



## Full wwPDB EM Validation Report ⓘ

Feb 19, 2025 – 12:19 pm GMT

PDB ID : 8P6P  
EMDB ID : EMD-17133  
Title : Mycoplasma pneumoniae small ribosomal subunit in chloramphenicol-treated cells  
Authors : Schacherl, M.; Xue, L.; Spahn, C.M.T.; Mahamid, J.  
Deposited on : 2023-05-27  
Resolution : 3.20 Å (reported)  
Based on initial models : 7OOC, 7OOD

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

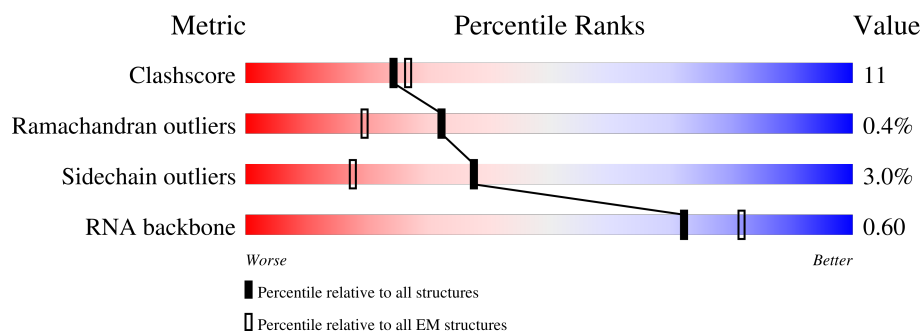
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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.




















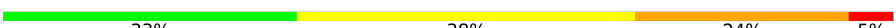

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	3	2907	99%
2	5	1520	52% 41% 6%
3	7	75	20% 17% 60%
4	8	76	20% 18% 61%
5	A	294	58% 31% 10%
6	B	273	67% 17% 15%
7	C	205	62% 36%

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Mol	Chain	Length	Quality of chain
8	D	219	
9	E	215	
10	F	155	
11	G	142	
12	H	132	
13	I	108	
14	J	121	
15	K	139	
16	L	124	
17	M	61	
18	N	86	
19	O	94	
20	P	85	
21	Q	104	
22	R	87	
23	S	87	
24	T	60	
25	Y	21	
26	x	97	

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 55465 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	3	24	Total	C	N	O	P	0	0
			512	229	93	166	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	1507	Total	C	N	O	P	0	0
			32258	14420	5847	10484	1507		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	1003	A	G	conflict	GB 26117688

- Molecule 3 is a RNA chain called tRNA-Asp (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	30	Total	C	N	O	P	0	0
			640	285	112	213	30		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	17	G	-	insertion	GB 26117688
7	55	C	U	conflict	GB 26117688

- Molecule 4 is a RNA chain called tRNA-Lys (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	30	Total	C	N	O	P	0	0
			639	286	114	209	30		

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	266	Total	C	N	O	S	0	0
			2138	1359	376	394	9		

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	232	Total	C	N	O	S	0	0
			1835	1158	343	329	5		

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	204	Total	C	N	O	S	0	0
			1669	1057	316	292	4		

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	155	Total	C	N	O	S	0	0
			1191	753	228	207	3		

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	184	Total	C	N	O	S	0	0
			1509	950	270	287	2		

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	155	Total	C	N	O	S	0	0
			1254	790	240	217	7		

- Molecule 11 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	141	Total	C	N	O	S	0	0
			1110	723	193	192	2		

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	129	Total	C	N	O	S	0	0
			1040	661	195	183	1		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	104	Total	C	N	O	S	0	0
			832	536	147	148	1		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	114	Total	C	N	O	S	0	0
			829	514	153	156	6		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	135	Total	C	N	O	S	0	0
			1071	677	212	180	2		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	L	123	Total	C	N	O	0	0
			991	618	200	173		

- Molecule 17 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	M	60	Total	C	N	O	0	0
			474	302	96	72	4	

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	N	85	Total	C	N	O	0	0
			689	436	130	123		

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	87	Total	C	N	O	S	0	0
			705	453	130	118	4		

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	85	Total	C	N	O	S	0	0
			693	436	138	118	1		

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	71	Total	C	N	O	S	0	0
			590	378	115	93	4		

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	86	Total	C	N	O	S	0	0
			700	444	132	122	2		

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	79	Total	C	N	O		0	0
			643	391	138	114			

- Molecule 24 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	59	Total	C	N	O	S	0	0
			519	326	111	80	2		

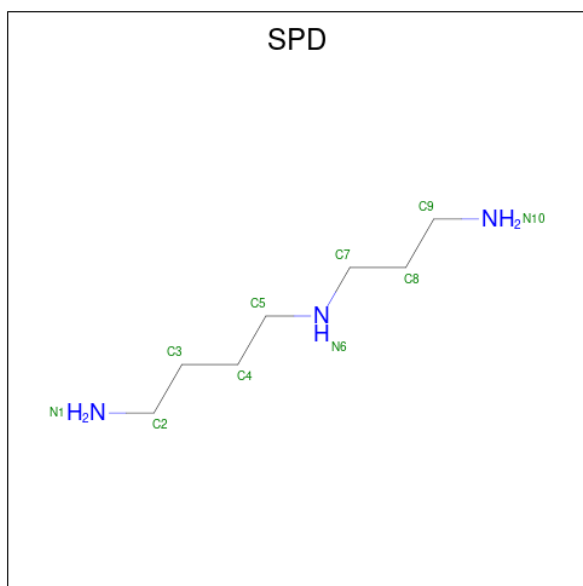
- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	21	Total	C	N	O	P	0	0
			446	200	79	146	21		

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

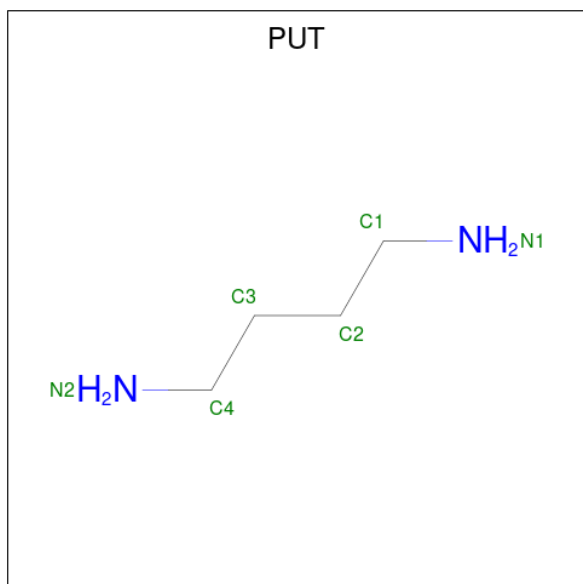
Mol	Chain	Residues	Atoms				AltConf	Trace
26	x	43	Total	C	N	O	0	0
			342	214	65	63		

- Molecule 27 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).



