: 71% 27%



- Molecule 12: 50S ribosomal protein L14

Chain 1O: 84% 16%



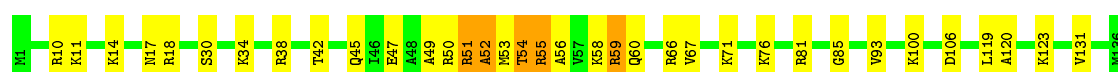
- Molecule 13: 50S ribosomal protein L15

Chain 1P: 81% 19%



- Molecule 14: 50S ribosomal protein L16

Chain 1Q: 74% 22%



- Molecule 15: 50S ribosomal protein L17

Chain 1R: 72% 26%





- Molecule 16: 50S ribosomal protein L18

Chain 1S: 78% 22%



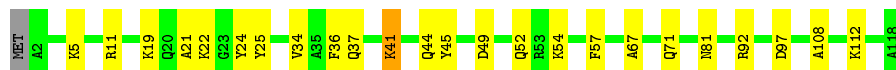
- Molecule 17: 50S ribosomal protein L19

Chain 1T: 70% 29% .



- Molecule 18: 50S ribosomal protein L20

Chain 1U: 79% 19% ..



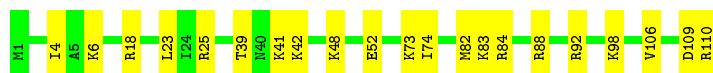
- Molecule 19: 50S ribosomal protein L21

Chain 1V: 83% 16% .



- Molecule 20: 50S ribosomal protein L22

Chain 1W: 81% 19%



- Molecule 21: 50S ribosomal protein L23

Chain 1X: 73% 20% 7%

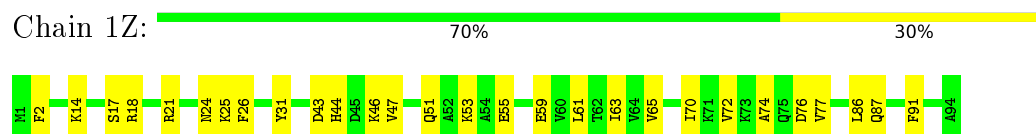


- Molecule 22: 50S ribosomal protein L24

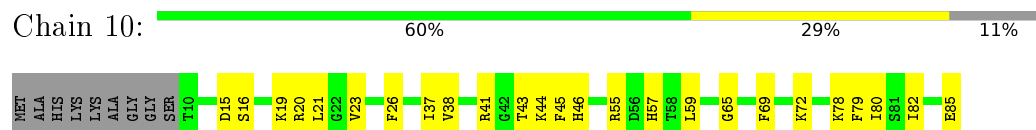
Chain 1Y: 79% 19% .



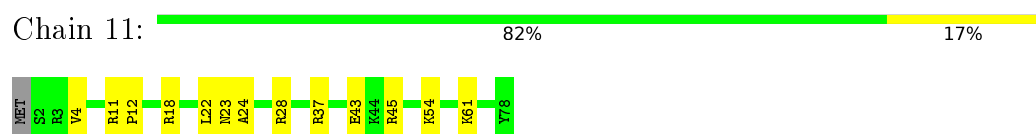
- Molecule 23: 50S ribosomal protein L25



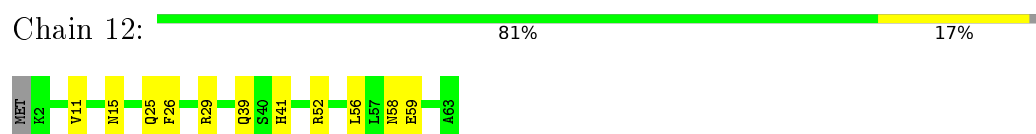
- Molecule 24: 50S ribosomal protein L27



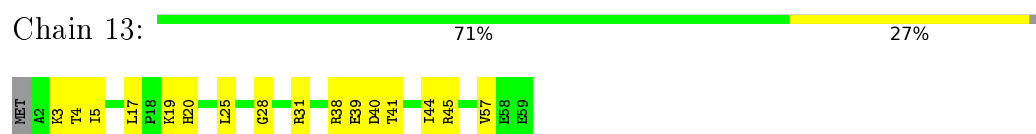
- Molecule 25: 50S ribosomal protein L28



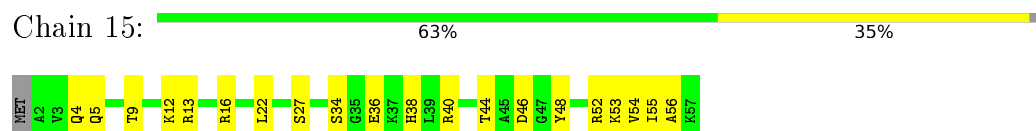
- Molecule 26: 50S ribosomal protein L29



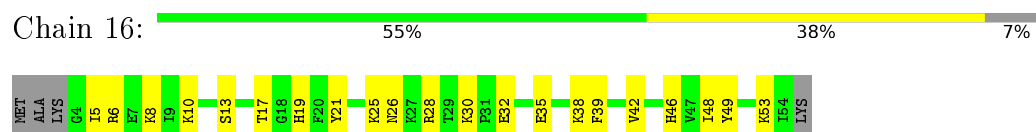
- Molecule 27: 50S ribosomal protein L30



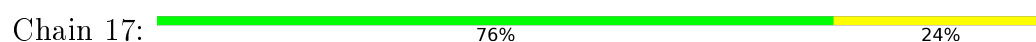
- Molecule 28: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L34





- Molecule 31: 50S ribosomal protein L35

Chain 18: 65% 34%



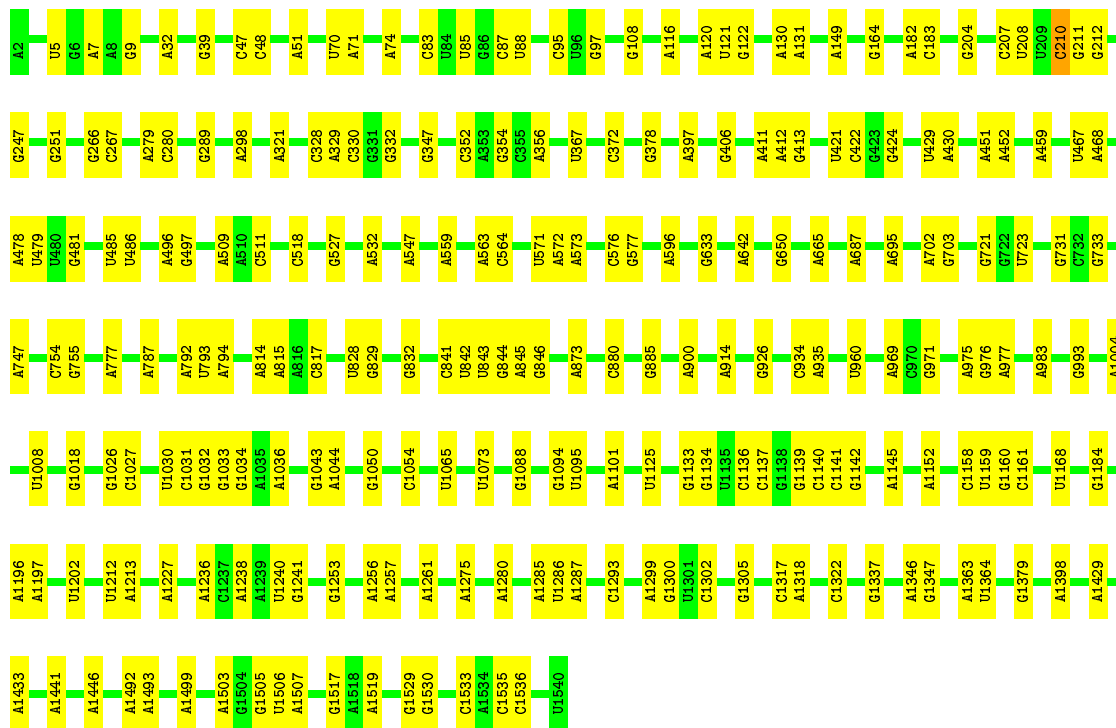
- Molecule 32: 50S ribosomal protein L36

Chain 19: 84% 16%



- Molecule 33: 16S Ribosomal RNA

Chain 1a: 85% 15%

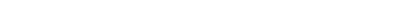


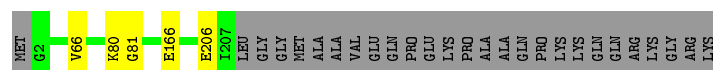
- Molecule 34: 30S ribosomal protein S2

Chain 1b: 87% 10%



- Molecule 35: 30S ribosomal protein S3

Chain 1c:  86% • 12%



- Molecule 36: 30S ribosomal protein S4

Chain 1d: 96% .



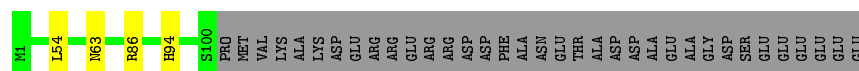
- Molecule 37: 30S ribosomal protein S5

Chain 1e:  86% 10%



- Molecule 38: 30S ribosomal protein S6

Chain 1f:  71% 0 26%



- Molecule 39: 30S ribosomal protein S7

Chain 1g: 84% 16%



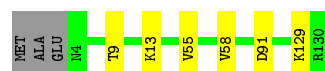
- Molecule 40: 30S ribosomal protein S8

Chain 1h:  99%



- Molecule 41: 30S ribosomal protein S9

Chain 1i:  93% 5% .

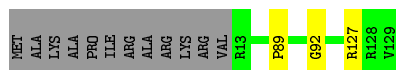


- Molecule 42: 30S ribosomal protein S10

Chain 1j:  89% 6% 5%



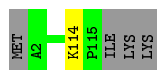
- Molecule 43: 30S ribosomal protein S11



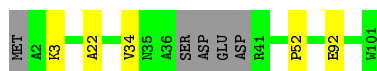
- Molecule 44: 30S ribosomal protein S12



- Molecule 45: 30S ribosomal protein S13



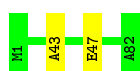
- Molecule 46: 30S ribosomal protein S14



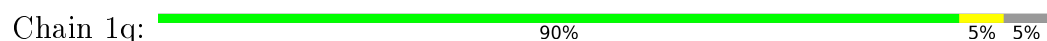
- Molecule 47: 30S ribosomal protein S15



- Molecule 48: 30S ribosomal protein S16



- Molecule 49: 30S ribosomal protein S17




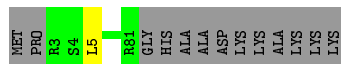
- Molecule 50: 30S ribosomal protein S18

Chain 1r:  73% 27%



- Molecule 51: 30S ribosomal protein S19

Chain 1s:  85% 14%



- Molecule 52: 30S ribosomal protein S20

Chain 1t:  95% ..



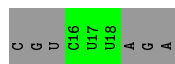
- Molecule 53: 30S ribosomal protein S21

Chain 1u:  65% 7% 28%




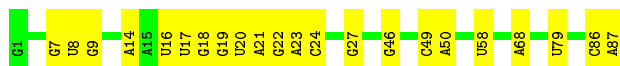
- Molecule 54: mRNA

Chain 1v:  33% 67%



- Molecule 55: P-site tRNA

Chain 1x:  75% 25%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	61651	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, ZN, OMG, OMU, G7M, H2U, 2MA, MEQ, 2MG, 5MC, 6UQ, 6MZ, 1MG, 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	1A	0.27	0/69297	0.81	26/108106 (0.0%)
10	1K	0.29	0/993	0.53	0/1341
11	1N	0.38	0/1152	0.54	0/1551
12	1O	0.30	0/955	0.51	0/1279
13	1P	0.28	0/1062	0.52	0/1413
14	1Q	0.29	0/1115	0.50	0/1488
15	1R	0.27	0/1006	0.49	0/1345
16	1S	0.28	0/910	0.48	0/1219
17	1T	0.29	0/929	0.53	0/1242
18	1U	0.29	0/960	0.43	0/1278
19	1V	0.27	0/829	0.51	0/1107
2	1B	0.23	0/2872	0.77	0/4478
20	1W	0.25	0/864	0.47	0/1156
21	1X	0.27	0/744	0.50	0/994
22	1Y	0.30	0/787	0.52	0/1051
23	1Z	0.28	0/766	0.48	0/1025
24	10	0.29	0/598	0.49	0/790
25	11	0.26	0/635	0.47	0/848
26	12	0.24	0/502	0.41	0/667
27	13	0.27	0/467	0.42	0/623
28	15	0.30	0/450	0.51	0/599
29	16	0.38	0/421	0.55	0/561
3	1D	0.29	0/2121	0.54	0/2852
30	17	0.32	0/380	0.59	0/498
31	18	0.27	0/513	0.49	0/676
32	19	0.26	0/303	0.48	0/397
33	1a	0.25	0/36966	0.73	12/57666 (0.0%)
34	1b	0.25	0/1735	0.42	0/2338
35	1c	0.24	0/1651	0.40	0/2225
36	1d	0.25	0/1665	0.43	0/2227
37	1e	0.26	0/1118	0.46	0/1504
38	1f	0.25	0/835	0.43	0/1128

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	1g	0.24	0/1195	0.39	0/1602
4	1E	0.28	0/1576	0.50	0/2119
40	1h	0.26	0/989	0.45	0/1326
41	1i	0.25	0/1034	0.47	0/1375
42	1j	0.25	0/796	0.49	0/1077
43	1k	0.25	0/893	0.43	0/1205
44	1l	0.27	0/969	0.48	0/1300
45	1m	0.23	0/892	0.43	0/1193
46	1n	0.23	0/785	0.41	0/1043
47	1o	0.24	0/718	0.41	0/959
48	1p	0.24	0/659	0.43	0/884
49	1q	0.26	0/657	0.47	0/881
5	1F	0.27	0/1571	0.47	0/2113
50	1r	0.24	0/462	0.40	0/621
51	1s	0.25	0/652	0.41	0/877
52	1t	0.23	0/671	0.38	0/888
53	1u	0.26	0/430	0.48	0/570
54	1v	0.33	0/65	0.91	0/98
55	1x	0.25	0/2080	0.76	0/3242
6	1G	0.30	0/1428	0.51	0/1919
7	1H	0.28	0/1343	0.49	0/1816
8	1I	0.29	0/1121	0.51	0/1515
9	1J	0.31	0/1037	0.59	0/1400
All	All	0.27	0/157624	0.72	38/235695 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1N	0	1
27	13	0	1
All	All	0	2

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	1a	1158	C	N1-C2-O2	8.80	124.18	118.90
1	1A	1584	U	C2-N1-C1'	8.32	127.68	117.70
1	1A	1584	U	N1-C2-O2	8.29	128.61	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	1a	1158	C	C2-N1-C1'	8.29	127.91	118.80
33	1a	210	C	N1-C2-O2	8.01	123.70	118.90
33	1a	1158	C	N3-C2-O2	-7.21	116.86	121.90
33	1a	210	C	C2-N1-C1'	7.04	126.55	118.80
1	1A	102	U	C2-N1-C1'	7.03	126.13	117.70
1	1A	1584	U	N3-C2-O2	-7.00	117.30	122.20
1	1A	1313	U	C2-N1-C1'	6.91	125.99	117.70
1	1A	102	U	N1-C2-O2	6.76	127.53	122.80
33	1a	754	C	C2-N1-C1'	6.63	126.09	118.80
33	1a	1433	A	O5'-P-OP1	-6.53	99.83	105.70
1	1A	1171	G	C4-N9-C1'	6.46	134.90	126.50
1	1A	2602	A	C2-N3-C4	6.37	113.78	110.60
1	1A	140	C	N1-C2-O2	6.11	122.56	118.90
1	1A	140	C	N3-C2-O2	-5.95	117.74	121.90
1	1A	613	A	O4'-C1'-N9	5.90	112.92	108.20
1	1A	12	U	N1-C2-O2	5.88	126.92	122.80
33	1a	1158	C	C6-N1-C1'	-5.85	113.78	120.80
1	1A	1584	U	C6-N1-C1'	-5.74	113.17	121.20
33	1a	210	C	N3-C2-O2	-5.72	117.90	121.90
1	1A	12	U	N3-C2-O2	-5.66	118.24	122.20
1	1A	2535	G	C2-N3-C4	5.54	114.67	111.90
1	1A	140	C	C6-N1-C2	-5.54	118.09	120.30
1	1A	512	G	O4'-C1'-N9	5.53	112.62	108.20
1	1A	102	U	N3-C2-O2	-5.46	118.38	122.20
1	1A	2602	A	C5-C6-N1	5.39	120.40	117.70
1	1A	1171	G	C8-N9-C1'	-5.27	120.15	127.00
1	1A	101	A	O4'-C1'-N9	5.25	112.40	108.20
33	1a	210	C	C6-N1-C1'	-5.21	114.55	120.80
1	1A	1172	C	C5-C6-N1	5.20	123.60	121.00
1	1A	1508	A	O4'-C1'-N9	5.17	112.33	108.20
33	1a	754	C	N1-C2-O2	5.10	121.96	118.90
1	1A	2471	A	C2-N3-C4	5.07	113.14	110.60
33	1a	1158	C	C6-N1-C2	-5.06	118.28	120.30
1	1A	2535	G	N3-C4-C5	-5.04	126.08	128.60
1	1A	2501	C	C2-N1-C1'	-5.00	113.30	118.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	13	3[B]	LYS	Peptide
11	1N	135	GLN	Peptide

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	1A	62361	0	31379	418	0
2	1B	2569	0	1301	18	0
3	1D	2082	0	2154	63	0
4	1E	1576	0	1627	44	0
5	1F	1552	0	1619	40	0
6	1G	1404	0	1433	34	0
7	1H	1323	0	1371	32	0
8	1I	1110	0	1148	20	0
9	1J	1023	0	1050	51	0
10	1K	979	0	1028	32	0
11	1N	1129	0	1162	41	0
12	1O	946	0	1023	12	0
13	1P	1053	0	1129	24	0
14	1Q	1090	0	1183	31	0
15	1R	993	0	1034	28	0
16	1S	900	0	935	24	0
17	1T	917	0	962	39	0
18	1U	947	0	1019	24	0
19	1V	816	0	839	21	0
20	1W	857	0	922	15	0
21	1X	738	0	807	15	0
22	1Y	779	0	831	18	0
23	1Z	753	0	780	23	0
24	10	591	0	606	25	0
25	11	625	0	652	13	0
26	12	501	0	531	10	0
27	13	463	0	504	12	0
28	15	444	0	458	23	0
29	16	414	0	442	21	0
30	17	377	0	418	15	0
31	18	504	0	572	22	0
32	19	302	0	340	5	0
33	1a	33015	0	16617	0	0
34	1b	1704	0	1732	0	0
35	1c	1624	0	1696	0	0
36	1d	1643	0	1707	0	0
37	1e	1105	0	1148	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	1f	817	0	808	0	0
39	1g	1181	0	1238	0	0
40	1h	979	0	1031	0	0
41	1i	1022	0	1070	0	0
42	1j	786	0	828	0	0
43	1k	877	0	887	0	0
44	1l	955	0	1016	0	0
45	1m	883	0	941	0	0
46	1n	774	0	824	0	0
47	1o	710	0	728	0	0
48	1p	649	0	666	0	0
49	1q	648	0	691	0	0
50	1r	455	0	478	0	0
51	1s	637	0	665	0	0
52	1t	665	0	714	0	0
53	1u	425	0	449	0	0
54	1v	60	0	32	0	0
55	1x	1861	0	938	0	0
56	1A	95	0	0	2	0
57	19	1	0	0	0	0
All	All	145689	0	98163	965	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 6.