Mol	Chain	Residues	Atoms			AltConf
27	5	1	Total	C	N	0
			10	7	3	
27	5	1	Total	C	N	0
			10	7	3	

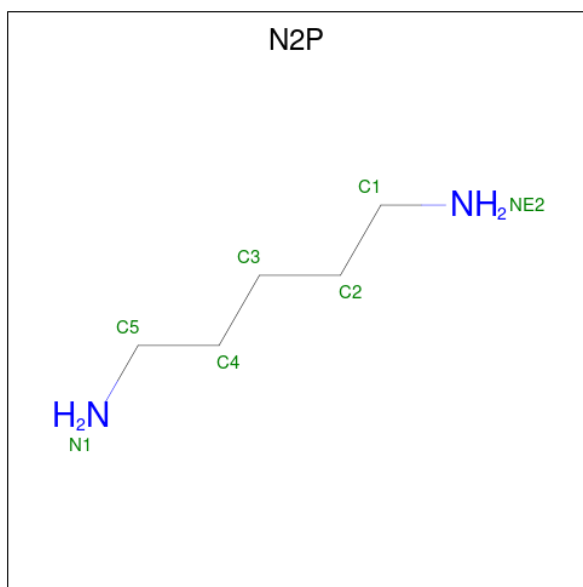
- Molecule 28 is 1,4-DIAMINOBTUTANE (three-letter code: PUT) (formula:  $C_4H_{12}N_2$ ).





Mol	Chain	Residues	Atoms			AltConf
28	5	1	Total	C	N	0
			6	4	2	
28	5	1	Total	C	N	0
			6	4	2	

- Molecule 29 is PENTANE-1,5-DIAMINE (three-letter code: N2P) (formula: C<sub>5</sub>H<sub>14</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
29	5	1	Total	C	N	0
			7	5	2	

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
30	5	96	Total	Mg	0
			96	96	
30	7	1	Total	Mg	0
			1	1	
30	8	1	Total	Mg	0
			1	1	
30	H	1	Total	Mg	0
			1	1	
30	K	1	Total	Mg	0
			1	1	
30	L	1	Total	Mg	0
			1	1	
30	P	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
30	Y	1	Total	Mg	0
			1	1	

- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	M	1	Total	Zn	0
			1	1	
31	Q	1	Total	Zn	0
			1	1	

- Molecule 32 is water.

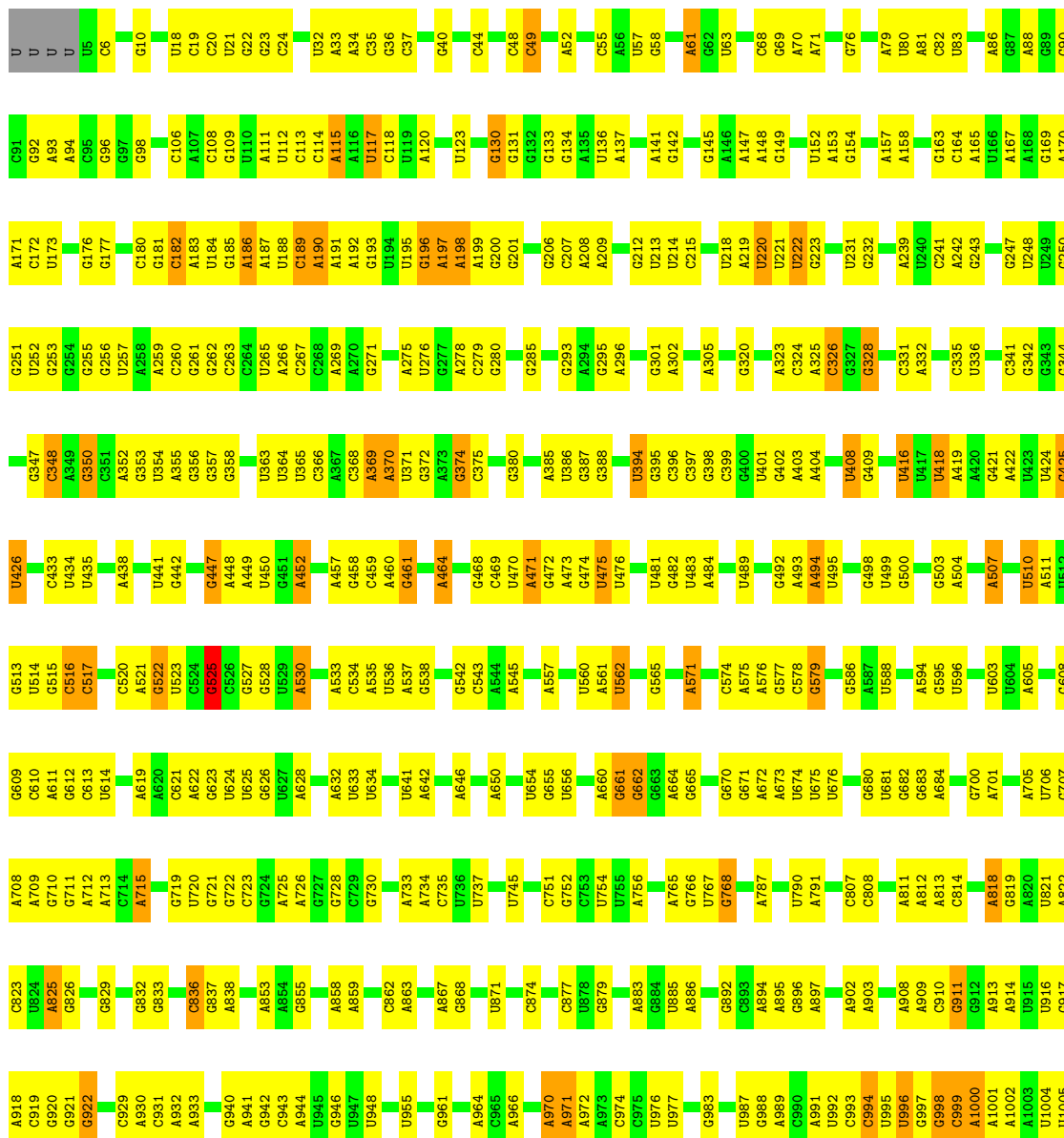
Mol	Chain	Residues	Atoms		AltConf
32	5	1	Total	O	0
			1	1	
32	A	1	Total	O	0
			1	1	



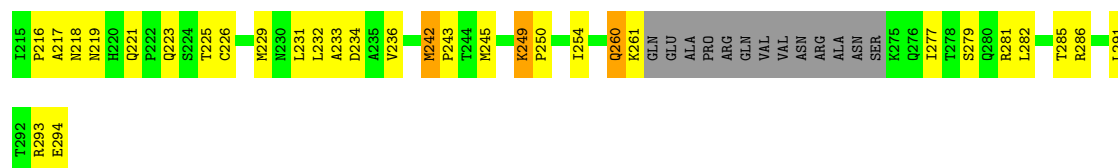
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U G U C G A G U G U U U U G G C C C G A A A G A U G U A A C G G C U A A G U U A C C C A A U U U A U G G A U  
A A G A U U A U C A A C U U G U G G U A G A C C G U U A A G C C U U A A G U C C A A G C G U A A C A G C C A U  
U G G U G G A U C A A A A A G G U G A G A C C G U U G A U U G G A A G U U G A A G U C C A A G C G U A A C C  
C A A A C C G A U U G A C U A A A G G U U U C C A A C C A G G U C C A G G U U C C A G G G U U A G U C C A C C U  
A A C C U G A G G C C U U A A A G C G U U G G A A G G C A C A A C C A A G U U A A U U C U G U A C A A G U U  
A G A C U G G A A A G A A A G G U U U U C C A C A C C C A A U A A U U G A A U U U G G G G A A A A U C C A  
U A A G G U G G U A A C A U A G G C A A A A A G C C A U U G A A G U A A U U C G A U G G A A A A U  
G A G U G A A A G A A G C A A G G A A A G G U U U A A A U C A U U C A A A A G A A A A G G U U A A  
U C U A G C U G U G U A A C C A A G U A G U C A A C G A A A C A C G U U C A A A G G A A G G U U A  
G C G A G U G A A C C A A U A G C C A A G G A A A C U C U G C C A A A U U A A G U U A A G C C G U  
G C U U A A A A A A G U A A G C C G G C A A G A A A G C G A G G A C C G A U U A A A A C A A C A A C  
U C U A A U C C A A A A C C U A A G A A G U U A A U A A G G U G A A C C A C C U U A A C C U A A A A C A A C  
A A G A A G G A A G G A A G C A A G C U U U U C C U U A C C U G G A A C C C A G A A A G G U U A  
G U A G C A A A U C U A G G G A A A A A U U C C C U U C C G U C C G A A A A A A A A A A A A A A A  
C U G U C C G G C U A A C C A A G A A A A A U C C A A G U U A C C G G U A A A A A A A A A A A A A  
C G G G A A C G G A A A A C C C A A G G U G A A A A G C U U U A A G U U A A A A A A A A A A A A A  
G U A G A A A A A A G G A A G C A A U G G A A A G U U A G C C G C U U A A A A A A A A A A A A A  
G A A U A C C U A C C G U U G U U G C C U U G C C U U A A A C U U G A A C C C A A A A A A A A A A  
U G U U A G G G A A G A A G A A C U U G A C C G G U C C A A A A A A A A A A A A A A A A A A  
G G U A C C U C G G U U G A  
U G A A A C A A A C A  
G A A A U G G C C A  
A G A G U U C A U A

- Molecule 2: 16S ribosomal RNA

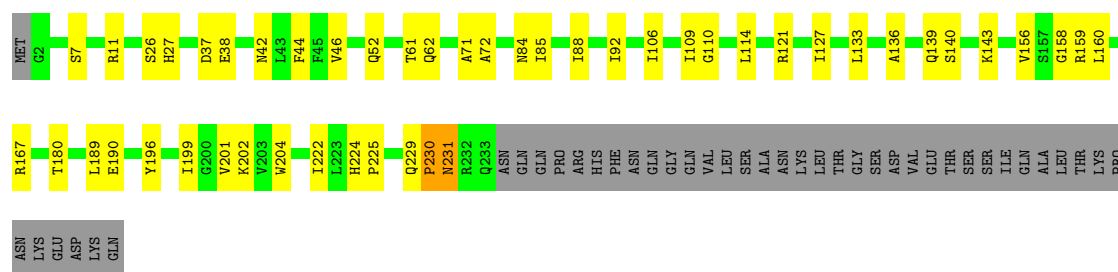
Chain 5:  52% 41% 6%







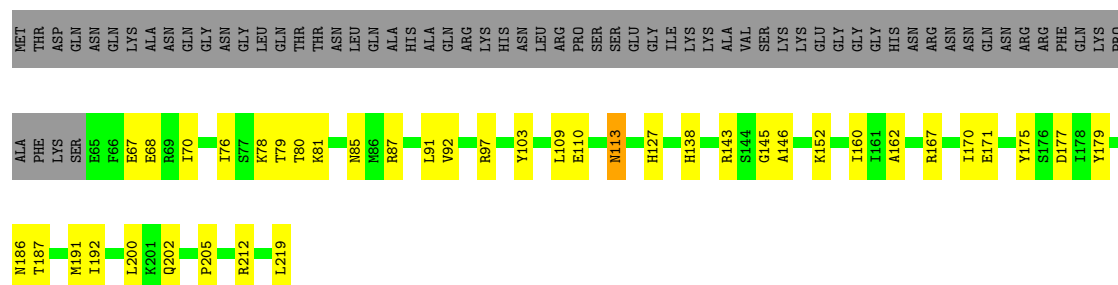
• Molecule 6: 30S ribosomal protein S3



• Molecule 7: 30S ribosomal protein S4

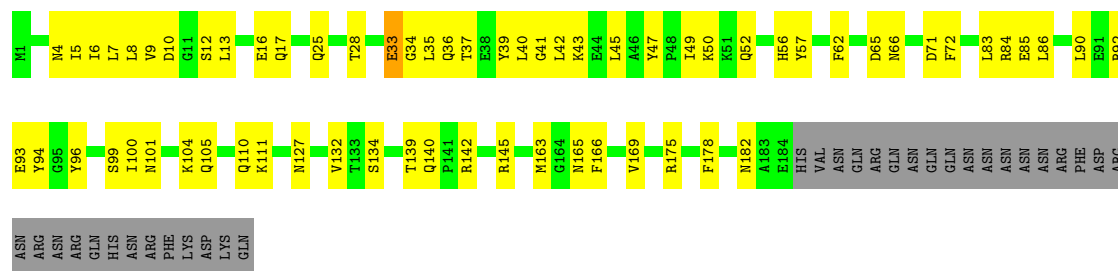


• Molecule 8: 30S ribosomal protein S5



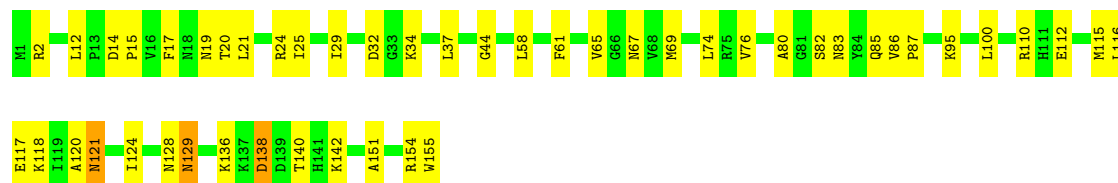
• Molecule 9: 30S ribosomal protein S6





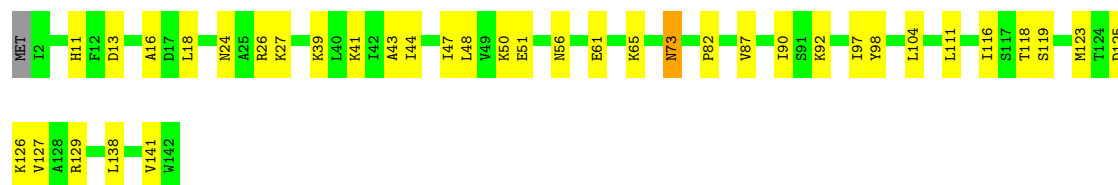
• Molecule 10: 30S ribosomal protein S7

Chain F: 69% 29% .