All (965) 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)
9:1J:22:ALA:HB2	9:1J:86:MET:SD	1.64	1.35
1:1A:1847:G:N2	1:1A:1848:A:H62	1.52	1.07
9:1J:22:ALA:CB	9:1J:86:MET:SD	2.48	1.02
1:1A:1847:G:H21	1:1A:1848:A:N6	1.63	0.97
1:1A:1799:G:OP1	3:1D:258:ARG:NH1	2.03	0.91
3:1D:65:VAL:HG21	3:1D:87:ARG:HH22	1.33	0.91
13:1P:62:PRO:HB2	31:18:30:ARG:HH11	1.36	0.88
1:1A:1083:U:H4'	9:1J:42:ARG:HH12	1.38	0.88
1:1A:827:U:H2'	1:1A:2068:U:C2	2.09	0.88
18:1U:44:GLN:HE21	19:1V:77:PHE:HB3	1.40	0.86
1:1A:2116:G:O6	1:1A:2171:A:N6	2.08	0.85
6:1G:33:LYS:HD3	6:1G:92:ARG:HH11	1.41	0.85
1:1A:674:G:H1'	5:1F:69:ARG:HE	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2683:C:OP1	17:1T:51:ARG:NH2	2.11	0.84
1:1A:2285:C:OP2	29:16:6:ARG:NH2	2.12	0.83
1:1A:1124:G:N3	32:19:37:GLN:NE2	2.28	0.82
8:1I:16:GLY:O	8:1I:51:ARG:NH2	2.12	0.81
9:1J:31:ARG:HH21	9:1J:79:PRO:HD3	1.43	0.80
1:1A:2419:U:OP1	31:18:41:LYS:NZ	2.13	0.80
5:1F:90:GLN:HE21	5:1F:92:HIS:HE1	1.30	0.80
11:1N:74:TYR:HD2	11:1N:92:MET:HG3	1.48	0.79
21:1X:38:ALA:O	21:1X:81:LYS:NZ	2.16	0.79
17:1T:63:LYS:NZ	17:1T:65:SER:OG	2.16	0.78
6:1G:158:THR:HG22	6:1G:160:ALA:H	1.48	0.78
16:1S:36:TYR:HD1	16:1S:52:SER:HB2	1.48	0.78
11:1N:31:GLU:HG2	11:1N:142:ILE:HG13	1.65	0.78
1:1A:320:A:N3	5:1F:163:ASN:ND2	2.31	0.78
30:17:34:ARG:HG3	30:17:39:ARG:HG3	1.66	0.77
1:1A:1266:G:N2	1:1A:1269:A:OP2	12.96	0.77
1:1A:2469:A:H1'	14:1Q:55:ARG:HH21	1.49	0.77
1:1A:958:U:OP2	14:1Q:14:LYS:NZ	2.17	0.77
1:1A:2822:G:O6	15:1R:2:ARG:NH1	2.17	0.77
1:1A:466:A:OP1	30:17:34:ARG:NH2	2.18	0.77
5:1F:117:ARG:NH2	5:1F:183:PHE:O	2.19	0.76
24:10:23:VAL:HB	24:10:26:PHE:HE1	1.51	0.75
1:1A:2845:U:O3'	17:1T:53:ARG:NH1	2.19	0.75
1:1A:2384:U:OP2	24:10:55:ARG:NH2	2.19	0.75
9:1J:92:ALA:HB1	9:1J:96:PHE:HE2	1.52	0.75
29:16:21:TYR:OH	29:16:39:PHE:O	2.03	0.75
23:1Z:21:ARG:NH2	23:1Z:87:GLN:O	2.20	0.75
5:1F:147:LEU:HB2	5:1F:183:PHE:HD2	1.51	0.74
1:1A:1112:G:O3'	7:1H:3:ARG:NH1	2.20	0.74
1:1A:1266:G:OP2	28:15:16:ARG:NH1	2.15	0.74
1:1A:1847:G:H21	1:1A:1848:A:H62	0.77	0.73
28:15:46:ASP:O	28:15:53:LYS:NZ	2.21	0.73
1:1A:2483:C:N3	14:1Q:123:LYS:NZ	2.37	0.73
1:1A:1655:A:H1'	4:1E:118:PHE:CE2	2.24	0.73
16:1S:48:LEU:O	16:1S:85:LYS:NZ	2.21	0.72
3:1D:152:GLY:O	3:1D:156:ARG:NH2	2.20	0.72
1:1A:827:U:H2'	1:1A:2068:U:O2	1.90	0.72
21:1X:8:LEU:O	26:12:29:ARG:NH1	2.23	0.71
22:1Y:28:VAL:HG12	22:1Y:34:VAL:HG12	1.71	0.71
29:16:6:ARG:HH21	29:16:26:ASN:HB2	1.54	0.71
1:1A:2561:U:O2'	12:1O:23:LYS:HG3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:124:ILE:HG23	3:1D:192:LEU:HD21	1.73	0.71
3:1D:171:TYR:HD1	3:1D:185:GLU:HA	1.56	0.71
1:1A:1508:A:O2'	1:1A:1509:A:O4'	2.08	0.71
7:1H:7:ALA:O	7:1H:69:ARG:NE	2.24	0.71
11:1N:31:GLU:HG2	11:1N:142:ILE:CG1	2.21	0.71
26:12:11:VAL:O	26:12:15:ASN:ND2	2.24	0.71
1:1A:568:U:H1'	1:1A:2030:6MZ:H9C1	1.72	0.71
8:1I:40:THR:OG1	8:1I:43:ASN:ND2	2.22	0.71
1:1A:728:G:H4'	3:1D:13:ARG:HD3	1.73	0.70
6:1G:112:ARG:NH1	6:1G:134:GLU:OE2	2.23	0.70
1:1A:920:A:OP1	27:13:19:LYS:NZ	2.24	0.70
9:1J:21:GLY:C	9:1J:86:MET:HE3	2.11	0.70
14:1Q:67:VAL:HG12	14:1Q:100:LYS:HD3	1.73	0.70
1:1A:1816:C:N4	3:1D:35:GLU:OE1	2.21	0.70
1:1A:1655:A:H1'	4:1E:118:PHE:HE2	1.56	0.70
28:15:13:ARG:HG3	28:15:16:ARG:HH12	1.57	0.70
1:1A:2305:U:C2	6:1G:151:GLY:HA3	2.27	0.70
1:1A:2223:G:O3'	3:1D:265:LYS:NZ	2.25	0.70
2:1B:57:A:H4'	6:1G:27:GLN:HE21	1.57	0.69
20:1W:4:ILE:HG12	20:1W:106:VAL:HG22	1.73	0.69
9:1J:22:ALA:CA	9:1J:86:MET:SD	2.80	0.69
13:1P:62:PRO:HB2	31:18:30:ARG:NH1	2.07	0.69
1:1A:2069:G7M:O2'	1:1A:2070:A:O5'	2.11	0.69
11:1N:23:LYS:NZ	11:1N:142:ILE:OXT	2.24	0.69
11:1N:118:MET:HA	11:1N:121:LYS:NZ	2.06	0.69
1:1A:301:G:OP2	22:1Y:82:ARG:NH1	2.25	0.69
23:1Z:26:PHE:HE2	23:1Z:44:HIS:HA	1.58	0.69
3:1D:78:VAL:HG21	3:1D:110:LEU:HD21	1.72	0.69
1:1A:136:G:H1	1:1A:143:C:N4	1.91	0.68
1:1A:2846:G:P	17:1T:53:ARG:HH12	2.16	0.68
1:1A:1798:U:OP2	3:1D:271:ARG:NH2	2.25	0.68
1:1A:1252:G:H1	18:1U:37:GLN:HE21	1.41	0.68
1:1A:2658:C:OP1	7:1H:158:LYS:NZ	2.27	0.68
1:1A:706:A:OP1	3:1D:7:LYS:NZ	2.26	0.68
16:1S:71:ALA:HB2	16:1S:102:ARG:HG3	1.74	0.68
7:1H:52:PHE:CE2	7:1H:69:ARG:HA	2.28	0.68
16:1S:36:TYR:CD1	16:1S:52:SER:HB2	2.29	0.68
10:1K:100:LYS:HB2	10:1K:141:GLU:HB2	1.76	0.68
12:1O:38:ILE:HD11	12:1O:112:PHE:HZ	1.58	0.68
1:1A:287:G:H1	1:1A:353:C:H42	1.42	0.68
11:1N:74:TYR:CD2	11:1N:92:MET:HG3	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:10:43:THR:HG23	24:10:57:HIS:HD2	1.58	0.67
1:1A:1340:U:OP1	21:1X:19:LYS:NZ	2.27	0.67
9:1J:22:ALA:N	9:1J:86:MET:CE	2.57	0.67
29:16:38:LYS:HB2	29:16:49:TYR:HE2	1.59	0.67
7:1H:99:LYS:NZ	7:1H:104:ASN:OD1	2.19	0.67
11:1N:13:ARG:NH1	11:1N:49:ASP:O	2.27	0.67
1:1A:2467:C:OP2	32:19:4:ARG:NH2	2.27	0.67
7:1H:95:ARG:HD2	7:1H:128:GLN:HB3	1.76	0.67
1:1A:2741:A:O3'	32:19:36:ARG:NH1	2.28	0.67
14:1Q:50:ARG:O	14:1Q:52:ALA:N	2.28	0.66
1:1A:1153:C:OP1	18:1U:92:ARG:NH2	2.28	0.66
21:1X:53:VAL:HG12	21:1X:92:ASN:HD22	1.61	0.66
1:1A:846:U:O2'	1:1A:847:U:OP2	2.13	0.66
7:1H:52:PHE:HE2	7:1H:69:ARG:HA	1.59	0.66
29:16:38:LYS:HB2	29:16:49:TYR:CE2	2.31	0.66
1:1A:1653:G:H3'	15:1R:2:ARG:HD2	1.78	0.66
1:1A:1095:A:H61	10:1K:30:GLN:HE22	1.44	0.66
15:1R:55:ALA:HA	15:1R:80:PHE:CE1	2.31	0.66
3:1D:115:GLN:O	3:1D:125:LYS:NZ	2.27	0.66
14:1Q:47:GLU:OE1	14:1Q:50:ARG:NH1	2.30	0.65
9:1J:31:ARG:HE	9:1J:79:PRO:HG3	1.61	0.65
23:1Z:51:GLN:HE22	23:1Z:86:LEU:HD21	1.61	0.65
29:16:25:LYS:NZ	29:16:32:GLU:O	2.22	0.65
18:1U:97:ASP:OD2	19:1V:13:ARG:NE	2.30	0.65
30:17:31:LEU:HB3	30:17:35:ARG:HH12	1.61	0.65
24:10:21:LEU:HD11	24:10:41[A]:ARG:HE	1.61	0.65
5:1F:62:GLN:HE22	5:1F:69:ARG:HD2	1.62	0.65
1:1A:2294:G:H5'	16:1S:98:GLN:HE22	1.61	0.65
1:1A:2371:G:O2'	29:16:46:HIS:ND1	2.24	0.65
10:1K:56:PRO:HD3	10:1K:75:PRO:HD3	1.78	0.64
20:1W:73:LYS:HB2	20:1W:106:VAL:HB	1.78	0.64
1:1A:1824:G:H5"	3:1D:52:ARG:HH11	1.62	0.64
25:11:18:ARG:HH21	25:11:24:ALA:HB2	1.61	0.64
17:1T:52:ASN:O	17:1T:53:ARG:NH1	2.31	0.64
1:1A:2127:G:O2'	1:1A:2128:G:O5'	2.15	0.64
11:1N:49:ASP:OD2	11:1N:121:LYS:NZ	2.30	0.64
11:1N:37:ARG:HD3	11:1N:39:LYS:HD3	1.80	0.64
23:1Z:63:ILE:HD11	23:1Z:91:PHE:CD2	2.33	0.64
1:1A:859:G:OP2	1:1A:869:G:N1	22.17	0.64
9:1J:132:TYR:H	9:1J:133:GLU:HB2	1.63	0.64
13:1P:81:ASP:HB3	13:1P:100:ILE:HD13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:48:U:P	16:1S:30:ARG:HH22	2.20	0.64
1:1A:7:G:O4'	11:1N:135:GLN:NE2	2.27	0.64
1:1A:1795:C:O2	3:1D:253:LYS:NZ	2.30	0.64
15:1R:32:GLU:HG2	15:1R:115:LEU:HD12	1.79	0.64
13:1P:23:ILE:HG12	19:1V:82:HIS:CD2	2.32	0.64
1:1A:2768:U:O2'	11:1N:95:ARG:NH2	2.31	0.63
9:1J:132:TYR:N	9:1J:133:GLU:HB2	2.12	0.63
1:1A:6:A:O2'	11:1N:135:GLN:NE2	2.29	0.63
5:1F:90:GLN:HE21	5:1F:92:HIS:CE1	2.14	0.63
1:1A:1151:A:H4'	18:1U:81:ASN:ND2	2.13	0.63
1:1A:444:C:OP2	5:1F:44:ARG:NH2	2.32	0.63
1:1A:1568:G:O4'	3:1D:58:HIS:HE1	1.80	0.63
1:1A:45:G:H5''	1:1A:46:G:H5'	1.80	0.63
5:1F:59:PRO:HG2	5:1F:78:TRP:HH2	1.64	0.63
2:1B:9:G:P	16:1S:25:ARG:HH12	2.22	0.63
17:1T:51:ARG:CZ	17:1T:53:ARG:HG3	2.29	0.63
22:1Y:85:PHE:HE1	22:1Y:94:ARG:HG2	1.63	0.63
23:1Z:26:PHE:CE2	23:1Z:44:HIS:HA	2.33	0.63
1:1A:2127:G:O2'	1:1A:2128:G:O4'	2.15	0.63
1:1A:2365:G:N7	31:18:39:LYS:NZ	2.41	0.62
8:1I:68:ARG:O	8:1I:72:ILE:HG12	2.00	0.62
21:1X:2:ILE:HG22	21:1X:7:LEU:HD21	1.80	0.62
8:1I:115:VAL:HG13	8:1I:132:PHE:HE1	1.63	0.62
15:1R:30:ARG:NH2	15:1R:72:ASP:OD2	2.32	0.62
1:1A:1252:G:H1	18:1U:37:GLN:NE2	1.96	0.62
1:1A:2511:U:H1'	4:1E:130:GLN:HE21	1.64	0.62
6:1G:110:ARG:NH1	6:1G:136:ILE:O	2.32	0.62
3:1D:76:ALA:HB2	3:1D:96:TYR:CD1	2.35	0.62
9:1J:69:PHE:HB3	9:1J:72:LEU:HD12	1.82	0.62
28:15:54:VAL:HG23	28:15:55:ILE:HG12	1.80	0.62
23:1Z:17:SER:HB3	23:1Z:21:ARG:HH12	1.65	0.62
14:1Q:17:ASN:O	14:1Q:38:ARG:NH1	2.32	0.61
28:15:27:SER:HB2	28:15:40:ARG:HD3	1.83	0.61
1:1A:65:U:H4'	21:1X:73:ARG:HE	1.65	0.61
15:1R:73:ASN:HA	15:1R:76:VAL:HG22	1.82	0.61
29:16:13:SER:HA	29:16:49:TYR:CD1	2.35	0.61
1:1A:405:U:O4	3:1D:2:ALA:N	105.52	0.61
17:1T:30:VAL:HG11	17:1T:72:ARG:HH22	1.65	0.60
12:1O:43:ILE:HD12	12:1O:56:ASP:HB2	1.83	0.60
1:1A:550:C:H2'	1:1A:551:G:H5''	1.83	0.60
7:1H:54:PRO:HG3	7:1H:62:TRP:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1V:44:GLY:O	19:1V:45:GLU:HG2	2.01	0.60
9:1J:4:ASN:OD1	9:1J:5:LEU:N	2.33	0.60
56:1A:3001:6UQ:OAT	56:1A:3001:6UQ:OAK	2.20	0.60
6:1G:63:GLN:HE21	6:1G:89:VAL:HG13	1.67	0.60
9:1J:21:GLY:C	9:1J:86:MET:CE	2.69	0.60
23:1Z:2:PHE:HB2	23:1Z:61:LEU:HD22	1.82	0.60
6:1G:99:PHE:HA	6:1G:102:ARG:HE	1.66	0.60
17:1T:106:LYS:HE3	17:1T:109:ARG:HH22	1.66	0.60
9:1J:18:VAL:HG11	9:1J:51:TYR:CD2	2.37	0.59
9:1J:22:ALA:N	9:1J:86:MET:SD	2.75	0.59
11:1N:37:ARG:NH1	11:1N:44:TYR:OH	2.35	0.59
15:1R:79:LEU:HD23	15:1R:83:LEU:HD12	1.84	0.59
1:1A:2200:C:OP2	25:11:37:ARG:NH1	2.36	0.59
21:1X:92:ASN:O	21:1X:93:LEU:HB2	2.01	0.59
1:1A:878:A:N6	1:1A:899:A:O2'	2.35	0.59
17:1T:88:ARG:NH2	17:1T:112:GLU:HB2	2.17	0.59
1:1A:1517:G:N3	1:1A:1919:A:O2'	103.07	0.59
1:1A:1721:G:HO2'	1:1A:1722:A:H8	1.50	0.59
1:1A:545:U:H2'	1:1A:546:U:O3'	2.02	0.59
6:1G:73:SER:OG	6:1G:81:GLN:N	2.36	0.59
10:1K:12:GLN:HG2	10:1K:56:PRO:HB3	1.85	0.59
7:1H:104:ASN:ND2	7:1H:114:ASP:OD1	2.36	0.59
10:1K:103:ARG:HA	10:1K:106:LEU:HD12	1.84	0.59
10:1K:113:LYS:O	10:1K:117:MET:N	2.36	0.59
30:17:16:HIS:HA	30:17:21:ARG:HH22	1.68	0.58
5:1F:41:GLN:HG2	5:1F:43:THR:HG23	1.85	0.58
31:18:31:HIS:ND1	31:18:32:ILE:HG13	2.19	0.58
9:1J:119:PRO:HG2	9:1J:122:GLN:HB2	1.85	0.58
5:1F:73:ILE:HA	5:1F:78:TRP:CZ3	2.38	0.58
9:1J:3:LEU:O	9:1J:8:LYS:NZ	2.37	0.58
11:1N:56:VAL:HB	11:1N:124:VAL:HG12	1.85	0.58
22:1Y:59:VAL:HG11	22:1Y:61:LYS:HE3	1.85	0.58
1:1A:6:A:C2'	11:1N:135:GLN:HE22	2.16	0.58
2:1B:103:U:HO2'	23:1Z:31:TYR:HH	1.49	0.58
1:1A:1606:C:H5'	1:1A:1607:C:OP1	2.03	0.58
1:1A:2886[A]:A:N1	28:15:40:ARG:HD2	2.18	0.58
1:1A:84:A:OP1	22:1Y:6:ARG:NH1	2.36	0.58
5:1F:52:VAL:HB	5:1F:74:LYS:HD2	1.85	0.58
12:1O:107:LEU:O	12:1O:109:SER:N	2.37	0.58
15:1R:63:ARG:HA	15:1R:80:PHE:CE2	2.39	0.58
15:1R:96:ARG:HH12	15:1R:116:VAL:HG13	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2070:A:H2'	1:1A:2071:A:C8	2.39	0.58
3:1D:227:PRO:HA	3:1D:233:GLY:HA2	1.85	0.58
30:17:34:ARG:CD	30:17:42:LEU:HA	2.34	0.58
1:1A:1482:G:H1'	1:1A:1509:A:H61	1.68	0.57
1:1A:536:G:H4'	18:1U:57:PHE:CZ	2.39	0.57
2:1B:90:C:H5'	14:1Q:18[A]:ARG:HG2	1.87	0.57
17:1T:51:ARG:NH1	17:1T:56:HIS:O	2.37	0.57
9:1J:61:ARG:NH2	9:1J:76:PHE:O	2.37	0.57
3:1D:84:ASP:OD2	3:1D:87:ARG:NH2	2.20	0.57
1:1A:1113:U:H5'	7:1H:3:ARG:HH12	1.69	0.57
7:1H:88:GLN:HE21	7:1H:163:ARG:HD2	1.69	0.57
8:1I:41:LYS:HA	8:1I:44:ILE:HG22	1.86	0.57
1:1A:250:G:O5'	13:1P:59:ARG:NH1	2.37	0.57
9:1J:92:ALA:HB1	9:1J:96:PHE:CE2	2.36	0.57
1:1A:2780:G:P	11:1N:120:ARG:HE	2.27	0.57
14:1Q:54:THR:O	14:1Q:59:ARG:HG3	2.04	0.57
30:17:31:LEU:HB3	30:17:35:ARG:NH1	2.18	0.57
24:10:23:VAL:HB	24:10:26:PHE:CE1	2.37	0.57
3:1D:260:ASN:OD1	3:1D:262:ARG:HG2	2.04	0.57
15:1R:87:PHE:HB3	15:1R:94:TYR:CE1	2.40	0.57
1:1A:2324:U:H3'	1:1A:2325:G:C5'	2.35	0.57
1:1A:2371:G:HO2'	29:16:46:HIS:CE1	2.19	0.57
2:1B:103:U:O2'	23:1Z:31:TYR:OH	2.22	0.57
5:1F:59:PRO:HG2	5:1F:78:TRP:CH2	2.39	0.57
20:1W:23:LEU:HD21	28:15:22:LEU:HB2	1.86	0.57
10:1K:21:SER:HB3	10:1K:22:PRO:HD3	1.87	0.56
1:1A:282:A:H2'	1:1A:283:G:C8	2.40	0.56
2:1B:30:C:OP1	16:1S:3:LYS:NZ	2.30	0.56
5:1F:147:LEU:HB2	5:1F:183:PHE:CD2	2.37	0.56
1:1A:930:G:H1'	27:13:25:LEU:HD21	1.87	0.56
10:1K:110:ALA:O	10:1K:114:ALA:N	2.39	0.56
1:1A:1825:U:H4'	3:1D:232:HIS:HE1	1.70	0.56
1:1A:1365:A:P	25:11:28:ARG:HH22	2.28	0.56
1:1A:141:G:OP2	1:1A:142:A:N6	2.38	0.56
28:15:38:HIS:HB3	28:15:44:THR:HG22	1.86	0.56
1:1A:2849:U:P	17:1T:93:ARG:HH21	2.29	0.56
6:1G:33:LYS:HB3	6:1G:92:ARG:HE	1.71	0.56
1:1A:747:5MU:H4'	20:1W:92:ARG:HH21	1.71	0.56
22:1Y:87:PHE:HE1	22:1Y:92:LYS:HE2	1.70	0.56
1:1A:784:G:H5'	1:1A:785:G:OP1	2.06	0.56
21:1X:69:ARG:HG2	21:1X:74:ILE:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:10:43:THR:HG23	24:10:57:HIS:CD2	2.39	0.56
1:1A:1536:C:H4'	1:1A:1537:G:H5''	1.88	0.56
2:1B:8:C:O3'	16:1S:25:ARG:NH1	2.38	0.56
8:1I:7:ASP:OD1	8:1I:8:LYS:N	2.39	0.56
1:1A:1046:A:O2'	9:1J:8:LYS:HE3	2.05	0.56
26:12:52:ARG:O	26:12:56:LEU:HG	2.06	0.56
12:1O:80:ASP:N	17:1T:68:GLU:OE2	2.39	0.56
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.71	0.55
1:1A:2330:G:O3'	24:10:44:LYS:NZ	2.31	0.55
11:1N:117:ALA:HA	11:1N:120:ARG:HH21	1.71	0.55
5:1F:178:VAL:HG23	13:1P:3:LEU:HD21	1.88	0.55
22:1Y:81:ASP:OD1	22:1Y:82:ARG:N	2.35	0.55
23:1Z:43:ASP:OD2	23:1Z:46:LYS:HG2	2.05	0.55
1:1A:1176:U:H2'	1:1A:1177:G:C8	2.42	0.55
1:1A:28:A:O2'	1:1A:296:U:OP1	51.10	0.55
4:1E:121:THR:HB	4:1E:127:PHE:CD2	2.41	0.55
1:1A:2813:A:H2	1:1A:2887[B]:A:H61	1.51	0.55
1:1A:871:U:H2'	1:1A:872:U:C6	2.42	0.55
17:1T:99:TYR:O	17:1T:103:ARG:NH1	2.39	0.55
1:1A:2886[B]:A:N3	1:1A:2886[B]:A:H2'	2.21	0.55
1:1A:790:U:O4	5:1F:61:ARG:NH2	2.39	0.55
12:1O:58:LEU:HA	12:1O:89:ASN:OD1	2.06	0.55
16:1S:30:ARG:HG3	16:1S:102:ARG:HD2	1.88	0.55
17:1T:62:ARG:NH2	17:1T:71:GLU:OE2	2.39	0.55
1:1A:995:C:O2	11:1N:3:THR:OG1	2.20	0.55
17:1T:89:ARG:HB3	17:1T:113:ARG:NH1	2.22	0.55
1:1A:2393:U:H5''	13:1P:62:PRO:HB3	1.88	0.55
7:1H:86:LYS:HG2	7:1H:132:VAL:HG22	1.87	0.55
29:16:21:TYR:HE2	29:16:38:LYS:HB2	1.72	0.55
1:1A:1170:C:H2'	1:1A:1171:G:C8	2.41	0.55
1:1A:1738:G:HO2'	1:1A:1739:A:H8	1.52	0.55
4:1E:48:ILE:HG23	4:1E:84:LEU:HD21	1.88	0.55
1:1A:1475:G:H4'	1:1A:1689:A:H4'	67.89	0.55
20:1W:25:ARG:NH2	20:1W:74:ILE:O	2.30	0.55
1:1A:2298:A:OP1	6:1G:71:ARG:NH2	2.37	0.55
3:1D:154:LEU:HD13	3:1D:176:LEU:HD21	1.88	0.55
1:1A:2313:C:H5''	6:1G:88:LYS:HD2	1.89	0.55
7:1H:27:LYS:NZ	7:1H:32:GLU:OE1	2.39	0.55
10:1K:113:LYS:O	10:1K:117:MET:HG2	2.07	0.55
21:1X:11:LEU:HD23	21:1X:34:VAL:HG12	1.88	0.55
1:1A:729:G:OP2	3:1D:207:LYS:NZ	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:127:PHE:HZ	4:1E:160:LYS:HB2	1.72	0.55
6:1G:67:ILE:HG22	6:1G:87:CYS:HB3	1.89	0.55
9:1J:118:ILE:HG22	9:1J:123:ILE:HG12	1.88	0.55
22:1Y:26:LYS:HD2	22:1Y:37:GLU:HG2	1.88	0.55
1:1A:922:C:H1'	24:10:26:PHE:CD2	2.42	0.54
1:1A:2172:U:H4'	1:1A:2173:A:H5'	1.88	0.54
1:1A:2849:U:OP1	17:1T:93:ARG:NH2	2.36	0.54
4:1E:116:LYS:HA	15:1R:1:MET:SD	2.47	0.54
20:1W:109:ASP:OD1	20:1W:110:ARG:N	2.40	0.54
1:1A:2251:OMG:OP1	14:1Q:81[A]:ARG:NH2	2.40	0.54
13:1P:51:GLU:OE1	13:1P:60:ARG:NH2	2.39	0.54
1:1A:2636:C:O2'	4:1E:45:TYR:OH	2.23	0.54
3:1D:71:LYS:NZ	3:1D:98:ASP:OD2	2.37	0.54
4:1E:186:LEU:HD21	17:1T:4:ILE:HG21	1.90	0.54
1:1A:1754:A:O2'	17:1T:103:ARG:NH2	2.39	0.54
6:1G:99:PHE:HB2	6:1G:102:ARG:HH11	1.72	0.54
25:11:43:GLU:OE1	25:11:45:ARG:NH2	2.33	0.54
1:1A:2351:G:O6	31:18:42:ARG:NH1	2.40	0.54
21:1X:11:LEU:HD22	21:1X:32:LEU:HD13	1.90	0.54
25:11:18:ARG:NH1	25:11:22:LEU:HB3	2.23	0.54
1:1A:1184:U:OP2	27:13:31:ARG:NH2	2.41	0.54
1:1A:827:U:C2'	1:1A:2068:U:C2	2.85	0.54
9:1J:22:ALA:HA	9:1J:86:MET:HA	1.90	0.54
1:1A:350:G:OP1	17:1T:3:ASN:N	133.58	0.54
1:1A:858:G:OP1	24:10:78:LYS:NZ	2.23	0.53
1:1A:1817:G:H5''	3:1D:87:ARG:HG3	1.89	0.53
11:1N:118:MET:HA	11:1N:121:LYS:HZ3	1.72	0.53
1:1A:2267:A:H5''	1:1A:2268:A:H5'	1.90	0.53
1:1A:2485:G:H5''	14:1Q:45:GLN:HE21	1.73	0.53
16:1S:92:PHE:HE2	16:1S:94:ARG:HB3	1.74	0.53
24:10:65:GLY:HA2	24:10:85:GLU:HG3	1.90	0.53
1:1A:7:G:H5'	11:1N:132:HIS:CE1	2.44	0.53
7:1H:22:GLN:NE2	7:1H:38:ASN:O	2.42	0.53
1:1A:2037:A:H2'	1:1A:2038:G:C8	2.43	0.53
1:1A:2286:G:OP1	29:16:30:LYS:NZ	2.38	0.53
4:1E:2:ILE:HG13	4:1E:100:LEU:HD21	1.89	0.53
4:1E:49:GLN:HE21	4:1E:79:LEU:HB3	1.73	0.53
13:1P:85:VAL:HB	13:1P:94:THR:HG22	1.90	0.53
22:1Y:81:ASP:OD2	22:1Y:96:PHE:HB3	2.09	0.53
1:1A:357:C:H2'	1:1A:358:U:C6	2.43	0.53