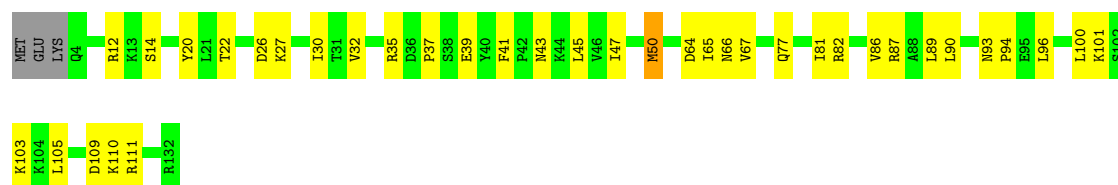
• Molecule 11: 30S ribosomal protein S8

Chain G: 73% 25% ..



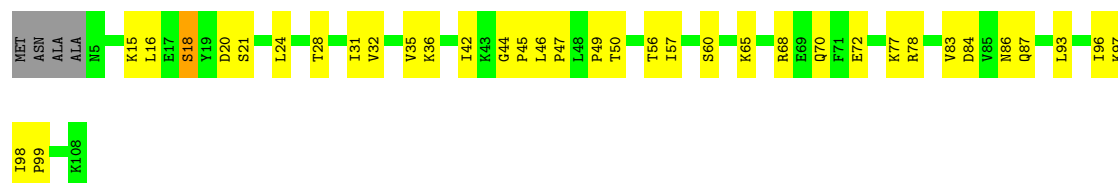
• Molecule 12: 30S ribosomal protein S9

Chain H: 70% 27% ..



• Molecule 13: 30S ribosomal protein S10

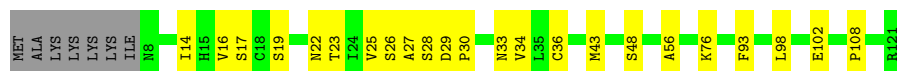
Chain I: 63% 32% . .



• Molecule 14: 30S ribosomal protein S11

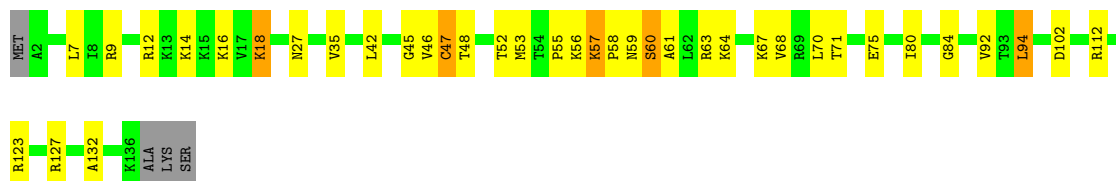


Chain J:  75% 19% 6%



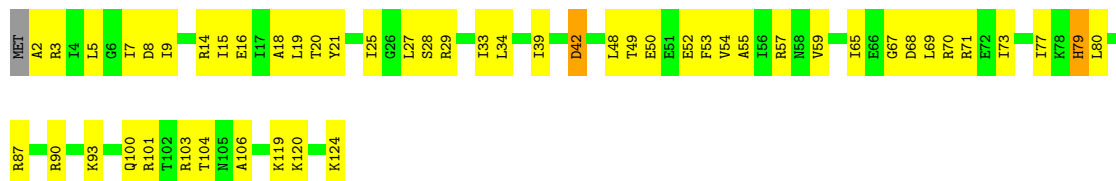
- Molecule 15: 30S ribosomal protein S12

Chain K:  70% 24% ..



- Molecule 16: 30S ribosomal protein S13

Chain L:  58% 40% ..



- Molecule 17: 30S ribosomal protein S14 type Z

Chain M:  69% 30% .



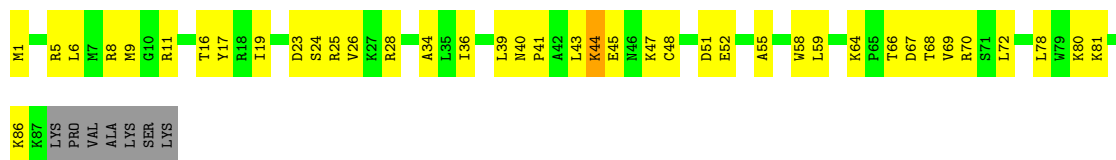
- Molecule 18: 30S ribosomal protein S15

Chain N:  72% 26% ..



- Molecule 19: 30S ribosomal protein S16

Chain O:  50% 41% 7%



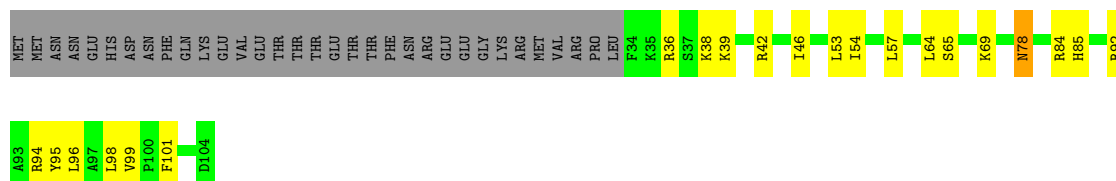
- Molecule 20: 30S ribosomal protein S17

Chain P:  66% 34%



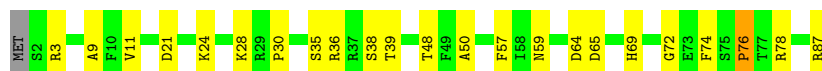
- Molecule 21: 30S ribosomal protein S18

Chain Q:  48% 19% 32%



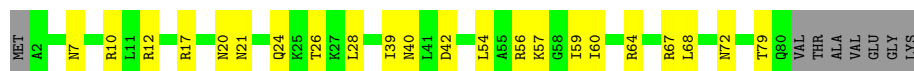
- Molecule 22: 30S ribosomal protein S19

Chain R:  72% 25% ..



- Molecule 23: 30S ribosomal protein S20

Chain S:  66% 25% 9%



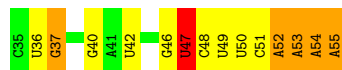
- Molecule 24: 30S ribosomal protein S21

Chain T:  75% 23% .



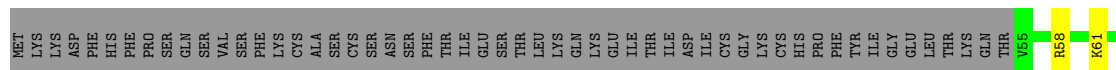
- Molecule 25: mRNA

Chain Y:  33% 38% 24% 5%



- Molecule 26: 50S ribosomal protein L31

Chain x:  42% 56%



1100

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	30774	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation and 3D CTF correction are done in Warp	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	137	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PUT, ZN, SPD, MA6, B8T, 5MC, MG, G7M, N2P

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  > 5$	RMSZ	# $ Z  > 5$
1	3	0.24	0/572	0.76	0/889
2	5	0.30	0/35992	0.77	4/56111 (0.0%)
3	7	0.25	0/713	0.77	0/1107
4	8	0.20	0/713	0.77	0/1106
5	A	0.26	0/2172	0.51	0/2934
6	B	0.28	0/1863	0.56	0/2516
7	C	0.37	1/1700 (0.1%)	0.69	3/2278 (0.1%)
8	D	0.27	0/1206	0.55	1/1616 (0.1%)
9	E	0.27	0/1536	0.54	0/2072
10	F	0.26	0/1274	0.55	0/1710
11	G	0.27	0/1126	0.52	0/1517
12	H	0.28	0/1056	0.61	0/1409
13	I	0.27	0/843	0.55	0/1132
14	J	0.31	0/844	0.66	2/1136 (0.2%)
15	K	0.26	0/1089	0.58	0/1461
16	L	0.26	0/1002	0.61	0/1340
17	M	0.30	0/483	0.58	0/643
18	N	0.25	0/695	0.54	0/926
19	O	0.34	0/718	0.74	2/962 (0.2%)
20	P	0.24	0/702	0.56	0/934
21	Q	0.26	0/601	0.57	0/801
22	R	0.30	0/716	0.62	1/958 (0.1%)
23	S	0.27	0/645	0.54	0/857
24	T	0.28	0/524	0.58	0/685
25	Y	0.27	0/498	0.87	1/773 (0.1%)
26	x	0.25	0/347	0.53	0/457
All	All	0.29	1/59630 (0.0%)	0.71	14/88330 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	152	PRO	CG-CD	-10.24	1.16	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	152	PRO	N-CD-CG	-13.35	83.17	103.20
14	J	108	PRO	CA-N-CD	-12.03	94.65	111.50
22	R	76	PRO	CA-N-CD	-9.30	98.48	111.50
19	O	41	PRO	CA-N-CD	-8.45	99.67	111.50
19	O	41	PRO	N-CD-CG	-6.60	93.30	103.20
8	D	205	PRO	CA-N-CD	-6.57	102.30	111.50
7	C	152	PRO	CA-CB-CG	-6.37	91.89	104.00
7	C	152	PRO	CA-N-CD	-6.22	102.79	111.50
2	5	994	C	C2-N1-C1'	6.20	125.62	118.80
25	Y	47	U	C2-N1-C1'	5.67	124.50	117.70
2	5	751	C	C2-N1-C1'	5.41	124.75	118.80
14	J	108	PRO	N-CD-CG	-5.28	95.28	103.20
2	5	1024	U	P-O3'-C3'	5.17	125.91	119.70
2	5	1134	C	C2-N1-C1'	5.05	124.35	118.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	512	0	260	1	0
2	5	32258	0	16204	502	0
3	7	640	0	324	15	0
4	8	639	0	324	9	0
5	A	2138	0	2204	59	0
6	B	1835	0	1909	36	0
7	C	1669	0	1729	58	0
8	D	1191	0	1284	27	0
9	E	1509	0	1520	48	0
10	F	1254	0	1320	32	0
11	G	1110	0	1226	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	H	1040	0	1107	25	0
13	I	832	0	918	26	0
14	J	829	0	855	16	0
15	K	1071	0	1165	27	0
16	L	991	0	1061	39	0
17	M	474	0	505	16	0
18	N	689	0	746	13	0
19	O	705	0	755	30	0
20	P	693	0	753	19	0
21	Q	590	0	625	23	0
22	R	700	0	709	15	0
23	S	643	0	694	18	0
24	T	519	0	578	8	0
25	Y	446	0	226	11	0
26	x	342	0	354	0	0
27	5	20	0	38	2	0
28	5	12	0	24	0	0
29	5	7	0	14	0	0
30	5	96	0	0	0	0
30	7	1	0	0	0	0
30	8	1	0	0	0	0
30	H	1	0	0	0	0
30	K	1	0	0	0	0
30	L	1	0	0	0	0
30	P	1	0	0	0	0
30	Y	1	0	0	0	0
31	M	1	0	0	0	0
31	Q	1	0	0	0	0
32	5	1	0	0	0	0
32	A	1	0	0	0	0
All	All	55465	0	39431	976	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 11.