1:1A:1046:A:H4'	9:1J:58:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:12:56:LEU:HA	26:12:59:GLU:HG2	1.90	0.53
29:16:10:LYS:HE3	29:16:53:LYS:O	2.08	0.53
30:17:34:ARG:HD2	30:17:42:LEU:HA	1.90	0.53
1:1A:2061:G:OP1	5:1F:63:LYS:NZ	2.35	0.53
4:1E:110:THR:HG21	4:1E:169:ARG:CZ	2.39	0.53
10:1K:33:VAL:HG22	10:1K:61:VAL:HG11	1.90	0.53
1:1A:1083:U:H4'	9:1J:42:ARG:NH1	2.18	0.53
9:1J:21:GLY:CA	9:1J:86:MET:HE1	2.38	0.53
15:1R:55:ALA:HA	15:1R:80:PHE:HE1	1.73	0.53
19:1V:73:LYS:NZ	19:1V:86:GLN:OE1	2.39	0.53
26:12:26:PHE:HD1	26:12:29:ARG:HH11	1.55	0.53
1:1A:142:A:H2'	1:1A:143:C:C6	2.44	0.53
1:1A:1478:G:H1	1:1A:1513:U:H3	1.56	0.53
22:1Y:33:LYS:HE2	22:1Y:66:GLN:NE2	2.24	0.53
1:1A:1171:G:C4	1:1A:1172:C:N4	2.76	0.52
7:1H:4:VAL:O	7:1H:69:ARG:HG2	2.09	0.52
10:1K:79:LEU:HD23	10:1K:82:LYS:HD3	1.91	0.52
10:1K:8:TYR:CE1	10:1K:60:THR:HG23	2.44	0.52
28:15:27:SER:O	28:15:40:ARG:HG3	2.09	0.52
8:1I:90:LEU:HD11	8:1I:146:VAL:HG11	1.91	0.52
1:1A:323:C:HO2'	1:1A:1205:A:H61	1.54	0.52
1:1A:17:G:H4'	18:1U:25:TYR:HE1	1.74	0.52
6:1G:103:LEU:HA	6:1G:107:ALA:HB3	1.91	0.52
17:1T:30:VAL:HG13	17:1T:80:VAL:HG12	1.91	0.52
1:1A:1140:C:OP2	11:1N:68:LYS:NZ	2.36	0.52
1:1A:1266:G:O2'	1:1A:2012:G:O6	2.25	0.52
11:1N:135:GLN:N	11:1N:135:GLN:OE1	2.43	0.52
15:1R:55:ALA:HA	15:1R:80:PHE:CD1	2.44	0.52
14:1Q:50:ARG:HA	14:1Q:53:MET:CG	2.39	0.52
1:1A:827:U:H2'	1:1A:2068:U:N3	2.24	0.52
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.44	0.52
1:1A:448:U:O4'	5:1F:79:ARG:NE	2.41	0.52
1:1A:1216:G:H5''	18:1U:11:ARG:HH12	1.74	0.52
3:1D:2:ALA:N	3:1D:20:VAL:O	2.43	0.52
4:1E:14:ILE:HA	17:1T:12:GLN:HE22	1.75	0.52
9:1J:57:ASN:ND2	9:1J:78:GLY:O	2.27	0.52
28:15:13:ARG:HG3	28:15:16:ARG:NH1	2.22	0.52
30:17:12:ARG:HH21	30:17:12:ARG:HG2	1.75	0.52
9:1J:21:GLY:CA	9:1J:86:MET:CE	2.88	0.52
27:13:28:GLY:HA3	27:13:38:ARG:HH21	1.75	0.52
31:18:9:GLY:O	31:18:13:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1K:98:VAL:HG23	10:1K:138:LEU:HD23	1.91	0.52
1:1A:139:U:O4	21:1X:2:ILE:HG13	2.10	0.52
1:1A:581:C:H2'	1:1A:582:A:C8	2.45	0.52
31:18:16:LYS:HA	31:18:22:PHE:HD1	1.75	0.51
7:1H:98:VAL:HG22	7:1H:103:ILE:HG12	1.90	0.51
8:1I:127:GLU:HG2	8:1I:145:ASN:HD22	1.74	0.51
1:1A:1223:G:N2	1:1A:1226:A:OP2	2.43	0.51
8:1I:113:SER:O	8:1I:116:ARG:NH1	2.41	0.51
16:1S:2:ASP:OD1	16:1S:5:SER:OG	2.18	0.51
13:1P:63:LYS:O	31:18:30:ARG:NH1	2.41	0.51
1:1A:137:U:H3	1:1A:142:A:H61	1.57	0.51
5:1F:61:ARG:HE	5:1F:65:THR:HG23	1.76	0.51
24:10:37:ILE:HD11	24:10:82:ILE:HD11	1.93	0.51
29:16:6:ARG:NH2	29:16:26:ASN:HB2	2.22	0.51
1:1A:1059:G:H4'	10:1K:117:MET:HE1	1.92	0.51
1:1A:2886[B]:A:H3'	1:1A:2887[B]:A:C5'	2.41	0.51
8:1I:21:VAL:HG21	8:1I:25:TYR:HD2	1.76	0.51
4:1E:46:ARG:NH2	4:1E:88:GLU:O	2.38	0.51
20:1W:83:LYS:O	20:1W:84:ARG:NH2	2.38	0.51
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.46	0.51
6:1G:25:VAL:O	6:1G:28:VAL:HG12	2.11	0.51
1:1A:137:U:H3	1:1A:142:A:N6	2.09	0.51
1:1A:1597:A:H5''	1:1A:1598:A:H5'	1.93	0.51
1:1A:1824:G:H5''	3:1D:52:ARG:NH1	2.25	0.51
1:1A:2162:G:H5''	1:1A:2171:A:H2'	1.93	0.51
1:1A:1869:G:N2	1:1A:1871:A:O2'	2.43	0.51
1:1A:2321:U:H5'	1:1A:2322:A:OP2	2.11	0.51
1:1A:2882:A:P	15:1R:96:ARG:HE	2.34	0.51
3:1D:130:LEU:HD11	3:1D:135:ILE:HG13	1.92	0.51
1:1A:1026:G:H2'	1:1A:1027:A:C8	2.46	0.51
1:1A:2000:C:OP1	15:1R:5:LYS:NZ	2.39	0.51
1:1A:639:U:H2'	1:1A:640:C:C6	2.46	0.51
13:1P:109:LYS:HG2	13:1P:126:ARG:HB2	1.92	0.51
1:1A:572:A:OP2	19:1V:79:ARG:NH1	2.44	0.51
1:1A:112:U:H5'	26:12:58:ASN:ND2	2.26	0.50
1:1A:2874:C:H5''	15:1R:4:ARG:HH21	1.76	0.50
1:1A:748:G:OP1	20:1W:88:ARG:NH1	2.43	0.50
1:1A:1799:G:H8	3:1D:180:GLU:OE1	1.93	0.50
4:1E:152:PRO:HG3	4:1E:156:PHE:CZ	2.46	0.50
1:1A:729:G:C6	3:1D:207:LYS:HB2	2.47	0.50
3:1D:58:HIS:ND1	3:1D:59:LYS:O	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:10:46:HIS:HB2	24:10:79:PHE:CD1	2.45	0.50
1:1A:827:U:C2'	1:1A:2068:U:O2	2.58	0.50
1:1A:2116:G:N7	1:1A:2165:C:N4	2.58	0.50
29:16:5:ILE:HG21	29:16:28:ARG:HE	1.76	0.50
1:1A:2784:U:H4'	4:1E:43:ASP:OD1	2.10	0.50
4:1E:152:PRO:HG3	4:1E:156:PHE:CE1	2.46	0.50
1:1A:2313:C:O4'	6:1G:37:ASN:ND2	2.44	0.50
14:1Q:49:ALA:HB1	14:1Q:120:ALA:HB1	1.92	0.50
16:1S:37:ALA:HB3	16:1S:78:VAL:HG11	1.94	0.50
13:1P:23:ILE:HG12	19:1V:82:HIS:HD2	1.75	0.50
19:1V:68:ARG:NH1	19:1V:90:ARG:HB2	2.26	0.50
13:1P:57:LEU:HG	31:18:14:PHE:HZ	1.77	0.50
31:18:39:LYS:HA	31:18:42:ARG:NH2	2.25	0.50
1:1A:1847:G:O5'	1:1A:1847:G:H8	1.95	0.50
7:1H:52:PHE:CZ	7:1H:72:LEU:HD22	2.47	0.50
1:1A:536:G:H4'	18:1U:57:PHE:HZ	1.76	0.50
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.46	0.50
10:1K:54:PRO:HD2	10:1K:78:VAL:HG11	1.94	0.50
1:1A:2428:G:N2	13:1P:54:GLN:HE21	2.10	0.50
1:1A:2020:A:H5'	28:15:9:THR:CG2	2.42	0.50
1:1A:84:A:N1	1:1A:98:G:O2'	2.38	0.50
1:1A:851:C:H2'	1:1A:852:U:C6	2.47	0.50
6:1G:13:VAL:O	6:1G:17:MET:HG2	2.12	0.50
26:12:39:GLN:HB3	26:12:41:HIS:CE1	2.47	0.50
29:16:25:LYS:HE2	29:16:30:LYS:O	2.11	0.50
9:1J:21:GLY:HA3	9:1J:86:MET:CE	2.42	0.50
9:1J:88:HIS:ND1	9:1J:89:PRO:O	2.45	0.50
1:1A:483:A:C4	22:1Y:58:ILE:HD11	2.47	0.50
1:1A:2291:U:H2'	1:1A:2292:U:C6	2.47	0.49
10:1K:20:PRO:HB2	10:1K:23:PRO:HD2	1.94	0.49
11:1N:72:LYS:HE3	11:1N:74:TYR:CE1	2.46	0.49
1:1A:142:A:C5	1:1A:143:C:C4	3.00	0.49
1:1A:1651:G:OP1	15:1R:40:LYS:NZ	2.43	0.49
1:1A:857:G:H5'	24:10:69:PHE:CD2	2.48	0.49
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.28	0.49
1:1A:245:G:N7	31:18:8:ARG:NH2	2.55	0.49
10:1K:59:ILE:HD11	10:1K:67:PHE:CD1	2.47	0.49
18:1U:108:ALA:O	18:1U:112:LYS:HG2	2.12	0.49
24:10:45:PHE:HE1	24:10:78:LYS:HD3	1.76	0.49
1:1A:900:A:H4'	1:1A:1832:C:H5''	87.64	0.49
11:1N:7:LYS:O	11:1N:11:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:929:U:H4'	27:13:38:ARG:NH2	2.27	0.49
1:1A:7:G:HO2'	11:1N:15:TRP:HZ2	1.61	0.49
18:1U:49:ASP:HA	18:1U:52:GLN:HB2	1.94	0.49
1:1A:1656:C:OP1	4:1E:141:ARG:NE	2.41	0.49
1:1A:781:A:P	3:1D:217:ARG:HH22	2.36	0.49
6:1G:73:SER:HB3	6:1G:80:ARG:HA	1.94	0.49
8:1I:21:VAL:CG2	8:1I:25:TYR:HD2	2.25	0.49
14:1Q:10:ARG:HH22	14:1Q:11:LYS:HE3	1.77	0.49
1:1A:551:G:H5'	1:1A:551:G:H8	1.78	0.49
29:16:35:GLU:OE2	29:16:48:ILE:HD11	2.13	0.49
1:1A:2547:A:H2'	1:1A:2548:U:C6	2.48	0.49
2:1B:66:A:H61	2:1B:107:G:H2'	1.77	0.49
1:1A:1656:C:P	4:1E:141:ARG:HE	2.36	0.49
1:1A:2547:A:H4'	12:1O:29:HIS:CE1	2.47	0.49
20:1W:82:MET:HB2	20:1W:98:LYS:HB2	1.95	0.49
1:1A:281:C:H2'	1:1A:282:A:C8	2.48	0.48
1:1A:2831:G:P	4:1E:56:LYS:HE2	2.53	0.48
14:1Q:10:ARG:NH2	14:1Q:11:LYS:HE3	2.28	0.48
15:1R:8:ARG:NH2	15:1R:39:PRO:HA	2.27	0.48
17:1T:86:VAL:HG11	17:1T:89:ARG:HG2	1.94	0.48
31:18:42:ARG:HG3	31:18:45:ARG:NH2	2.28	0.48
1:1A:2067:G:O2'	1:1A:2069:G7M:H5''	2.14	0.48
9:1J:33:VAL:HG21	9:1J:106:PHE:CE2	2.47	0.48
12:1O:30:ARG:NH2	12:1O:37:ASP:OD2	2.46	0.48
9:1J:72:LEU:HD21	9:1J:112:ALA:HB2	1.95	0.48
22:1Y:85:PHE:CE1	22:1Y:94:ARG:HG2	2.45	0.48
23:1Z:55:GLU:HB3	23:1Z:59:GLU:CD	2.33	0.48
1:1A:337:C:OP2	22:1Y:4:LYS:NZ	2.39	0.48
1:1A:479:A:N3	1:1A:481:G:H5''	2.28	0.48
1:1A:781:A:OP1	3:1D:217:ARG:NH2	2.46	0.48
6:1G:67:ILE:HA	6:1G:87:CYS:HA	1.93	0.48
11:1N:110:PRO:O	11:1N:115:GLY:HA3	2.13	0.48
2:1B:48:U:H4'	16:1S:100:HIS:HD2	1.78	0.48
25:11:12:PRO:CB	25:11:28:ARG:HH21	2.26	0.48
23:1Z:76:ASP:OD1	23:1Z:77:VAL:N	2.45	0.48
1:1A:1172:C:C4	1:1A:1173:U:H1'	2.48	0.48
1:1A:2079:U:O2'	25:11:23:ASN:OD1	2.30	0.48
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.29	0.48
1:1A:2845:U:H5''	17:1T:52:ASN:O	2.14	0.48
4:1E:5:VAL:HG11	4:1E:80:TRP:CZ3	2.48	0.48
1:1A:1432:G:O5'	17:1T:106:LYS:HG2	54.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1412:U:H2'	1:1A:1413:A:C8	2.49	0.48
6:1G:69:LYS:HE3	6:1G:84:PRO:HG3	1.96	0.48
6:1G:5:HIS:NE2	6:1G:9:LYS:HE3	2.28	0.48
1:1A:355:U:H2'	1:1A:356:G:C8	2.49	0.48
1:1A:674:G:H1'	5:1F:69:ARG:NE	2.20	0.48
23:1Z:63:ILE:HG22	23:1Z:65:VAL:HG23	1.95	0.48
1:1A:1040:A:OP1	23:1Z:46:LYS:NZ	2.47	0.48
1:1A:1847:G:N2	1:1A:1848:A:N6	2.37	0.48
1:1A:30:G:OP2	18:1U:5:LYS:NZ	2.39	0.48
1:1A:906:U:O2'	14:1Q:66:ARG:NH2	2.29	0.47
10:1K:12:GLN:HA	10:1K:56:PRO:HA	1.95	0.47
10:1K:61:VAL:HG12	10:1K:67:PHE:HB3	1.96	0.47
17:1T:89:ARG:HB3	17:1T:113:ARG:HH12	1.78	0.47
1:1A:323:C:H2'	5:1F:163:ASN:OD1	2.14	0.47
1:1A:594:U:H2'	1:1A:595:C:C6	2.48	0.47
3:1D:243:HIS:O	3:1D:245:VAL:HG13	2.14	0.47
9:1J:33:VAL:HG22	9:1J:105:LYS:HE2	1.97	0.47
11:1N:102:GLU:HG3	11:1N:124:VAL:HG21	1.97	0.47
14:1Q:34:LYS:HE3	14:1Q:131:VAL:HG11	1.95	0.47
16:1S:35:ILE:HD12	16:1S:102:ARG:HG2	1.96	0.47
9:1J:18:VAL:O	9:1J:86:MET:SD	2.72	0.47
11:1N:140:LEU:HG	11:1N:142:ILE:HB	1.96	0.47
18:1U:44:GLN:NE2	19:1V:77:PHE:HB3	2.18	0.47
18:1U:67:ALA:O	18:1U:71:GLN:HG2	2.14	0.47
1:1A:2362:C:H5''	31:18:40:ARG:NH1	2.29	0.47
1:1A:832:U:H2'	1:1A:833:A:C8	2.49	0.47
1:1A:1827:U:OP2	3:1D:221:ARG:NH1	2.47	0.47
6:1G:71:ARG:HG2	6:1G:72:LYS:HG2	1.97	0.47
7:1H:43:VAL:HG23	7:1H:52:PHE:HE1	1.80	0.47
20:1W:48:LYS:HE2	20:1W:52:GLU:OE2	2.15	0.47
1:1A:2189:U:H2'	1:1A:2190:G:O4'	2.15	0.47
1:1A:2886[B]:A:H3'	1:1A:2887[B]:A:H5'	1.96	0.47
1:1A:340:A:O2'	5:1F:162:ARG:NH1	2.47	0.47
1:1A:494:G:H4'	20:1W:6:LYS:HB2	1.95	0.47
1:1A:644:A:H2'	1:1A:645:C:O4'	2.15	0.47
1:1A:1902:C:H5''	3:1D:240:PHE:CE2	2.49	0.47
10:1K:79:LEU:HA	10:1K:82:LYS:HG2	1.95	0.47
14:1Q:76:LYS:NZ	14:1Q:85:GLY:O	2.46	0.47
16:1S:17:LYS:HA	16:1S:20:GLU:OE2	2.14	0.47
30:17:16:HIS:HA	30:17:21:ARG:NH2	2.28	0.47
1:1A:1868:C:H2'	1:1A:1869:G:O4'	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.50	0.47
1:1A:2386:A:N3	24:10:41[A]:ARG:HG3	2.30	0.47
1:1A:2461:A:H1'	1:1A:2492:U:C2	2.50	0.47
1:1A:2812:G:H2'	1:1A:2813:A:O4'	2.15	0.47
4:1E:4:LEU:HD22	4:1E:32:ASN:HD22	1.80	0.47
5:1F:70:SER:HB2	5:1F:78:TRP:CH2	2.50	0.47
1:1A:2874:C:OP1	15:1R:4:ARG:NH2	2.48	0.47
16:1S:92:PHE:CE2	16:1S:94:ARG:HB3	2.50	0.47
23:1Z:70:ILE:HG22	23:1Z:72:VAL:HG13	1.97	0.47
29:16:21:TYR:CD2	29:16:38:LYS:HD3	2.49	0.47
1:1A:572:A:H5'	19:1V:79:ARG:NH2	2.30	0.47
11:1N:69:ARG:O	11:1N:90:GLU:HB2	2.13	0.47
1:1A:2888[A]:C:H2'	1:1A:2889:C:C6	2.50	0.47
15:1R:63:ARG:HA	15:1R:80:PHE:HE2	1.80	0.47
31:18:26:HIS:CE1	31:18:48:ALA:HB2	2.49	0.46
1:1A:2615:U:C2	28:15:4:GLN:HA	2.50	0.46
1:1A:289:G:H2'	1:1A:290:U:O4'	2.15	0.46
56:1A:3001:6UQ:CLAG	14:1Q:54:THR:HG22	2.53	0.46
4:1E:13:ARG:HH11	17:1T:56:HIS:HA	1.79	0.46
4:1E:35:THR:HG22	4:1E:73:VAL:HG21	1.98	0.46
5:1F:29:HIS:CE1	5:1F:33:VAL:HG21	2.51	0.46
7:1H:11:VAL:HG21	7:1H:17:VAL:HG23	1.97	0.46
1:1A:2529:G:H4'	7:1H:175:LYS:HG3	1.97	0.46
6:1G:147:ASP:OD1	6:1G:150:ARG:NH1	2.32	0.46
4:1E:13:ARG:HG2	17:1T:56:HIS:HE1	1.81	0.46
1:1A:65:U:O3'	21:1X:73:ARG:NH1	2.43	0.46
4:1E:14:ILE:HD13	17:1T:12:GLN:HE22	1.81	0.46
11:1N:26:GLY:O	11:1N:30:THR:HG23	2.15	0.46
24:10:38:VAL:HG12	24:10:59:LEU:HB2	1.97	0.46
1:1A:2019:A:H4'	18:1U:34:VAL:HG21	1.97	0.46
9:1J:29:ASP:OD1	9:1J:30:SER:N	2.49	0.46
13:1P:110:VAL:HG11	13:1P:135:ILE:HD11	1.98	0.46
28:15:53:LYS:HE3	28:15:56:ALA:HA	1.98	0.46
1:1A:1183:U:H2'	1:1A:1184:U:C6	2.51	0.46
5:1F:49:ARG:HH11	5:1F:72:SER:HB3	1.80	0.46
14:1Q:50:ARG:HA	14:1Q:53:MET:HG3	1.98	0.46
18:1U:36:PHE:HZ	19:1V:84:ARG:NH2	2.13	0.46
30:17:34:ARG:HG2	30:17:42:LEU:HD23	1.98	0.46
10:1K:59:ILE:HD12	10:1K:69:PHE:HB3	1.97	0.46
1:1A:2054:A:H2'	28:15:5:GLN:HE22	1.81	0.46
1:1A:2813:A:H2	1:1A:2887[B]:A:N6	2.11	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:30:PHE:HB3	3:1D:103:TYR:OH	2.16	0.46
3:1D:130:LEU:HD13	3:1D:134:ASN:HB2	1.97	0.46
5:1F:23:PHE:HB2	5:1F:111:GLU:OE2	2.15	0.46
14:1Q:30:SER:H	14:1Q:106:ASP:HB3	1.79	0.46
14:1Q:42:THR:HG22	14:1Q:93:VAL:HG12	1.97	0.46
16:1S:1:MET:SD	16:1S:6:ALA:HA	2.56	0.46
17:1T:106:LYS:HA	17:1T:109:ARG:NH2	2.31	0.46
1:1A:2485:G:H5''	14:1Q:45:GLN:NE2	2.31	0.46
1:1A:726:G:O2'	1:1A:727:A:OP2	2.34	0.46
1:1A:588:U:H1'	5:1F:85:PHE:CD1	2.51	0.46
10:1K:22:PRO:HB2	10:1K:23:PRO:HD3	1.97	0.46
11:1N:49:ASP:HB2	11:1N:114:LEU:HD11	1.98	0.46
1:1A:2069:G7M:HN71	1:1A:2069:G7M:O6	2.15	0.46
1:1A:1007:C:OP1	11:1N:37:ARG:NH2	2.49	0.46
15:1R:32:GLU:HB3	15:1R:118:ARG:HG3	1.98	0.46
1:1A:1171:G:H2'	1:1A:1172:C:C5	2.50	0.46
1:1A:2011:U:OP1	20:1W:42:LYS:NZ	2.25	0.46
3:1D:131:PRO:HG3	3:1D:189:ARG:NE	2.31	0.46
12:1O:4:GLU:O	12:1O:5:GLN:HB2	2.16	0.46
23:1Z:24:ASN:OD1	23:1Z:44:HIS:HB3	2.16	0.46
28:15:52:ARG:HG3	28:15:54:VAL:HG13	1.98	0.45
17:1T:27:GLU:OE1	17:1T:87:LYS:HE3	2.17	0.45
23:1Z:21:ARG:HA	23:1Z:25:LYS:O	2.16	0.45
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.51	0.45
1:1A:742:A:H2'	1:1A:743:A:C8	2.51	0.45
7:1H:9:VAL:O	7:1H:49:THR:HA	2.16	0.45
12:1O:58:LEU:HD11	12:1O:86:LEU:HD22	1.97	0.45
17:1T:106:LYS:HE3	17:1T:109:ARG:NH2	2.30	0.45
22:1Y:2:ALA:HA	22:1Y:85:PHE:HE2	1.80	0.45
3:1D:261:LYS:HA	3:1D:264:ASP:OD2	2.16	0.45
1:1A:2772:C:H5'	4:1E:173:GLN:NE2	2.31	0.45
8:1I:115:VAL:HA	8:1I:132:PHE:CD1	2.52	0.45
8:1I:72:ILE:HG23	8:1I:142:VAL:HG23	1.97	0.45
10:1K:80:LEU:HD23	10:1K:109:ILE:HD13	1.98	0.45
10:1K:21:SER:O	10:1K:26:PRO:HD2	2.17	0.45
1:1A:335:C:H5''	22:1Y:82:ARG:HD3	1.99	0.45
1:1A:155:A:H2'	1:1A:156:A:C8	2.52	0.45
1:1A:900:A:H4'	1:1A:1832:C:C5'	87.12	0.45
4:1E:25:THR:HG21	4:1E:193:VAL:HG22	1.97	0.45
6:1G:16:LEU:HD13	6:1G:29:PRO:HD2	1.98	0.45
8:1I:53:GLU:O	8:1I:57:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1K:18:ALA:C	10:1K:20:PRO:HD3	2.37	0.45
1:1A:2636:C:H4'	4:1E:81:GLU:OE1	2.17	0.45
5:1F:151:GLY:HA3	5:1F:191:ASP:OD2	2.16	0.45
1:1A:2667:C:H1'	7:1H:109:PHE:CD1	2.51	0.45
1:1A:953:G:OP2	14:1Q:18[B]:ARG:NH1	2.50	0.45
1:1A:1224:U:H4'	19:1V:88:GLY:O	2.16	0.45
30:17:34:ARG:HD3	30:17:42:LEU:HA	1.98	0.45
1:1A:154:U:O4	1:1A:155:A:N6	3.08	0.45
4:1E:99:GLU:HG2	4:1E:182:ALA:HB2	1.99	0.45
17:1T:43:PHE:HE2	17:1T:61:VAL:HB	1.80	0.45
1:1A:1442:U:H2'	1:1A:1443:U:C6	2.52	0.45
1:1A:2895:G:H2'	1:1A:2896:C:C6	2.52	0.45
1:1A:845:A:H5'	1:1A:846:U:OP2	2.17	0.45
8:1I:127:GLU:HG2	8:1I:145:ASN:ND2	2.32	0.45
2:1B:90:C:H5'	14:1Q:18[B]:ARG:CG	2.46	0.45
15:1R:10:LEU:HB3	15:1R:12:ARG:NH2	2.32	0.45
17:1T:22:PRO:HD3	17:1T:50:ILE:HD12	1.99	0.45
21:1X:6:ARG:O	21:1X:10:VAL:HG23	2.16	0.45
14:1Q:56:ALA:HB2	14:1Q:119:LEU:HD12	1.99	0.45
24:10:15:ASP:OD1	24:10:16:SER:N	2.49	0.45
1:1A:1297:C:OP1	1:1A:2710:C:H4'	2.16	0.45
3:1D:69:ARG:NH2	3:1D:116:ILE:HD12	2.32	0.45
3:1D:43:ARG:HA	3:1D:48:ARG:O	2.17	0.45
9:1J:27:VAL:HG13	9:1J:80:THR:HG23	1.99	0.45
10:1K:53:LEU:HD21	10:1K:82:LYS:NZ	2.32	0.45
11:1N:30:THR:O	11:1N:34:ARG:HG3	2.15	0.45
1:1A:464:U:H5'	30:17:5:PHE:CD1	2.52	0.45
1:1A:1794:A:H2'	1:1A:1795:C:C6	2.52	0.45
1:1A:26:G:C6	1:1A:27:G:N1	2.85	0.45
1:1A:254:G:H4'	14:1Q:71:LYS:HZ1	73.23	0.45
1:1A:95:A:O2'	26:12:41:HIS:ND1	2.32	0.44
1:1A:1084:A:C8	9:1J:54:VAL:HB	2.52	0.44
1:1A:1418:G:H2'	1:1A:1579:A:N6	2.32	0.44
1:1A:427:U:OP1	3:1D:13:ARG:NH2	89.09	0.44
3:1D:34:LEU:HD21	3:1D:63:ARG:HD3	1.99	0.44
1:1A:523:C:H4'	1:1A:540:C:O2	2.17	0.44
2:1B:48:U:H2'	2:1B:49:C:C6	2.52	0.44
4:1E:4:LEU:HD22	4:1E:32:ASN:ND2	2.32	0.44
5:1F:149:ILE:HB	5:1F:188:MET:HG2	1.99	0.44
5:1F:49:ARG:NH1	5:1F:72:SER:HB3	2.32	0.44
8:1I:4:ILE:HG21	8:1I:47:PHE:CD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:102:U:H2'	1:1A:102:U:O2	2.18	0.44
1:1A:1239:G:H2'	1:1A:1240:U:O4'	2.17	0.44
1:1A:1540:G:H2'	1:1A:1541:C:C6	2.53	0.44
1:1A:395:U:O2'	1:1A:396:G:N7	2.39	0.44
1:1A:57:C:H2'	1:1A:58:G:O4'	2.17	0.44
3:1D:171:TYR:HE1	3:1D:185:GLU:HB3	1.82	0.44
3:1D:201:MET:HG3	3:1D:202:LEU:HD12	1.98	0.44
1:1A:2772:C:H5'	4:1E:173:GLN:HE21	1.82	0.44
5:1F:62:GLN:NE2	5:1F:69:ARG:HD2	2.30	0.44
6:1G:56:ASP:OD2	6:1G:150:ARG:NH2	2.51	0.44
17:1T:106:LYS:CE	17:1T:109:ARG:HH22	2.29	0.44
1:1A:572:A:H5'	19:1V:79:ARG:HH22	1.82	0.44
1:1A:518:G:O5'	20:1W:18:ARG:NH1	2.51	0.44
1:1A:1808:A:C5	25:11:28:ARG:NH1	2.86	0.44
15:1R:98:LEU:HD12	28:15:55:ILE:HD11	1.99	0.44
1:1A:184:C:H2'	1:1A:185:G:C8	2.53	0.44
1:1A:1869:G:H5'	1:1A:1870:C:OP2	2.18	0.44
3:1D:133:ARG:NH2	3:1D:187:ASP:OD1	2.51	0.44
16:1S:17:LYS:O	16:1S:20:GLU:HG2	2.16	0.44
21:1X:70:HIS:N	21:1X:73:ARG:O	2.50	0.44
1:1A:1225:G:H4'	19:1V:86:GLN:HE21	1.81	0.44
1:1A:1847:G:P	1:1A:1847:G:H8	2.41	0.44
1:1A:571:U:H5'	1:1A:819:A:C5	19.07	0.44
1:1A:612:G:H2'	1:1A:614:A:C8	2.52	0.44
7:1H:69:ARG:NH1	7:1H:73:ASN:HB2	2.33	0.44
16:1S:71:ALA:HB2	16:1S:102:ARG:CG	2.46	0.44
18:1U:19:LYS:HG3	18:1U:22:LYS:HE2	2.00	0.44
30:17:12:ARG:NH2	30:17:13:ASN:OD1	2.50	0.44
3:1D:244:PRO:O	3:1D:252:THR:HG22	2.17	0.44
5:1F:168:ASP:OD2	5:1F:170:ARG:NH1	2.50	0.44
5:1F:59:PRO:HB2	5:1F:60:TRP:CE3	2.52	0.44
27:13:40:ASP:OD1	27:13:45:ARG:NE	2.49	0.44
1:1A:1668:A:O2'	1:1A:1674:G:N7	2.45	0.44
1:1A:851:C:OP1	27:13:19:LYS:HD3	2.18	0.44
1:1A:2031:A:C6	1:1A:2498:OMC:H1'	2.53	0.44
3:1D:171:TYR:CE1	3:1D:185:GLU:HB3	2.52	0.44
9:1J:32:GLY:O	9:1J:105:LYS:HD2	2.18	0.44
11:1N:142:ILE:HA	11:1N:142:ILE:HD12	1.74	0.44
1:1A:301:G:P	22:1Y:82:ARG:HH12	2.41	0.44
23:1Z:51:GLN:NE2	23:1Z:86:LEU:HD21	2.29	0.44
29:16:13:SER:HA	29:16:49:TYR:HD1	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1125:G:C6	1:1A:1126:A:N6	2.86	0.44
1:1A:550:C:C2'	1:1A:551:G:H5''	2.46	0.44
2:1B:28:C:OP1	16:1S:31:THR:HG21	2.18	0.44
9:1J:92:ALA:O	9:1J:95:LEU:N	2.51	0.44
10:1K:100:LYS:HA	10:1K:139:VAL:O	2.17	0.44
32:19:2:LYS:HB3	32:19:35:GLN:HG2	1.99	0.43
1:1A:725:G:C6	1:1A:726:G:N1	2.86	0.43
5:1F:124:PHE:HE2	5:1F:157:LEU:HD11	1.81	0.43
1:1A:2667:C:H1'	7:1H:109:PHE:HD1	1.83	0.43
8:1I:26:ALA:HA	8:1I:30:LEU:HB2	2.00	0.43
18:1U:21:ALA:HA	18:1U:24:TYR:CE2	2.53	0.43
18:1U:41:LYS:NZ	18:1U:45:TYR:OH	2.46	0.43
1:1A:2339:C:H2'	1:1A:2340:A:C8	2.53	0.43
1:1A:1638:C:H4'	1:1A:2710:C:O2	2.17	0.43
3:1D:262:ARG:HG3	3:1D:263:THR:HG23	1.99	0.43
9:1J:113:PHE:CD2	9:1J:114:GLU:HG3	2.53	0.43
24:10:72:LYS:HB2	24:10:79:PHE:CE2	2.53	0.43
25:11:4:VAL:HG22	25:11:11:ARG:HE	1.83	0.43
1:1A:2017:U:H4'	28:15:5:GLN:O	2.18	0.43
1:1A:1881:C:H2'	1:1A:1882:U:O4'	2.18	0.43
1:1A:2636:C:H2'	1:1A:2637:U:C6	2.53	0.43
1:1A:493:G:H2'	1:1A:494:G:O4'	2.18	0.43
4:1E:118:PHE:CE1	4:1E:163:GLY:HA2	2.53	0.43
4:1E:186:LEU:HD23	4:1E:186:LEU:HA	1.81	0.43
1:1A:1223:G:N1	1:1A:1226:A:OP2	2.49	0.43
1:1A:2039:U:H2'	1:1A:2040:G:C8	2.54	0.43
1:1A:2421:G:P	29:16:8:LYS:HZ1	2.42	0.43
4:1E:56:LYS:HE3	4:1E:56:LYS:HB3	1.79	0.43
5:1F:70:SER:HB2	5:1F:78:TRP:CZ2	2.53	0.43
17:1T:43:PHE:CE1	17:1T:63:LYS:HE3	2.53	0.43
1:1A:372:G:O2'	25:11:54:LYS:NZ	2.39	0.43
1:1A:518:G:H4'	20:1W:18:ARG:CZ	2.49	0.43
19:1V:68:ARG:HH11	19:1V:90:ARG:HB2	1.83	0.43
1:1A:1447:C:H2'	1:1A:1448:G:C8	2.53	0.43
1:1A:2532:G:O2'	1:1A:2657:A:N1	2.50	0.43
1:1A:2886[A]:A:C6	1:1A:2887[A]:A:C5	3.07	0.43
1:1A:651:G:H5'	31:18:19:LYS:HG3	2.01	0.43
1:1A:720:U:H2'	1:1A:721:A:C8	2.53	0.43
6:1G:105:THR:HG22	6:1G:106:ILE:HG23	1.99	0.43
15:1R:102:PHE:HD1	15:1R:109:PRO:HA	1.84	0.43
1:1A:1007:C:H5''	11:1N:37:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2800:A:C2	1:1A:2895:G:H1'	2.54	0.43
1:1A:713:G:H5'	3:1D:175:ARG:HH22	57.62	0.43
5:1F:90:GLN:HG3	5:1F:92:HIS:CE1	2.54	0.43
13:1P:123:ARG:NH2	13:1P:143:GLU:OE2	2.49	0.43
1:1A:2262:U:P	24:10:19:LYS:HZ3	2.40	0.43
27:13:41:THR:OG1	27:13:44:ILE:HG12	2.18	0.43
1:1A:1997:C:OP2	4:1E:129:THR:OG1	2.29	0.43
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.54	0.43
3:1D:210:ALA:O	3:1D:214:ARG:NH1	2.51	0.43
9:1J:68:PRO:HD2	9:1J:69:PHE:CE2	2.53	0.43
24:10:37:ILE:HG21	24:10:80:ILE:HG21	2.01	0.43
31:18:39:LYS:HG3	31:18:42:ARG:NH1	2.34	0.43
1:1A:2386:A:C2	24:10:41[A]:ARG:HG3	2.53	0.43
3:1D:144:VAL:HB	3:1D:154:LEU:HB2	2.00	0.43
11:1N:72:LYS:HE3	11:1N:74:TYR:HE1	1.84	0.43
1:1A:2394:C:H5''	13:1P:63:LYS:HE2	2.00	0.43
1:1A:1187:G:H5''	19:1V:83:TYR:CZ	2.54	0.43
1:1A:1095:A:H61	10:1K:30:GLN:NE2	2.13	0.43
1:1A:191:A:H2'	1:1A:192:C:C6	2.54	0.43
1:1A:545:U:H3'	1:1A:546:U:H4'	2.01	0.43
1:1A:728:G:H4'	3:1D:13:ARG:CD	2.46	0.43
6:1G:36:LEU:HD12	6:1G:61:SER:HB3	2.00	0.43
23:1Z:47:VAL:O	23:1Z:51:GLN:HG2	2.19	0.43
28:15:34:SER:HB3	28:15:48:TYR:CD2	2.54	0.42
31:18:42:ARG:HA	31:18:45:ARG:NH1	2.34	0.42
1:1A:1182:G:H2'	1:1A:1183:U:O4'	2.19	0.42
1:1A:1746:A:H2'	1:1A:1747:U:C6	2.54	0.42
6:1G:67:ILE:O	6:1G:67:ILE:HG13	2.19	0.42
6:1G:73:SER:CB	6:1G:80:ARG:HA	2.48	0.42
8:1I:142:VAL:HG12	8:1I:143:ILE:N	2.34	0.42
13:1P:132:ARG:HG3	13:1P:142:ILE:HD13	2.00	0.42
18:1U:44:GLN:NE2	19:1V:77:PHE:HD2	2.17	0.42
20:1W:39:THR:HG22	20:1W:41:LYS:HG2	2.00	0.42
1:1A:1417:C:H2'	1:1A:1418:G:O4'	2.19	0.42
1:1A:1992:G:N2	1:1A:1996:C:O2'	2.52	0.42
1:1A:2819:G:H2'	1:1A:2821:A:N7	2.34	0.42
1:1A:335:C:OP2	22:1Y:82:ARG:NH2	2.53	0.42
1:1A:362:A:H3'	1:1A:363:G:H8	1.83	0.42
1:1A:2600:A:N7	3:1D:236:GLU:HG2	2.34	0.42
4:1E:13:ARG:HG2	17:1T:56:HIS:CE1	2.53	0.42
5:1F:73:ILE:HA	5:1F:78:TRP:HZ3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:40:VAL:HG23	6:1G:86:GLY:HA2	2.01	0.42
26:12:26:PHE:HD1	26:12:29:ARG:NH1	2.15	0.42
1:1A:2184:A:H2'	1:1A:2185:U:C6	2.53	0.42
2:1B:13:G:H1	2:1B:69:G:HO2'	1.68	0.42
7:1H:95:ARG:HD2	7:1H:128:GLN:CB	2.46	0.42
14:1Q:51:ARG:O	14:1Q:55:ARG:NH1	2.52	0.42
1:1A:833:A:H2'	1:1A:834:G:C8	2.54	0.42
25:11:18:ARG:NH2	25:11:24:ALA:HB2	2.31	0.42
28:15:48:TYR:CE1	28:15:53:LYS:HD3	2.54	0.42
1:1A:1799:G:H3'	3:1D:258:ARG:HH12	1.84	0.42
1:1A:2117:A:H61	1:1A:2171:A:H61	1.66	0.42
1:1A:280:U:H2'	1:1A:281:C:C6	2.54	0.42
1:1A:1806:C:H1'	3:1D:44:ASN:HD21	1.83	0.42
10:1K:93:PRO:HB3	10:1K:137:GLY:N	2.34	0.42
13:1P:78:ARG:HG2	13:1P:113:ALA:HB3	2.02	0.42
1:1A:1365:A:OP1	25:11:28:ARG:NH2	2.46	0.42
1:1A:2020:A:H5'	28:15:9:THR:HG22	2.02	0.42
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.55	0.42
4:1E:13:ARG:NH1	17:1T:56:HIS:HA	2.34	0.42
9:1J:103:ASN:O	9:1J:105:LYS:N	2.52	0.42
9:1J:21:GLY:HA3	9:1J:86:MET:HE1	2.01	0.42
21:1X:34:VAL:HG21	21:1X:43:ILE:HD11	2.01	0.42
1:1A:1796:U:H2'	1:1A:1797:G:H8	1.84	0.42
1:1A:2566:A:H4'	1:1A:2567:G:H5''	2.01	0.42
3:1D:161:TYR:HB3	3:1D:194:GLU:HG2	2.02	0.42
7:1H:94:TYR:CD1	7:1H:107:LEU:HA	2.55	0.42
8:1I:85:GLY:HA2	8:1I:91:PHE:CZ	2.55	0.42
1:1A:1665:A:O2'	12:1O:1:MET:HB3	2.19	0.42
12:1O:2:ILE:HD12	12:1O:8:LEU:HD11	2.02	0.42
13:1P:85:VAL:HB	13:1P:94:THR:CG2	2.48	0.42
16:1S:53:THR:HB	16:1S:65:THR:HB	2.02	0.42
1:1A:139:U:O2'	1:1A:141:G:N1	2.51	0.42
1:1A:1650:A:H4'	15:1R:103:ARG:NH2	2.34	0.42
1:1A:2831:G:OP1	4:1E:56:LYS:HE2	2.20	0.42
9:1J:24:SER:OG	9:1J:85:SER:OG	2.09	0.42
17:1T:71:GLU:OE2	17:1T:101:ARG:NE	2.52	0.42
1:1A:927:A:O2'	27:13:39:GLU:OE2	2.35	0.42
1:1A:394:C:N4	1:1A:395:U:O4	2.53	0.42
1:1A:933:A:H5'	1:1A:934:U:OP2	2.20	0.42
9:1J:107:GLU:O	9:1J:108:VAL:HB	2.19	0.42
13:1P:85:VAL:HG21	13:1P:90:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1R:35:LYS:HE3	15:1R:100:CYS:SG	2.59	0.42
1:1A:372:G:H5''	25:11:61:LYS:HD3	2.01	0.42
26:12:25:GLN:O	26:12:29:ARG:HG3	2.20	0.42
1:1A:12:U:O2	1:1A:12:U:H2'	2.20	0.42
3:1D:79:GLU:OE2	3:1D:95:LEU:HB2	2.20	0.42
13:1P:56:PRO:O	13:1P:60:ARG:HG3	2.20	0.42
27:13:45:ARG:HH22	27:13:57:VAL:HG11	1.85	0.41
1:1A:937:C:OP1	31:18:52:LYS:HD2	2.20	0.41
9:1J:65:GLU:HA	9:1J:70:GLU:HG2	2.01	0.41
11:1N:47:HIS:CE1	11:1N:48:VAL:HG23	2.55	0.41
27:13:17:LEU:HD12	27:13:20:HIS:CE1	2.55	0.41
27:13:5:ILE:HG21	27:13:45:ARG:NH1	2.35	0.41
1:1A:1385:A:O2'	1:1A:1396:U:O2	2.36	0.41
1:1A:118:A:N3	1:1A:178:G:H1'	2.35	0.41
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.20	0.41
1:1A:2095:A:H2'	1:1A:2096:C:O4'	2.20	0.41
1:1A:2346:A:H3'	1:1A:2347:C:H5''	2.01	0.41
3:1D:29:PRO:HG2	3:1D:34:LEU:HD11	2.03	0.41
9:1J:31:ARG:NE	9:1J:79:PRO:HG3	2.31	0.41
9:1J:8:LYS:HE2	9:1J:8:LYS:HB2	1.87	0.41
31:18:7:VAL:HB	31:18:61:CYS:HB3	2.01	0.41
1:1A:2054:A:H2'	28:15:5:GLN:OE1	2.20	0.41
1:1A:2530:A:N6	7:1H:156:PRO:HG3	2.35	0.41
1:1A:388:G:N7	1:1A:390:U:H2'	2.35	0.41
2:1B:104:A:H2'	2:1B:105:G:O4'	2.20	0.41
5:1F:26:ALA:HB2	13:1P:9:ALA:HB2	2.02	0.41
11:1N:31:GLU:OE2	11:1N:35:ARG:NE	2.53	0.41
1:1A:2728:U:O2'	1:1A:2729:G:H5''	2.20	0.41
1:1A:2751:G:OP2	7:1H:3:ARG:HD2	2.19	0.41
1:1A:576:U:H2'	1:1A:577:G:C8	2.55	0.41
1:1A:679:C:H42	1:1A:711:G:H1	85.29	0.41
2:1B:66:A:N6	2:1B:107:G:H2'	2.35	0.41
7:1H:52:PHE:HZ	7:1H:72:LEU:HD22	1.83	0.41
10:1K:106:LEU:HD11	10:1K:140:VAL:HG11	2.01	0.41
1:1A:2262:U:H5''	24:10:41[A]:ARG:HH12	1.84	0.41
31:18:62:LEU:HB3	31:18:65:ALA:HB2	2.02	0.41
7:1H:170:ARG:NH2	32:19:29:ALA:O	2.42	0.41
1:1A:2311:A:C2	6:1G:77:PHE:HB3	2.56	0.41
1:1A:2489:U:C4	1:1A:2490:G:C6	3.09	0.41
7:1H:166:ASP:OD1	7:1H:167:GLU:N	2.54	0.41
14:1Q:55:ARG:HB2	14:1Q:55:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1V:41:ILE:HD13	19:1V:103:ALA:HA	2.02	0.41
29:16:17:THR:HG21	29:16:42:VAL:HB	2.02	0.41
1:1A:1175:A:N3	1:1A:1175:A:H2'	2.36	0.41
1:1A:2328:A:H2'	1:1A:2329:U:C6	2.55	0.41
1:1A:588:U:H2'	1:1A:589:U:C6	2.55	0.41
1:1A:634:C:H2'	1:1A:635:C:C6	2.55	0.41
30:17:34:ARG:HG3	30:17:39:ARG:CG	2.41	0.41
1:1A:1087:G:N2	1:1A:1099:G:H1'	17.29	0.41
1:1A:1539:U:H2'	1:1A:1540:G:C8	2.56	0.41
1:1A:1740:G:H2'	1:1A:1741:C:O4'	2.21	0.41
1:1A:2168:G:H2'	1:1A:2168:G:N3	2.34	0.41
1:1A:2272:U:H5''	1:1A:2273:A:OP1	2.21	0.41
1:1A:45:G:N7	1:1A:215:G:O2'	2.49	0.41
4:1E:55:LYS:HD3	4:1E:60:VAL:HG22	2.03	0.41
5:1F:154:ASP:HB3	5:1F:157:LEU:HB3	2.01	0.41
11:1N:118:MET:HA	11:1N:121:LYS:HZ1	1.84	0.41
17:1T:4:ILE:HD12	17:1T:4:ILE:H	1.85	0.41
24:10:41[B]:ARG:HD3	24:10:41[B]:ARG:HA	1.88	0.41
31:18:16:LYS:HA	31:18:22:PHE:CD1	2.54	0.41
1:1A:1199:U:H2'	1:1A:1200:C:C6	2.54	0.41
1:1A:747:5MU:O2	1:1A:2014:A:H1'	2.20	0.41
1:1A:2324:U:H3'	1:1A:2325:G:H5''	2.02	0.41
1:1A:48:G:N2	1:1A:49:A:N1	2.68	0.41
1:1A:544:C:H3'	1:1A:545:U:C2	2.56	0.41
2:1B:90:C:H5'	14:1Q:18[B]:ARG:HG2	2.01	0.41
4:1E:38:LYS:O	4:1E:46:ARG:HA	2.20	0.41
11:1N:136:GLN:HG3	11:1N:136:GLN:H	1.30	0.41
13:1P:19:LEU:HD23	13:1P:27:LEU:HB3	2.02	0.41
1:1A:2822:G:O6	15:1R:2:ARG:HD3	2.20	0.41
18:1U:44:GLN:HE22	19:1V:77:PHE:HD2	1.67	0.41
23:1Z:21:ARG:HE	23:1Z:87:GLN:HA	1.85	0.41
23:1Z:53:LYS:HB3	23:1Z:55:GLU:OE1	2.21	0.41
24:10:69:PHE:CD1	24:10:80:ILE:HG12	2.56	0.41
1:1A:1585:C:H2'	1:1A:1586:A:O4'	2.21	0.41
1:1A:1655:A:H1'	4:1E:118:PHE:CD2	2.56	0.41
1:1A:640:C:H2'	1:1A:641:U:C6	2.56	0.41
1:1A:1817:G:H5''	3:1D:87:ARG:CG	2.50	0.41
4:1E:52:THR:HG23	4:1E:77:ARG:NH2	2.36	0.41
7:1H:26:ILE:HG22	7:1H:79:VAL:HG21	2.03	0.41
15:1R:28:LEU:HD23	15:1R:48:VAL:HG11	2.03	0.41
29:16:19:HIS:HE1	29:16:21:TYR:CE1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:608:A:C6	1:1A:609:A:C6	3.08	0.41
4:1E:47:ALA:HA	4:1E:84:LEU:HG	2.03	0.41
10:1K:117:MET:HG3	10:1K:125:MET:HB3	2.02	0.41
19:1V:61:ALA:HB2	19:1V:98:ILE:HD13	2.03	0.41
23:1Z:74:ALA:HA	23:1Z:91:PHE:HD1	1.86	0.41
28:15:9:THR:OG1	28:15:12:LYS:HG2	2.21	0.41
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.55	0.41
1:1A:1939:5MU:OP1	1:1A:2604:PSU:O2'	2.35	0.41
1:1A:629:G:H4'	1:1A:650:C:O2	2.21	0.41
1:1A:686:U:H2'	1:1A:788:A:N1	2.36	0.41
11:1N:32:LEU:O	11:1N:36:LEU:HG	2.20	0.41
1:1A:1494:A:HO2'	1:1A:1495:A:P	2.43	0.40
1:1A:1796:U:H2'	1:1A:1797:G:C8	2.57	0.40
1:1A:945:A:C4	1:1A:2448:A:C2	3.09	0.40
1:1A:2069:G7M:C2'	1:1A:2070:A:O5'	2.69	0.40
1:1A:851:C:H2'	1:1A:852:U:H6	1.86	0.40
1:1A:729:G:C5	3:1D:207:LYS:HB2	2.57	0.40
5:1F:195:GLN:O	5:1F:199:MET:HG3	2.21	0.40
18:1U:36:PHE:HZ	19:1V:84:ARG:HH22	1.69	0.40
1:1A:994:C:H3'	18:1U:54:LYS:HE3	2.03	0.40
28:15:36:GLU:OE1	28:15:44:THR:HB	2.21	0.40
1:1A:2528:U:H2'	1:1A:2530:A:O5'	2.22	0.40
1:1A:2312:U:H2'	6:1G:37:ASN:HD21	1.86	0.40
9:1J:29:ASP:OD1	9:1J:79:PRO:HG2	2.20	0.40
10:1K:32:GLY:O	10:1K:65:ARG:HB3	2.22	0.40
1:1A:17:G:H2'	1:1A:18:U:C6	2.57	0.40
1:1A:2356:U:O3'	24:10:20:ARG:HD3	2.22	0.40
1:1A:620:G:H4'	1:1A:621:A:O5'	2.22	0.40
1:1A:745:1MG:HM11	1:1A:745:1MG:HN21	1.74	0.40
14:1Q:52:ALA:O	14:1Q:56:ALA:N	2.54	0.40
16:1S:51:ALA:HB3	16:1S:78:VAL:HG13	2.04	0.40
22:1Y:87:PHE:CE1	22:1Y:92:LYS:HE2	2.54	0.40
23:1Z:14:LYS:HD3	23:1Z:18:ARG:NH2	2.36	0.40
1:1A:1367:A:O2'	30:17:25:LYS:HE3	2.22	0.40
1:1A:2305:U:O2'	6:1G:133:ARG:NE	2.55	0.40
1:1A:634:C:O5'	1:1A:634:C:H6	2.05	0.40
1:1A:910:A:C6	1:1A:911:A:C6	3.09	0.40
1:1A:934:U:H2'	1:1A:935:C:C6	2.56	0.40
2:1B:48:U:P	16:1S:30:ARG:NH2	2.93	0.40
3:1D:24:LEU:HD23	3:1D:83:TYR:HB2	2.03	0.40
8:1I:121:VAL:HG12	8:1I:121:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1J:38:MET:O	9:1J:42:ARG:HG2	2.20	0.40
1:1A:1083:U:C4'	9:1J:42:ARG:HH12	2.22	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	
3	1D	269/273 (98%)	251 (93%)	17 (6%)	1 (0%)	39	80
4	1E	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
5	1F	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
6	1G	175/179 (98%)	164 (94%)	11 (6%)	0	100	100
7	1H	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
8	1I	147/149 (99%)	132 (90%)	13 (9%)	2 (1%)	14	59
9	1J	133/165 (81%)	114 (86%)	13 (10%)	6 (4%)	3	31
10	1K	132/142 (93%)	122 (92%)	6 (4%)	4 (3%)	5	44
11	1N	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
12	1O	121/123 (98%)	116 (96%)	4 (3%)	1 (1%)	24	69
13	1P	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	1Q	136/136 (100%)	126 (93%)	8 (6%)	2 (2%)	13	57
15	1R	123/127 (97%)	117 (95%)	5 (4%)	1 (1%)	24	69
16	1S	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
17	1T	112/115 (97%)	108 (96%)	3 (3%)	1 (1%)	21	67
18	1U	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
19	1V	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	19	66
20	1W	108/110 (98%)	105 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	1X	91/100 (91%)	87 (96%)	3 (3%)	1 (1%)	17	64
22	1Y	100/104 (96%)	96 (96%)	3 (3%)	1 (1%)	19	66
23	1Z	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
24	10	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
25	11	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
26	12	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
27	13	57/59 (97%)	55 (96%)	1 (2%)	1 (2%)	11	54
28	15	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
29	16	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
30	17	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
31	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	19	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
34	1b	216/241 (90%)	189 (88%)	19 (9%)	8 (4%)	4	38
35	1c	204/233 (88%)	180 (88%)	19 (9%)	5 (2%)	7	48
36	1d	203/206 (98%)	187 (92%)	8 (4%)	8 (4%)	4	36
37	1e	148/167 (89%)	124 (84%)	17 (12%)	7 (5%)	3	30
38	1f	98/135 (73%)	84 (86%)	10 (10%)	4 (4%)	3	34
39	1g	149/179 (83%)	141 (95%)	7 (5%)	1 (1%)	26	72
40	1h	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
41	1i	125/130 (96%)	113 (90%)	6 (5%)	6 (5%)	3	30
42	1j	96/103 (93%)	83 (86%)	7 (7%)	6 (6%)	2	23
43	1k	115/129 (89%)	99 (86%)	13 (11%)	3 (3%)	7	46
44	1l	121/124 (98%)	106 (88%)	9 (7%)	6 (5%)	3	29
45	1m	112/118 (95%)	102 (91%)	9 (8%)	1 (1%)	21	67
46	1n	92/101 (91%)	79 (86%)	8 (9%)	5 (5%)	2	27
47	1o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
48	1p	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	7	48
49	1q	78/84 (93%)	62 (80%)	12 (15%)	4 (5%)	2	28
50	1r	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
51	1s	77/92 (84%)	72 (94%)	4 (5%)	1 (1%)	15	60
52	1t	83/87 (95%)	77 (93%)	4 (5%)	2 (2%)	7	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	1u	49/71 (69%)	36 (74%)	8 (16%)	5 (10%)	1	11
All	All	5755/6150 (94%)	5333 (93%)	326 (6%)	96 (2%)	16	55