All (976) 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)
3:7:34:G:H1	25:Y:42:U:H3	1.16	0.92
2:5:169:G:N2	2:5:219:A:O2'	2.13	0.81
2:5:983:G:H21	2:5:1012:A:H8	1.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:26:VAL:HG11	18:N:78:LEU:HD21	1.62	0.81
2:5:452:A:OP1	19:O:70:ARG:NH2	2.14	0.80
2:5:543:C:OP1	7:C:57:LYS:NZ	2.16	0.78
10:F:69:MET:HG2	10:F:95:LYS:HG2	1.65	0.78
2:5:369:A:O2'	2:5:448:A:N7	2.16	0.78
22:R:35:SER:HG	22:R:38:SER:HG	1.31	0.78
5:A:95:LEU:HD11	5:A:226:CYS:HA	1.67	0.77
2:5:1153:G:N7	12:H:101:LYS:NZ	2.33	0.76
2:5:424:U:OP1	7:C:12:ARG:NH2	2.20	0.75
6:B:224:HIS:HB3	6:B:225:PRO:HD3	1.68	0.75
20:P:61:VAL:HG12	20:P:80:ILE:HG12	1.67	0.75
2:5:1269:U:O2'	16:L:14:ARG:NH1	2.20	0.74
5:A:82:ILE:HG22	5:A:175:LEU:HB3	1.69	0.74
5:A:20:LEU:HG	5:A:62:ARG:HH21	1.53	0.74
24:T:6:VAL:HG12	24:T:8:ASN:H	1.53	0.74
2:5:206:G:N2	2:5:209:A:OP2	2.21	0.73
9:E:12:SER:OG	9:E:17:GLN:NE2	2.20	0.73
2:5:1332:U:OP1	17:M:35:SER:OG	2.07	0.72
6:B:85:ILE:HG21	6:B:231:ASN:HD21	1.55	0.72
18:N:77:ASN:O	18:N:81:THR:HG23	1.91	0.71
2:5:1508:C:H42	5:A:294:GLU:HG2	1.53	0.71
2:5:177:G:H1	2:5:188:U:H3	1.39	0.71
9:E:40:LEU:HB2	9:E:57:TYR:HB2	1.73	0.70
6:B:61:THR:HG22	6:B:62:GLN:H	1.56	0.70
2:5:521:A:N6	15:K:102:ASP:OD2	2.24	0.70
2:5:1045:C:H42	25:Y:46:G:H22	1.38	0.70
2:5:661:G:OP1	21:Q:84:ARG:NH1	2.25	0.70
5:A:28:THR:O	5:A:61:GLN:NE2	2.24	0.70
2:5:710:G:H2'	2:5:711:G:C8	2.27	0.69
2:5:1354:G:O6	10:F:2:ARG:NH2	2.24	0.69
22:R:9:ALA:HB1	22:R:39:THR:HG21	1.74	0.69
2:5:1009:G:H21	2:5:1012:A:H2	1.41	0.69
6:B:110:GLY:HA3	6:B:225:PRO:HD2	1.75	0.69
2:5:787:A:OP1	3:7:38:C:O2'	2.09	0.69
9:E:90:LEU:HA	9:E:93:GLU:HG2	1.75	0.69
2:5:145:G:N2	2:5:148:A:OP2	2.26	0.69
2:5:181:G:O2'	20:P:3:ARG:NH1	2.26	0.69
5:A:32:MET:SD	5:A:281:ARG:NH1	2.66	0.69
12:H:12:ARG:NH2	12:H:109:ASP:OD2	2.26	0.69
2:5:1330:A:H2'	2:5:1331:A:H8	1.58	0.68
2:5:408:U:H1'	7:C:28:GLY:HA2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:11:VAL:HG12	22:R:38:SER:HB3	1.75	0.68
3:7:27:U:H3	3:7:43:G:H1	1.40	0.68
12:H:20:TYR:HB2	12:H:66:ASN:HB3	1.74	0.68
5:A:49:ARG:HG3	5:A:50:LYS:H	1.59	0.68
2:5:715:A:N7	21:Q:69:LYS:NZ	2.39	0.68
16:L:14:ARG:NH2	16:L:42:ASP:OD2	2.21	0.68
2:5:670:G:H2'	2:5:671:G:C8	2.29	0.68
5:A:65:LEU:HD21	5:A:231:LEU:HD13	1.76	0.67
2:5:874:C:OP1	15:K:9:ARG:NH2	2.27	0.67
2:5:386:U:H4'	19:O:28:ARG:HH21	1.60	0.67
13:I:65:LYS:HE3	13:I:68:ARG:HH22	1.60	0.67
2:5:996:U:O2	2:5:1030:G:O6	2.13	0.67
2:5:1425:A:H2'	2:5:1427:U:H3	1.60	0.67
7:C:97:LEU:HD12	7:C:136:LEU:HD21	1.76	0.66
2:5:515:G:N2	2:5:528:G:OP1	2.28	0.66
2:5:1192:C:OP1	17:M:9:LYS:NZ	2.29	0.66
2:5:1330:A:H2'	2:5:1331:A:C8	2.31	0.66
16:L:52:GLU:OE1	16:L:52:GLU:N	2.26	0.66
2:5:998:G:O2'	2:5:1000:A:OP1	2.14	0.66
2:5:92:G:N7	23:S:10:ARG:NH2	2.44	0.65
9:E:12:SER:H	9:E:17:GLN:HE21	1.44	0.65
11:G:123:MET:HG3	11:G:127:VAL:HG13	1.78	0.65
2:5:404:A:OP1	7:C:111:ARG:NH2	2.26	0.65
2:5:1241:G:N2	2:5:1244:A:OP2	2.20	0.65
2:5:941:A:H2'	2:5:942:G:H8	1.62	0.65
2:5:1270:C:H5'	16:L:14:ARG:NH1	2.11	0.65
8:D:143:ARG:NH2	8:D:145:GLY:O	2.30	0.65
2:5:535:A:H5''	15:K:123:ARG:HH12	1.62	0.64
2:5:1193:U:H2'	2:5:1194:A:H8	1.63	0.64
2:5:989:A:O2'	17:M:12:ARG:NH1	2.30	0.64
5:A:93:LYS:HG3	5:A:109:THR:HB	1.78	0.64
10:F:110:ARG:HG2	10:F:112:GLU:HG3	1.78	0.64
2:5:195:U:H2'	2:5:196:G:H8	1.62	0.64
11:G:104:LEU:O	11:G:129:ARG:NH2	2.29	0.64
2:5:499:U:H2'	2:5:500:G:H8	1.62	0.64
10:F:25:ILE:HB	10:F:100:LEU:HD22	1.80	0.64
2:5:473:A:H2'	2:5:474:G:H8	1.61	0.64
15:K:42:LEU:HD12	15:K:94:LEU:HD21	1.80	0.64
2:5:735:C:OP2	9:E:92:ARG:NH2	2.31	0.64
2:5:808:C:O2'	2:5:895:A:N1	2.31	0.64
7:C:68:ASP:OD1	7:C:69:LYS:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:57:ILE:HG23	17:M:41:ARG:HB2	1.80	0.63
2:5:1113:U:O4	2:5:1114:A:N6	2.32	0.63
2:5:1467:A:N6	15:K:60:SER:OG	2.31	0.63
16:L:49:THR:OG1	16:L:52:GLU:OE1	2.17	0.63
7:C:94:GLU:O	7:C:99:ASN:ND2	2.32	0.63
12:H:30:ILE:HG13	12:H:65:ILE:HG13	1.81	0.63
2:5:259:A:OP1	23:S:67:ARG:NH1	2.31	0.63
2:5:902:A:H2'	2:5:903:A:H8	1.64	0.63
16:L:80:LEU:HD21	16:L:87:ARG:HG2	1.80	0.63
2:5:499:U:H2'	2:5:500:G:C8	2.34	0.62
8:D:68:GLU:OE1	8:D:68:GLU:N	2.31	0.62
12:H:12:ARG:HH22	12:H:111:ARG:HH21	1.47	0.62
2:5:918:A:O2'	2:5:1374:C:OP2	2.15	0.62
19:O:52:GLU:HG2	19:O:78:LEU:HD11	1.80	0.62
2:5:838:A:OP2	9:E:110:GLN:NE2	2.32	0.62
5:A:45:ILE:HD11	5:A:204:THR:HG23	1.80	0.62