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	1K	15	ALA
10	1K	19	ASN
14	1Q	51	ARG
22	1Y	52	LEU
36	1d	30	THR
37	1e	105	ILE
41	1i	55	VAL
41	1i	91	ASP
41	1i	129	LYS
43	1k	127	ARG
44	1l	34	CYS
46	1n	92	GLU
49	1q	51	ASN
53	1u	9	ASN
53	1u	40	LYS
8	1I	118	PRO
9	1J	67	THR
9	1J	106	PHE
9	1J	108	VAL
10	1K	23	PRO
10	1K	25	GLY
12	1O	108	ARG
14	1Q	52	ALA
19	1V	44	GLY
34	1b	82	ASP
34	1b	193	PRO
35	1c	206	GLU
36	1d	28	ILE
37	1e	12	GLN
37	1e	122	ASN
37	1e	158	GLY
39	1g	114	LYS
41	1i	9	THR
41	1i	13	LYS
41	1i	58	VAL
42	1j	57	VAL

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Mol	Chain	Res	Type
43	1k	89	PRO
44	1l	23	ALA
44	1l	24	LEU
44	1l	76	GLU
45	1m	114	LYS
48	1p	43	ALA
49	1q	17	MET
52	1t	41	ALA
53	1u	24	GLU
9	1J	104	ALA
17	1T	105	GLY
27	13	4	THR
34	1b	68	LEU
36	1d	153	SER
36	1d	165	ARG
36	1d	175	ALA
37	1e	24	THR
38	1f	54	LEU
38	1f	86	ARG
42	1j	95	GLY
46	1n	22	ALA
51	1s	5	LEU
53	1u	10	GLU
34	1b	19	GLN
34	1b	75	ALA
35	1c	80	LYS
35	1c	166	GLU
36	1d	192	SER
36	1d	193	ALA
37	1e	101	GLU
38	1f	63	ASN
44	1l	43	LYS
44	1l	78	SER
46	1n	3	LYS
48	1p	47	GLU
49	1q	76	VAL
53	1u	35	ARG
3	1D	253	LYS
8	1I	122	LEU
15	1R	106	ASP
34	1b	34	ALA
34	1b	149	GLY

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Mol	Chain	Res	Type
34	1b	168	HIS
36	1d	167	LYS
38	1f	94	HIS
42	1j	36	VAL
46	1n	52	PRO
49	1q	80	GLU
52	1t	68	HIS
9	1J	130	PRO
42	1j	41	PRO
42	1j	42	LEU
21	1X	90	GLY
35	1c	66	VAL
37	1e	143	GLY
42	1j	100	ILE
9	1J	88	HIS
35	1c	81	GLY
43	1k	92	GLY
46	1n	34	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	216/218 (99%)	216 (100%)	0	100	100
4	1E	163/163 (100%)	163 (100%)	0	100	100
5	1F	165/165 (100%)	165 (100%)	0	100	100
6	1G	147/150 (98%)	146 (99%)	1 (1%)	88	96
7	1H	137/138 (99%)	136 (99%)	1 (1%)	88	96
8	1I	114/114 (100%)	114 (100%)	0	100	100
9	1J	103/123 (84%)	102 (99%)	1 (1%)	82	93
10	1K	104/110 (94%)	104 (100%)	0	100	100
11	1N	116/116 (100%)	114 (98%)	2 (2%)	68	89
12	1O	104/104 (100%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	1P	103/103 (100%)	103 (100%)	0	100	100
14	1Q	111/109 (102%)	106 (96%)	5 (4%)	34	74
15	1R	102/103 (99%)	101 (99%)	1 (1%)	82	93
16	1S	87/87 (100%)	87 (100%)	0	100	100
17	1T	99/100 (99%)	99 (100%)	0	100	100
18	1U	89/90 (99%)	88 (99%)	1 (1%)	80	92
19	1V	84/84 (100%)	84 (100%)	0	100	100
20	1W	93/93 (100%)	93 (100%)	0	100	100
21	1X	80/84 (95%)	80 (100%)	0	100	100
22	1Y	83/85 (98%)	83 (100%)	0	100	100
23	1Z	78/78 (100%)	78 (100%)	0	100	100
24	10	58/63 (92%)	58 (100%)	0	100	100
25	11	67/68 (98%)	67 (100%)	0	100	100
26	12	54/55 (98%)	54 (100%)	0	100	100
27	13	49/49 (100%)	49 (100%)	0	100	100
28	15	47/48 (98%)	47 (100%)	0	100	100
29	16	45/49 (92%)	45 (100%)	0	100	100
30	17	38/38 (100%)	38 (100%)	0	100	100
31	18	51/52 (98%)	51 (100%)	0	100	100
32	19	34/34 (100%)	34 (100%)	0	100	100
34	1b	180/199 (90%)	180 (100%)	0	100	100
35	1c	170/190 (90%)	170 (100%)	0	100	100
36	1d	172/173 (99%)	172 (100%)	0	100	100
37	1e	113/126 (90%)	113 (100%)	0	100	100
38	1f	87/116 (75%)	87 (100%)	0	100	100
39	1g	124/147 (84%)	124 (100%)	0	100	100
40	1h	104/105 (99%)	104 (100%)	0	100	100
41	1i	105/107 (98%)	105 (100%)	0	100	100
42	1j	86/90 (96%)	86 (100%)	0	100	100
43	1k	90/99 (91%)	90 (100%)	0	100	100
44	1l	103/104 (99%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	1m	92/96 (96%)	92 (100%)	0	100	100
46	1n	79/84 (94%)	79 (100%)	0	100	100
47	1o	75/77 (97%)	75 (100%)	0	100	100
48	1p	65/65 (100%)	65 (100%)	0	100	100
49	1q	74/78 (95%)	74 (100%)	0	100	100
50	1r	48/65 (74%)	48 (100%)	0	100	100
51	1s	70/79 (89%)	70 (100%)	0	100	100
52	1t	65/66 (98%)	65 (100%)	0	100	100
53	1u	44/61 (72%)	44 (100%)	0	100	100
All	All	4767/5000 (95%)	4755 (100%)	12 (0%)	95	99