2:5:1463:A:H2'	2:5:1464:G:C8	2.34	0.62
3:7:10:G:H1	3:7:25:U:H3	1.45	0.62
2:5:1472:G:H1'	2:5:1493:MA6:H2	1.82	0.62
2:5:621:C:H2'	2:5:622:A:H8	1.65	0.62
2:5:1197:G:OP2	2:5:1296:C:N4	2.33	0.62
9:E:16:GLU:N	9:E:16:GLU:OE1	2.32	0.62
6:B:140:SER:HA	6:B:143:LYS:HE3	1.80	0.62
10:F:117:GLU:OE1	10:F:117:GLU:N	2.29	0.62
6:B:156:VAL:HG22	6:B:201:VAL:HG12	1.81	0.62
17:M:21:TYR:HE1	17:M:23:ARG:HE	1.46	0.62
5:A:84:PHE:CE1	5:A:177:ILE:HD12	2.35	0.61
15:K:127:ARG:HB2	15:K:132:ALA:HB3	1.82	0.61
2:5:133:G:H2'	2:5:134:G:C8	2.35	0.61
7:C:92:VAL:O	7:C:96:ARG:NH1	2.31	0.61
2:5:577:G:H5'	2:5:725:A:H1'	1.82	0.61
2:5:398:G:OP1	7:C:73:ARG:NH1	2.34	0.61
2:5:483:U:H2'	2:5:484:A:H8	1.66	0.61
2:5:1463:A:H2'	2:5:1464:G:H8	1.65	0.61
2:5:681:U:H1'	14:J:33:ASN:HA	1.81	0.61
6:B:109:ILE:HA	6:B:222:ILE:HG23	1.81	0.61
21:Q:42:ARG:O	21:Q:46:ILE:HG12	2.01	0.61
2:5:206:G:O2'	2:5:209:A:N6	2.34	0.61
7:C:81:GLN:HB2	7:C:85:LEU:HD11	1.82	0.61
2:5:460:A:H2'	2:5:461:G:H8	1.66	0.60
2:5:1329:G:H2'	2:5:1330:A:H8	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:711:G:H2'	2:5:712:A:C8	2.37	0.60
2:5:1123:G:O2'	2:5:1124:U:O5'	2.20	0.60
9:E:25:GLN:HE22	9:E:37:THR:HG22	1.67	0.60
16:L:50:GLU:OE2	16:L:50:GLU:N	2.33	0.60
10:F:115:MET:HA	10:F:118:LYS:HB2	1.83	0.60
2:5:371:U:OP1	19:O:68:THR:OG1	2.17	0.60
2:5:941:A:H2'	2:5:942:G:C8	2.36	0.60
16:L:69:LEU:O	16:L:73:ILE:HG13	2.01	0.60
6:B:127:ILE:HD11	6:B:133:LEU:HD13	1.83	0.60
8:D:177:ASP:N	8:D:177:ASP:OD1	2.30	0.60
17:M:7:LYS:O	17:M:11:THR:HG23	2.02	0.60
16:L:16:GLU:OE1	16:L:16:GLU:N	2.29	0.59
9:E:84:ARG:NH1	21:Q:95:TYR:O	2.34	0.59
11:G:13:ASP:OD2	11:G:16:ALA:HB3	2.03	0.59
7:C:96:ARG:HB2	7:C:99:ASN:HB3	1.84	0.59
2:5:473:A:H2'	2:5:474:G:C8	2.37	0.59
2:5:1193:U:H2'	2:5:1194:A:C8	2.36	0.59
9:E:6:ILE:HD13	21:Q:54:ILE:HD11	1.85	0.59
2:5:1329:G:H2'	2:5:1330:A:C8	2.38	0.59
2:5:733:A:OP1	21:Q:92:ARG:NH1	2.36	0.59
2:5:460:A:H2'	2:5:461:G:C8	2.38	0.59
5:A:249:LYS:HG3	5:A:250:PRO:HD2	1.84	0.58
19:O:78:LEU:HA	19:O:81:LYS:HD2	1.85	0.58
2:5:265:U:H2'	2:5:266:A:C8	2.39	0.58
2:5:403:A:H5''	7:C:111:ARG:HH11	1.68	0.58
2:5:1213:A:H5'	2:5:1310:C:H41	1.69	0.58
5:A:181:PRO:HD3	5:A:200:ALA:HB1	1.85	0.58
20:P:31:LYS:HE3	20:P:36:HIS:HB3	1.86	0.58
2:5:354:U:H2'	2:5:355:A:H8	1.68	0.58
2:5:537:A:H2'	2:5:538:G:C8	2.38	0.58
5:A:68:ALA:O	5:A:72:VAL:HG12	2.03	0.58
6:B:11:ARG:NH1	6:B:180:THR:O	2.35	0.58
23:S:68:LEU:O	23:S:72:ASN:ND2	2.34	0.58
8:D:167:ARG:NH1	8:D:171:GLU:OE2	2.32	0.58
16:L:50:GLU:O	16:L:54:VAL:HG22	2.04	0.58
7:C:70:GLN:O	7:C:74:LEU:HG	2.04	0.58
2:5:916:U:O2	8:D:79:THR:OG1	2.22	0.58
13:I:18:SER:OG	13:I:20:ASP:O	2.22	0.57
14:J:22:ASN:OD1	14:J:23:THR:N	2.33	0.57
2:5:1144:A:H2'	2:5:1145:A:C8	2.39	0.57
21:Q:64:LEU:HD12	21:Q:99:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:447:G:H5''	2:5:448:A:H3'	1.86	0.57
5:A:30:VAL:O	5:A:218:ASN:ND2	2.29	0.57
7:C:34:ILE:HG13	7:C:39:GLY:HA2	1.85	0.57
2:5:365:U:H3	2:5:388:G:H1	1.52	0.57
2:5:712:A:H2'	2:5:713:A:C8	2.39	0.57
7:C:14:LEU:O	7:C:59:ARG:NH2	2.37	0.57
8:D:212:ARG:NH2	11:G:51:GLU:OE1	2.34	0.57
10:F:15:PRO:HG2	12:H:45:LEU:HD21	1.86	0.57
9:E:163:MET:SD	11:G:50:LYS:NZ	2.77	0.57
2:5:76:G:N2	2:5:79:A:OP2	2.37	0.57
2:5:821:U:O2	11:G:11:HIS:NE2	2.37	0.57
2:5:537:A:H2'	2:5:538:G:H8	1.69	0.57
16:L:25:ILE:HG23	16:L:29:ARG:HG2	1.86	0.57
2:5:520:C:H41	15:K:63:ARG:NH2	2.02	0.57
2:5:1332:U:H3	2:5:1338:A:N6	2.01	0.57
5:A:53:ASN:ND2	5:A:279:SER:O	2.34	0.57
2:5:1448:A:H2'	2:5:1449:G:C8	2.40	0.57
8:D:70:ILE:HD12	8:D:92:VAL:HG22	1.85	0.57
9:E:93:GLU:OE1	21:Q:92:ARG:NH2	2.38	0.57
17:M:10:GLN:HG3	17:M:23:ARG:HG3	1.86	0.56
2:5:821:U:H2'	2:5:822:A:H8	1.70	0.56
5:A:214:ILE:HG22	5:A:216:PRO:HD3	1.86	0.56
9:E:33:GLU:OE1	9:E:34:GLY:N	2.38	0.56
13:I:46:LEU:HD23	13:I:46:LEU:H	1.69	0.56
2:5:399:C:H5''	7:C:132:PRO:HD2	1.88	0.56
2:5:709:A:H2'	2:5:710:G:C8	2.40	0.56
2:5:534:C:H2'	2:5:535:A:H8	1.71	0.56
2:5:612:G:H1	2:5:624:U:H3	1.54	0.56
19:O:68:THR:O	19:O:72:LEU:HG	2.06	0.56
15:K:67:LYS:HE2	15:K:75:GLU:HB3	1.88	0.56
2:5:1264:G:OP1	10:F:34:LYS:NZ	2.39	0.56
6:B:38:GLU:OE1	17:M:26:ARG:NH1	2.39	0.56
7:C:168:GLU:HG3	7:C:177:THR:HG23	1.88	0.56
12:H:35:ARG:HD2	12:H:39:GLU:HG2	1.88	0.56
16:L:65:ILE:HG22	16:L:67:GLY:H	1.70	0.56
8:D:170:ILE:HG23	8:D:175:TYR:HB2	1.88	0.55
2:5:733:A:H2'	2:5:734:A:H8	1.71	0.55
2:5:1139:A:H2'	2:5:1140:A:H8	1.71	0.55