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	1G	67	ILE
7	1H	43	VAL
9	1J	82	ILE
11	1N	136	GLN
11	1N	142	ILE
14	1Q	54	THR
14	1Q	55	ARG
14	1Q	58	LYS
14	1Q	59	ARG
14	1Q	60	GLN
15	1R	63	ARG
18	1U	41	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	200	HIS
3	1D	239	ASN
4	1E	32	ASN
4	1E	49	GLN
4	1E	130	GLN
5	1F	92	HIS
5	1F	165	HIS
6	1G	37	ASN

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Mol	Chain	Res	Type
6	1G	63	GLN
7	1H	88	GLN
7	1H	139	GLN
8	1I	66	ASN
8	1I	145	ASN
10	1K	30	GLN
11	1N	80	HIS
14	1Q	13	HIS
16	1S	29	HIS
16	1S	98	GLN
16	1S	100	HIS
17	1T	12	GLN
17	1T	56	HIS
18	1U	37	GLN
18	1U	44	GLN
21	1X	92	ASN
22	1Y	66	GLN
24	10	57	HIS
25	11	17	ASN
25	11	34	HIS
26	12	58	ASN
27	13	20	HIS
28	15	42	HIS
29	16	19	HIS
31	18	26	HIS
34	1b	15	HIS
35	1c	102	ASN
36	1d	116	GLN
36	1d	136	GLN
38	1f	37	HIS
38	1f	55	HIS
39	1g	28	ASN
40	1h	4	GLN
43	1k	118	HIS
43	1k	119	ASN
44	1l	5	ASN
46	1n	43	ASN
46	1n	49	GLN
48	1p	18	GLN
48	1p	63	GLN
49	1q	31	HIS
50	1r	52	GLN

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Mol	Chain	Res	Type
51	1s	57	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2884/2904 (99%)	360 (12%)	10 (0%)
2	1B	119/120 (99%)	8 (6%)	0
33	1a	1538/1539 (99%)	226 (14%)	0
54	1v	2/9 (22%)	0	0
55	1x	86/87 (98%)	22 (25%)	0
All	All	4629/4659 (99%)	616 (13%)	10 (0%)

All (616) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	A
1	1A	12	U
1	1A	15	G
1	1A	34	U
1	1A	46	G
1	1A	63	A
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	80	G
1	1A	101	A
1	1A	102	U
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	135	U
1	1A	136	G
1	1A	137	U
1	1A	138	U
1	1A	139	U
1	1A	140	C
1	1A	141	G
1	1A	142	A
1	1A	196	A
1	1A	199	A
1	1A	216	A

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Mol	Chain	Res	Type
1	1A	221	A
1	1A	222	A
1	1A	248	G
1	1A	266	G
1	1A	272	A
1	1A	276	U
1	1A	277	G
1	1A	279	A
1	1A	283	G
1	1A	285	G
1	1A	291	G
1	1A	302	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	331	C
1	1A	353	C
1	1A	358	U
1	1A	361	G
1	1A	362	A
1	1A	370	G
1	1A	372	G
1	1A	383	C
1	1A	386	G
1	1A	396	G
1	1A	411	G
1	1A	412	A
1	1A	424	G
1	1A	425	G
1	1A	435	C
1	1A	451	U
1	1A	481	G
1	1A	491	G
1	1A	504	A
1	1A	505	A
1	1A	508	A
1	1A	531	C
1	1A	532	A
1	1A	543	G
1	1A	546	U
1	1A	547	A
1	1A	548	G

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Mol	Chain	Res	Type
1	1A	549	G
1	1A	550	C
1	1A	551	G
1	1A	563	A
1	1A	573	U
1	1A	575	A
1	1A	603	A
1	1A	613	A
1	1A	614	A
1	1A	615	U
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	647	G
1	1A	654	A
1	1A	686	U
1	1A	730	A
1	1A	747	5MU
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	G
1	1A	785	G
1	1A	790	U
1	1A	792	A
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	845	A
1	1A	846	U
1	1A	847	U
1	1A	858	G
1	1A	859	G
1	1A	866	A
1	1A	878	A
1	1A	885	C
1	1A	893	C
1	1A	896	A
1	1A	897	C
1	1A	910	A
1	1A	914	G

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Mol	Chain	Res	Type
1	1A	915	C
1	1A	931	U
1	1A	946	C
1	1A	961	C
1	1A	974	G
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	G
1	1A	1033	U
1	1A	1046	A
1	1A	1047	G
1	1A	1070	A
1	1A	1083	U
1	1A	1088	A
1	1A	1090	A
1	1A	1112	G
1	1A	1128	G
1	1A	1130	U
1	1A	1132	U
1	1A	1133	A
1	1A	1135	C
1	1A	1136	G
1	1A	1142	A
1	1A	1168	G
1	1A	1171	G
1	1A	1172	C
1	1A	1175	A
1	1A	1176	U
1	1A	1177	G
1	1A	1182	G
1	1A	1238	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	G
1	1A	1301	A
1	1A	1352	U

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Mol	Chain	Res	Type
1	1A	1365	A
1	1A	1379	U
1	1A	1383	A
1	1A	1416	G
1	1A	1417	C
1	1A	1428	C
1	1A	1452	G
1	1A	1453	A
1	1A	1482	G
1	1A	1490	A
1	1A	1493	C
1	1A	1494	A
1	1A	1495	A
1	1A	1497	U
1	1A	1510	G
1	1A	1515	A
1	1A	1523	U
1	1A	1532	A
1	1A	1533	C
1	1A	1535	A
1	1A	1536	C
1	1A	1537	G
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1583	A
1	1A	1584	U
1	1A	1585	C
1	1A	1606	C
1	1A	1607	C
1	1A	1608	A
1	1A	1647	U
1	1A	1648	U
1	1A	1649	G
1	1A	1674	G
1	1A	1714	U
1	1A	1715	G
1	1A	1725	U
1	1A	1727	C
1	1A	1729	U
1	1A	1730	C

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Mol	Chain	Res	Type
1	1A	1731	G
1	1A	1738	G
1	1A	1740	G
1	1A	1744	A
1	1A	1755	A
1	1A	1764	C
1	1A	1773	A
1	1A	1782	U
1	1A	1800	C
1	1A	1801	A
1	1A	1808	A
1	1A	1816	C
1	1A	1829	A
1	1A	1858	A
1	1A	1859	U
1	1A	1870	C
1	1A	1871	A
1	1A	1872	A
1	1A	1873	G
1	1A	1876	A
1	1A	1906	G
1	1A	1907	G
1	1A	1913	A
1	1A	1914	C
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1967	C
1	1A	1970	A
1	1A	1972	G
1	1A	1991	U
1	1A	1993	U
1	1A	1997	C
1	1A	2023	C
1	1A	2031	A
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A

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Mol	Chain	Res	Type
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G7M
1	1A	2070	A
1	1A	2093	G
1	1A	2097	A
1	1A	2101	A
1	1A	2105	U
1	1A	2108	A
1	1A	2111	U
1	1A	2112	G
1	1A	2113	U
1	1A	2115	G
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2119	A
1	1A	2121	G
1	1A	2123	G
1	1A	2126	A
1	1A	2128	G
1	1A	2131	U
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2136	G
1	1A	2137	U
1	1A	2145	C
1	1A	2146	C
1	1A	2147	A
1	1A	2148	G
1	1A	2149	U
1	1A	2159	G
1	1A	2160	C
1	1A	2161	C
1	1A	2162	G
1	1A	2163	A
1	1A	2164	C
1	1A	2165	C
1	1A	2167	U
1	1A	2168	G
1	1A	2169	A

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Mol	Chain	Res	Type
1	1A	2170	A
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2177	C
1	1A	2178	C
1	1A	2179	C
1	1A	2181	U
1	1A	2185	U
1	1A	2187	U
1	1A	2188	U
1	1A	2190	G
1	1A	2198	A
1	1A	2204	G
1	1A	2211	A
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2273	A
1	1A	2283	C
1	1A	2286	G
1	1A	2287	A
1	1A	2305	U
1	1A	2308	G
1	1A	2325	G
1	1A	2327	A
1	1A	2333	A
1	1A	2335	A
1	1A	2339	C
1	1A	2347	C
1	1A	2383	G
1	1A	2385	C
1	1A	2406	A
1	1A	2424	C
1	1A	2425	A
1	1A	2435	A
1	1A	2441	U
1	1A	2448	A
1	1A	2476	A
1	1A	2491	U
1	1A	2502	G

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Mol	Chain	Res	Type
1	1A	2504	PSU
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2547	A
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2585	U
1	1A	2586	U
1	1A	2603	G
1	1A	2609	U
1	1A	2613	U
1	1A	2629	U
1	1A	2663	G
1	1A	2682	A
1	1A	2689	U
1	1A	2690	U
1	1A	2714	G
1	1A	2726	A
1	1A	2744	G
1	1A	2748	A
1	1A	2765	A
1	1A	2778	A
1	1A	2791	G
1	1A	2792	A
1	1A	2798	U
1	1A	2799	A
1	1A	2811	G
1	1A	2818	U
1	1A	2820	A
1	1A	2821	A
1	1A	2825	G
1	1A	2836	U
1	1A	2867	G
1	1A	2873	A
1	1A	2874	C
1	1A	2880	C
1	1A	2883	A
1	1A	2891	U
2	1B	25	U
2	1B	35	C

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Mol	Chain	Res	Type
2	1B	45	A
2	1B	56	G
2	1B	66	A
2	1B	89	U
2	1B	90	C
2	1B	109	A
33	1a	5	U
33	1a	7	A
33	1a	9	G
33	1a	32	A
33	1a	39	G
33	1a	47	C
33	1a	48	C
33	1a	51	A
33	1a	70	U
33	1a	71	A
33	1a	74	A
33	1a	83	C
33	1a	85	U
33	1a	87	C
33	1a	88	U
33	1a	95	C
33	1a	97	G
33	1a	108	G
33	1a	116	A
33	1a	120	A
33	1a	121	U
33	1a	122	G
33	1a	130	A
33	1a	131	A
33	1a	149	A
33	1a	164	G
33	1a	182	A
33	1a	183	C
33	1a	204	G
33	1a	207	C
33	1a	208	U
33	1a	210	C
33	1a	211	G
33	1a	212	G
33	1a	247	G
33	1a	251	G

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Mol	Chain	Res	Type
33	1a	266	G
33	1a	267	C
33	1a	279	A
33	1a	280	C
33	1a	289	G
33	1a	298	A
33	1a	321	A
33	1a	328	C
33	1a	329	A
33	1a	330	C
33	1a	332	G
33	1a	347	G
33	1a	352	C
33	1a	354	G
33	1a	356	A
33	1a	367	U
33	1a	372	C
33	1a	378	G
33	1a	397	A
33	1a	406	G
33	1a	411	A
33	1a	412	A
33	1a	413	G
33	1a	421	U
33	1a	422	C
33	1a	424	G
33	1a	429	U
33	1a	430	A
33	1a	451	A
33	1a	452	A
33	1a	459	A
33	1a	467	U
33	1a	468	A
33	1a	478	A
33	1a	479	U
33	1a	481	G
33	1a	485	U
33	1a	486	U
33	1a	496	A
33	1a	497	G
33	1a	509	A
33	1a	511	C

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Mol	Chain	Res	Type
33	1a	518	C
33	1a	527	G
33	1a	532	A
33	1a	547	A
33	1a	559	A
33	1a	563	A
33	1a	564	C
33	1a	571	U
33	1a	572	A
33	1a	573	A
33	1a	576	C
33	1a	577	G
33	1a	596	A
33	1a	633	G
33	1a	642	A
33	1a	650	G
33	1a	665	A
33	1a	687	A
33	1a	695	A
33	1a	702	A
33	1a	703	G
33	1a	721	G
33	1a	723	U
33	1a	731	G
33	1a	733	G
33	1a	747	A
33	1a	755	G
33	1a	777	A
33	1a	787	A
33	1a	792	A
33	1a	793	U
33	1a	794	A
33	1a	814	A
33	1a	815	A
33	1a	817	C
33	1a	828	U
33	1a	829	G
33	1a	832	G
33	1a	841	C
33	1a	842	U
33	1a	843	U
33	1a	844	G

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Mol	Chain	Res	Type
33	1a	845	A
33	1a	846	G
33	1a	873	A
33	1a	880	C
33	1a	885	G
33	1a	900	A
33	1a	914	A
33	1a	926	G
33	1a	934	C
33	1a	935	A
33	1a	960	U
33	1a	969	A
33	1a	971	G
33	1a	975	A
33	1a	976	G
33	1a	977	A
33	1a	983	A
33	1a	993	G
33	1a	1004	A
33	1a	1008	U
33	1a	1018	G
33	1a	1026	G
33	1a	1027	C
33	1a	1030	U
33	1a	1031	C
33	1a	1032	G
33	1a	1033	G
33	1a	1034	G
33	1a	1036	A
33	1a	1043	G
33	1a	1044	A
33	1a	1050	G
33	1a	1054	C
33	1a	1065	U
33	1a	1073	U
33	1a	1088	G
33	1a	1094	G
33	1a	1095	U
33	1a	1101	A
33	1a	1125	U
33	1a	1133	G
33	1a	1134	G

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Mol	Chain	Res	Type
33	1a	1136	C
33	1a	1137	C
33	1a	1139	G
33	1a	1140	C
33	1a	1141	C
33	1a	1142	G
33	1a	1145	A
33	1a	1152	A
33	1a	1159	U
33	1a	1160	G
33	1a	1161	C
33	1a	1168	U
33	1a	1184	G
33	1a	1196	A
33	1a	1197	A
33	1a	1202	U
33	1a	1212	U
33	1a	1213	A
33	1a	1227	A
33	1a	1236	A
33	1a	1238	A
33	1a	1240	U
33	1a	1241	G
33	1a	1253	G
33	1a	1256	A
33	1a	1257	A
33	1a	1261	A
33	1a	1275	A
33	1a	1280	A
33	1a	1285	A
33	1a	1286	U
33	1a	1287	A
33	1a	1293	C
33	1a	1299	A
33	1a	1300	G
33	1a	1302	C
33	1a	1305	G
33	1a	1317	C
33	1a	1318	A
33	1a	1322	C
33	1a	1337	G
33	1a	1346	A

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Mol	Chain	Res	Type
33	1a	1347	G
33	1a	1363	A
33	1a	1364	U
33	1a	1379	G
33	1a	1398	A
33	1a	1429	A
33	1a	1441	A
33	1a	1446	A
33	1a	1492	A
33	1a	1493	A
33	1a	1499	A
33	1a	1503	A
33	1a	1505	G
33	1a	1506	U
33	1a	1507	A
33	1a	1517	G
33	1a	1519	A
33	1a	1529	G
33	1a	1530	G
33	1a	1533	C
33	1a	1535	C
33	1a	1536	C
55	1x	7	G
55	1x	8	U
55	1x	9	G
55	1x	14	A
55	1x	16	U
55	1x	17	U
55	1x	18	G
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	22	G
55	1x	23	A
55	1x	24	C
55	1x	27	G
55	1x	46	G
55	1x	49	C
55	1x	50	A
55	1x	58	U
55	1x	68	A
55	1x	79	U

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Mol	Chain	Res	Type
55	1x	86	C
55	1x	87	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	784	G
1	1A	1494	A
1	1A	1730	C
1	1A	2118	U
1	1A	2127	G
1	1A	2158	A
1	1A	2324	U
1	1A	2406	A
1	1A	2585	U
1	1A	2873	A

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

26 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	6MZ	1A	1618	1	17,25,26	1.00	1 (5%)	15,36,39	2.49	2 (13%)
1	2MG	1A	1835	1	18,26,27	1.16	2 (11%)	21,38,41	2.19	6 (28%)
1	PSU	1A	1911	1	15,21,22	1.36	1 (6%)	16,30,33	2.22	4 (25%)
1	PSU	1A	1915	1	15,21,22	1.37	1 (6%)	16,30,33	2.21	4 (25%)
1	PSU	1A	1917	1	15,21,22	1.34	1 (6%)	16,30,33	2.21	4 (25%)
1	5MU	1A	1939	1	13,22,23	0.59	0	16,32,35	2.47	2 (12%)
1	5MC	1A	1962	1	14,22,23	1.33	1 (7%)	17,32,35	0.82	1 (5%)
1	6MZ	1A	2030	1	17,25,26	0.92	1 (5%)	15,36,39	2.82	3 (20%)
1	G7M	1A	2069	1	18,26,27	0.99	1 (5%)	21,39,42	2.67	8 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	1A	2251	1,55	18,26,27	1.18	2 (11%)	21,38,41	1.92	4 (19%)
1	2MG	1A	2445	1	18,26,27	1.14	2 (11%)	21,38,41	2.30	7 (33%)
1	H2U	1A	2449	1	17,21,22	1.04	2 (11%)	23,30,33	1.95	5 (21%)
1	PSU	1A	2457	1	15,21,22	1.35	1 (6%)	16,30,33	2.06	3 (18%)
1	OMC	1A	2498	1	15,22,23	0.62	0	20,31,34	2.07	1 (5%)
1	2MA	1A	2503	1	17,25,26	1.55	3 (17%)	18,37,40	2.67	1 (5%)
1	PSU	1A	2504	1	15,21,22	1.30	1 (6%)	16,30,33	2.32	4 (25%)
1	OMU	1A	2552	1	14,22,23	0.67	0	19,31,34	1.52	1 (5%)
1	PSU	1A	2580	1	15,21,22	1.46	2 (13%)	16,30,33	2.15	3 (18%)
1	PSU	1A	2604	1	15,21,22	1.33	1 (6%)	16,30,33	2.39	4 (25%)
1	PSU	1A	2605	1	15,21,22	1.42	1 (6%)	16,30,33	2.29	4 (25%)
1	1MG	1A	745	1	17,26,27	1.34	2 (11%)	19,39,42	0.71	0
1	PSU	1A	746	1	15,21,22	1.51	2 (13%)	16,30,33	2.19	3 (18%)
1	5MU	1A	747	1	13,22,23	0.55	0	16,32,35	2.56	2 (12%)
1	PSU	1A	955	1	15,21,22	1.37	1 (6%)	16,30,33	2.09	4 (25%)
4	MEQ	1E	150[A]	4	7,9,10	0.51	0	8,10,12	1.08	1 (12%)
4	MEQ	1E	150[B]	4	7,9,10	0.56	0	8,10,12	1.14	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6MZ	1A	1618	1	-	0/5/27/28	0/3/3/3
1	2MG	1A	1835	1	-	0/5/27/28	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/3/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/3/25/26	0/2/2/2
1	6MZ	1A	2030	1	-	0/5/27/28	0/3/3/3
1	G7M	1A	2069	1	-	0/3/25/26	0/3/3/3
1	OMG	1A	2251	1,55	-	0/5/27/28	0/3/3/3
1	2MG	1A	2445	1	-	0/5/27/28	0/3/3/3
1	H2U	1A	2449	1	-	0/7/38/39	0/2/2/2
1	PSU	1A	2457	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	2498	1	-	0/5/27/28	0/2/2/2
1	2MA	1A	2503	1	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	2504	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1	-	0/5/27/28	0/2/2/2
1	PSU	1A	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2604	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	1MG	1A	745	1	-	0/3/25/26	0/3/3/3
1	PSU	1A	746	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	747	1	-	0/3/25/26	0/2/2/2
1	PSU	1A	955	1	-	0/7/25/26	0/2/2/2
4	MEQ	1E	150[A]	4	-	0/7/9/11	0/0/0/0
4	MEQ	1E	150[B]	4	-	1/7/9/11	0/0/0/0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	746	PSU	C5-C1'	-4.55	1.48	1.52
1	1A	2580	PSU	C5-C1'	-4.49	1.48	1.52
1	1A	2605	PSU	C5-C1'	-4.45	1.48	1.52
1	1A	1911	PSU	C5-C1'	-4.21	1.48	1.52
1	1A	1915	PSU	C5-C1'	-4.20	1.48	1.52
1	1A	955	PSU	C5-C1'	-4.19	1.48	1.52
1	1A	2604	PSU	C5-C1'	-4.16	1.48	1.52
1	1A	2457	PSU	C5-C1'	-4.09	1.48	1.52
1	1A	1917	PSU	C5-C1'	-4.06	1.48	1.52
1	1A	2504	PSU	C5-C1'	-3.86	1.48	1.52
1	1A	2449	H2U	C4-N3	-2.63	1.33	1.37
1	1A	2449	H2U	C2-N3	-2.49	1.33	1.38
1	1A	2580	PSU	O4'-C1'	-2.21	1.41	1.44
1	1A	746	PSU	O4'-C1'	-2.01	1.41	1.44
1	1A	2069	G7M	C6-C5	2.10	1.45	1.41
1	1A	2030	6MZ	C5-C4	2.79	1.46	1.40
1	1A	2445	2MG	C5-C4	2.92	1.47	1.40
1	1A	2503	2MA	C5-C4	3.04	1.47	1.40
1	1A	1835	2MG	C5-C4	3.05	1.47	1.40
1	1A	2251	OMG	C5-C4	3.09	1.47	1.40
1	1A	1618	6MZ	C5-C4	3.16	1.47	1.40
1	1A	745	1MG	C5-C4	3.16	1.47	1.40
1	1A	2445	2MG	C6-C5	3.50	1.48	1.41
1	1A	1835	2MG	C6-C5	3.52	1.48	1.41
1	1A	2503	2MA	C6-N6	3.59	1.35	1.29
1	1A	2251	OMG	C6-C5	3.61	1.48	1.41
1	1A	745	1MG	C6-C5	3.94	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2503	2MA	C6-C5	3.96	1.48	1.40
1	1A	1962	5MC	C5-C4	4.67	1.48	1.41

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	747	5MU	C5-C4-N3	-7.70	118.88	125.35
1	1A	1939	5MU	C5-C4-N3	-7.47	119.07	125.35
1	1A	2030	6MZ	N3-C2-N1	-7.03	123.35	128.87
1	1A	2069	G7M	C2'-C1'-N9	-6.32	96.53	113.47
1	1A	1618	6MZ	N3-C2-N1	-6.09	124.09	128.87
1	1A	2449	H2U	C5-C6-N1	-5.70	104.52	110.76
1	1A	2069	G7M	C1'-N9-C4	-4.98	121.24	126.81
1	1A	2069	G7M	C5-C6-N1	-4.98	117.01	123.52
1	1A	2449	H2U	C4-N3-C2	-4.76	121.46	125.77
1	1A	2604	PSU	C5-C1'-C2'	-4.66	107.53	115.44
1	1A	2504	PSU	C5-C1'-C2'	-4.52	107.76	115.44
1	1A	2605	PSU	C5-C1'-C2'	-4.51	107.77	115.44
1	1A	1835	2MG	C5-C6-N1	-4.33	117.86	123.52
1	1A	2445	2MG	C5-C6-N1	-4.28	117.92	123.52
1	1A	2251	OMG	C5-C6-N1	-4.21	118.02	123.52
1	1A	2605	PSU	C5-C6-N1	-4.15	118.60	124.38
1	1A	746	PSU	C5-C1'-C2'	-4.14	108.41	115.44
1	1A	746	PSU	C5-C6-N1	-4.12	118.64	124.38
1	1A	2580	PSU	C5-C6-N1	-4.09	118.67	124.38
1	1A	1915	PSU	C5-C6-N1	-3.96	118.86	124.38
1	1A	955	PSU	C5-C6-N1	-3.96	118.86	124.38
1	1A	1911	PSU	C5-C6-N1	-3.87	118.99	124.38
1	1A	2457	PSU	C5-C6-N1	-3.75	119.15	124.38
1	1A	1917	PSU	C5-C6-N1	-3.72	119.19	124.38
1	1A	2604	PSU	C5-C6-N1	-3.72	119.19	124.38
1	1A	1917	PSU	C5-C1'-C2'	-3.67	109.20	115.44
1	1A	1915	PSU	C5-C1'-C2'	-3.67	109.21	115.44
1	1A	2251	OMG	N3-C2-N1	-3.61	122.65	127.56
1	1A	2445	2MG	C6-C5-C4	-3.59	116.76	120.86
1	1A	2069	G7M	N3-C2-N1	-3.45	122.86	127.56
1	1A	2030	6MZ	C1'-N9-C4	-3.43	122.98	126.81
1	1A	2445	2MG	CM2-N2-C2	-3.34	119.28	123.03
1	1A	1911	PSU	C5-C1'-C2'	-3.31	109.81	115.44
1	1A	2251	OMG	C6-C5-C4	-3.17	117.23	120.86
1	1A	2504	PSU	C5-C6-N1	-3.15	119.99	124.38
1	1A	1835	2MG	C6-C5-C4	-2.99	117.44	120.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1835	2MG	CM2-N2-C2	-2.94	119.73	123.03
1	1A	955	PSU	C5-C1'-C2'	-2.90	110.50	115.44
1	1A	2069	G7M	O2'-C2'-C3'	-2.46	103.91	111.86
1	1A	2449	H2U	O2-C2-N1	-2.22	120.27	123.17
1	1A	2445	2MG	N3-C2-N1	-2.21	122.88	126.19
4	1E	150[A]	MEQ	O-C-CA	-2.18	119.88	125.72
1	1A	2069	G7M	O3'-C3'-C2'	-2.18	104.82	111.86
1	1A	1835	2MG	N3-C2-N1	-2.14	122.99	126.19
4	1E	150[B]	MEQ	O-C-CA	-2.12	120.03	125.72
4	1E	150[B]	MEQ	CG-CB-CA	-2.10	109.26	114.03
1	1A	2445	2MG	N2-C2-N1	2.19	119.48	116.94
1	1A	1962	5MC	N4-C4-N3	2.28	120.27	116.92
1	1A	2504	PSU	O4'-C1'-C2'	2.29	107.17	104.69
1	1A	2604	PSU	O4'-C1'-C2'	2.46	107.35	104.69
1	1A	1917	PSU	O4'-C1'-C2'	2.66	107.57	104.69
1	1A	2605	PSU	O4'-C1'-C2'	2.68	107.59	104.69
1	1A	1915	PSU	O4'-C1'-C2'	2.69	107.59	104.69
1	1A	955	PSU	O4'-C1'-C2'	2.69	107.60	104.69
1	1A	1911	PSU	O4'-C1'-C2'	2.81	107.73	104.69
1	1A	2449	H2U	N3-C2-N1	2.88	119.31	116.64
1	1A	2457	PSU	O4'-C1'-C2'	3.00	107.93	104.69
1	1A	2069	G7M	O4'-C1'-N9	3.24	114.23	108.11
1	1A	2449	H2U	C6-N1-C2	3.29	127.24	122.16
1	1A	2580	PSU	O4'-C1'-C2'	3.56	108.54	104.69
1	1A	2069	G7M	C6-N1-C2	4.64	121.31	115.88
1	1A	1835	2MG	C6-N1-C2	4.95	122.33	115.24
1	1A	2445	2MG	C6-N1-C2	4.98	122.37	115.24
1	1A	2445	2MG	C2-N3-C4	5.22	120.72	114.99
1	1A	1835	2MG	C2-N3-C4	5.35	120.86	114.99
1	1A	2251	OMG	C6-N1-C2	5.54	122.38	115.88
1	1A	955	PSU	C4-N3-C2	5.78	119.98	115.16
1	1A	2605	PSU	C4-N3-C2	5.86	120.05	115.16
1	1A	2552	OMU	C4-N3-C2	5.97	120.50	114.21
1	1A	1915	PSU	C4-N3-C2	6.12	120.27	115.16
1	1A	1939	5MU	C4-N3-C2	6.14	120.28	115.16
1	1A	746	PSU	C4-N3-C2	6.19	120.32	115.16
1	1A	2580	PSU	C4-N3-C2	6.20	120.33	115.16
1	1A	2457	PSU	C4-N3-C2	6.26	120.38	115.16
1	1A	1917	PSU	C4-N3-C2	6.30	120.42	115.16
1	1A	1911	PSU	C4-N3-C2	6.39	120.49	115.16
1	1A	747	5MU	C4-N3-C2	6.49	120.57	115.16
1	1A	2604	PSU	C4-N3-C2	6.67	120.72	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2504	PSU	C4-N3-C2	6.69	120.74	115.16
1	1A	1618	6MZ	C2-N1-C6	7.18	121.63	116.47
1	1A	2030	6MZ	C2-N1-C6	7.32	121.73	116.47
1	1A	2498	OMC	C6-C5-C4	8.45	120.75	117.44
1	1A	2503	2MA	C2-N3-C4	10.70	120.44	115.29

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	1E	150[B]	MEQ	CG-CD-NE2-CE

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1939	5MU	1	0
1	1A	2030	6MZ	1	0
1	1A	2069	G7M	4	0
1	1A	2251	OMG	1	0
1	1A	2498	OMC	1	0
1	1A	2604	PSU	1	0
1	1A	745	1MG	1	0
1	1A	747	5MU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	6UQ	1A	3001	1	101,105,105	1.59	13 (12%)	125,164,164	2.09	38 (30%)

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
56	6UQ	1A	3001	1	-	0/47/211/211	0/11/11/11

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1A	3001	6UQ	CDF-CAC	-5.41	1.40	1.51
56	1A	3001	6UQ	CAD-CAJ	-4.02	1.40	1.50
56	1A	3001	6UQ	CCL-CCM	-3.35	1.48	1.54
56	1A	3001	6UQ	O1-C1	2.21	1.47	1.41
56	1A	3001	6UQ	OAL-CAM	2.21	1.48	1.44
56	1A	3001	6UQ	OBE-CAX	2.80	1.46	1.41
56	1A	3001	6UQ	OCG-CCB	2.87	1.48	1.41
56	1A	3001	6UQ	OCQ-CCR	2.99	1.46	1.41
56	1A	3001	6UQ	OCP-CCO	3.11	1.48	1.44
56	1A	3001	6UQ	OBQ-CAX	3.25	1.48	1.41
56	1A	3001	6UQ	OCS-CCR	3.45	1.47	1.41
56	1A	3001	6UQ	OBQ-CBP	5.38	1.55	1.43
56	1A	3001	6UQ	OCP-CCJ	6.29	1.47	1.40

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1A	3001	6UQ	CCC-OCH-CCU	-7.83	105.14	118.06
56	1A	3001	6UQ	CCZ-CCO-CCN	-6.58	104.75	114.68
56	1A	3001	6UQ	CBC-CBF-CBG	-6.25	104.14	115.04
56	1A	3001	6UQ	OCI-CCD-CCE	-5.08	97.02	103.51
56	1A	3001	6UQ	CAP-OAQ-CAR	-4.05	104.69	114.31
56	1A	3001	6UQ	OCK-CCE-CCD	-3.82	97.00	103.48
56	1A	3001	6UQ	CDG-CAR-CAM	-3.61	107.44	113.38
56	1A	3001	6UQ	CDF-CAC-CAB	-3.59	115.94	121.42
56	1A	3001	6UQ	CAP-OAS-CAU	-3.44	107.27	114.69
56	1A	3001	6UQ	CDJ-CBC-CBF	-3.40	107.17	112.07
56	1A	3001	6UQ	CAX-CAW-CAV	-3.32	106.58	112.67
56	1A	3001	6UQ	CAP-CAO-CAN	-3.17	105.94	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1A	3001	6UQ	CAA-CAB-CAC	-3.10	119.84	122.56
56	1A	3001	6UQ	CDE-ODD-CAE	-2.75	107.49	114.82
56	1A	3001	6UQ	O4-CBO-OBN	-2.63	103.84	110.69
56	1A	3001	6UQ	CCF-CCE-CCD	-2.61	106.90	112.66
56	1A	3001	6UQ	O2-C2-C3	-2.61	104.10	110.16
56	1A	3001	6UQ	OAY-CAX-CAW	-2.56	107.28	110.87
56	1A	3001	6UQ	CDM-ODL-CBL	-2.53	107.51	114.58
56	1A	3001	6UQ	CCB-O1-C1	-2.49	110.49	114.40
56	1A	3001	6UQ	CDK-CBM-CBL	-2.48	109.29	113.38
56	1A	3001	6UQ	CBK-CBL-CBM	-2.40	107.07	110.45
56	1A	3001	6UQ	CDH-CAZ-CAU	-2.32	109.55	113.38
56	1A	3001	6UQ	C3-C4-C5	-2.28	105.65	110.85
56	1A	3001	6UQ	CDF-CAC-CAD	2.04	124.09	121.27
56	1A	3001	6UQ	OAQ-CAR-CAM	2.08	112.91	109.09
56	1A	3001	6UQ	O4-C4-C5	2.12	114.97	109.33
56	1A	3001	6UQ	O4-C4-C3	2.26	113.07	107.18
56	1A	3001	6UQ	OBBCBC-CBF	2.39	115.57	109.85
56	1A	3001	6UQ	OCP-CCO-CCN	2.48	113.16	109.77
56	1A	3001	6UQ	CAA-CAB-CLAI	2.89	121.07	117.99
56	1A	3001	6UQ	OBE-CBD-CBI	2.95	113.68	108.26
56	1A	3001	6UQ	OAY-CAZ-CDH	3.01	109.58	105.74
56	1A	3001	6UQ	OBBCBC-CDJ	3.26	115.78	108.63
56	1A	3001	6UQ	O1-C1-C2	3.37	116.02	109.10
56	1A	3001	6UQ	O1-CCB-OCG	3.81	117.57	109.23
56	1A	3001	6UQ	CAA-CAF-CLAG	3.86	122.11	117.99
56	1A	3001	6UQ	CAF-CAA-CAB	4.02	121.57	117.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	1A	3001	6UQ	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.