8:D:212:ARG:NH1	11:G:111:LEU:O	2.39	0.55
12:H:32:VAL:HG22	12:H:67:VAL:HG11	1.88	0.55
19:O:5:ARG:HA	19:O:69:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S:60:ILE:HD11	23:S:64:ARG:HD3	1.88	0.55
2:5:433:C:H2'	2:5:434:U:C6	2.42	0.55
2:5:1009:G:N2	2:5:1012:A:OP2	2.35	0.55
2:5:1141:U:HO2'	2:5:1142:G:H8	1.55	0.55
24:T:36:LEU:HD13	24:T:40:MET:HG2	1.89	0.55
2:5:1337:U:O5'	2:5:1338:A:H5'	2.07	0.55
5:A:221:GLN:O	5:A:225:THR:HG22	2.07	0.55
9:E:4:ASN:HB2	9:E:90:LEU:HD11	1.88	0.55
10:F:83:ASN:O	10:F:85:GLN:NE2	2.39	0.55
20:P:64:VAL:HG23	20:P:76:ARG:HG2	1.88	0.55
2:5:293:G:N2	2:5:296:A:OP2	2.36	0.55
2:5:707:G:H2'	2:5:708:A:H8	1.71	0.55
2:5:80:U:H2'	2:5:81:A:H8	1.72	0.55
2:5:435:U:O2'	2:5:438:A:N6	2.40	0.55
2:5:970:A:H8	2:5:1331:A:HO2'	1.55	0.55
5:A:131:ASN:O	5:A:135:GLU:HG2	2.07	0.55
12:H:22:THR:HB	12:H:64:ASP:HB3	1.89	0.55
2:5:946:G:OP2	16:L:101:ARG:NH2	2.40	0.55
6:B:52:GLN:HB2	6:B:72:ALA:HB3	1.89	0.55
11:G:11:HIS:ND1	11:G:13:ASP:OD1	2.40	0.55
2:5:733:A:H2'	2:5:734:A:C8	2.41	0.54
2:5:1384:A:H2'	2:5:1385:A:H8	1.70	0.54
12:H:77:GLN:O	12:H:81:ILE:HG12	2.07	0.54
2:5:1127:A:H5''	13:I:50:THR:HG23	1.90	0.54
21:Q:94:ARG:HB3	21:Q:101:PHE:CE1	2.42	0.54
2:5:212:G:O2'	2:5:464:A:N6	2.29	0.54
2:5:1505:G:H2'	2:5:1506:A:H8	1.71	0.54
7:C:117:VAL:HG22	7:C:122:VAL:HG11	1.88	0.54
7:C:16:PHE:CD1	7:C:190:GLY:HA2	2.42	0.54
11:G:87:VAL:HG12	11:G:141:VAL:HG22	1.90	0.54
12:H:103:LYS:HG3	12:H:105:LEU:HG	1.89	0.54
2:5:1261:A:H2'	2:5:1262:A:C8	2.43	0.54
2:5:1402:U:H2'	2:5:1403:A:H8	1.73	0.54
13:I:31:ILE:HD11	13:I:96:ILE:HG21	1.90	0.54
22:R:50:ALA:HB1	22:R:57:PHE:HB3	1.88	0.54
2:5:350:G:O2'	2:5:385:A:OP1	2.25	0.54
2:5:527:G:O6	15:K:59:ASN:HA	2.07	0.54
13:I:24:LEU:HD21	13:I:78:ARG:HG2	1.89	0.54
10:F:25:ILE:O	10:F:29:ILE:HG12	2.08	0.54
2:5:1074:U:O2'	2:5:1093:A:OP2	2.26	0.54
2:5:1316:C:H2'	2:5:1317:A:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:29:ARG:O	16:L:33:ILE:HG13	2.08	0.54
9:E:36:GLN:OE1	9:E:36:GLN:N	2.31	0.54
2:5:1281:U:H5''	16:L:100:GLN:HE22	1.73	0.53
2:5:1320:A:H2	2:5:1350:A:H62	1.56	0.53
8:D:80:THR:OG1	8:D:81:LYS:N	2.41	0.53
10:F:44:GLY:HA3	10:F:116:LEU:HD11	1.89	0.53
2:5:22:G:H2'	2:5:23:G:C8	2.43	0.53
2:5:259:A:H2'	2:5:260:C:C6	2.44	0.53
2:5:1058:A:N1	2:5:1099:G:O2'	2.36	0.53
2:5:1068:G:N2	2:5:1071:A:OP2	2.33	0.53
5:A:177:ILE:HG12	5:A:199:VAL:HG22	1.91	0.53
2:5:197:A:H4'	23:S:56:ARG:NH2	2.23	0.53
12:H:14:SER:O	12:H:14:SER:OG	2.26	0.53
22:R:21:ASP:O	22:R:24:LYS:HG2	2.09	0.53
2:5:710:G:H2'	2:5:711:G:H8	1.72	0.53
7:C:102:TYR:HD2	7:C:110:ARG:HB2	1.73	0.53
2:5:352:A:N3	2:5:364:U:O2'	2.36	0.53
5:A:199:VAL:HG12	5:A:213:PHE:HB2	1.90	0.53
2:5:182:C:O2'	2:5:183:A:N7	2.42	0.53
2:5:940:G:C2	2:5:941:A:C8	2.96	0.53
2:5:1102:A:N1	6:B:180:THR:HG22	2.24	0.53
7:C:26:SER:OG	7:C:27:LYS:N	2.41	0.53
2:5:1245:A:H2'	2:5:1246:A:H8	1.72	0.53
5:A:285:THR:HG23	5:A:286:ARG:HD3	1.89	0.53
6:B:229:GLN:HG3	6:B:230:PRO:CD	2.39	0.53
9:E:13:LEU:O	9:E:17:GLN:HG2	2.08	0.53
20:P:8:VAL:HG12	20:P:64:VAL:HG12	1.91	0.53
2:5:1295:U:O3'	22:R:78:ARG:NH2	2.42	0.53
5:A:18:VAL:HG11	5:A:231:LEU:HD11	1.91	0.53
2:5:250:G:H2'	2:5:251:G:H8	1.74	0.52
2:5:1071:A:H5''	8:D:76:ILE:HD12	1.91	0.52
4:8:43:U:H2'	4:8:44:G:C8	2.44	0.52
9:E:132:VAL:HG12	9:E:132:VAL:O	2.09	0.52
20:P:70:SER:O	20:P:74:ARG:NH1	2.42	0.52
2:5:20:C:H5''	8:D:146:ALA:HB3	1.91	0.52
2:5:1150:G:H2'	2:5:1151:A:H8	1.74	0.52
16:L:14:ARG:HE	16:L:42:ASP:HA	1.73	0.52
2:5:93:A:H5'	2:5:94:A:H5''	1.92	0.52
2:5:662:G:H1'	2:5:730:G:H5'	1.90	0.52
2:5:1385:A:H2'	2:5:1386:C:C6	2.45	0.52
2:5:181:G:N2	2:5:184:U:OP2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:992:U:H2'	2:5:993:C:H6	1.74	0.52
14:J:16:VAL:HG22	14:J:25:VAL:HG13	1.92	0.52
5:A:242:MET:HB2	5:A:243:PRO:HD2	1.92	0.52
19:O:23:ASP:OD1	19:O:24:SER:N	2.43	0.52
2:5:624:U:H2'	2:5:625:U:C6	2.44	0.52
6:B:159:ARG:HH21	6:B:196:TYR:HB3	1.74	0.52
7:C:123:LEU:HD22	7:C:128:THR:HG22	1.92	0.52
2:5:37:C:O2'	2:5:499:U:OP1	2.27	0.52
2:5:88:A:OP1	23:S:12:ARG:NH1	2.41	0.52
2:5:712:A:H2'	2:5:713:A:H8	1.75	0.52
2:5:1432:A:H5''	23:S:26:THR:HG22	1.90	0.52
3:7:11:U:H2'	3:7:12:G:C8	2.45	0.52
9:E:8:LEU:HD11	9:E:57:TYR:CZ	2.45	0.52
9:E:71:ASP:OD1	9:E:71:ASP:N	2.41	0.52
16:L:9:ILE:HD12	16:L:18:ALA:HB1	1.92	0.52
16:L:73:ILE:O	16:L:77:ILE:HG12	2.10	0.52
20:P:53:VAL:O	20:P:55:ALA:N	2.43	0.52
2:5:250:G:H5''	20:P:73:LYS:HE2	1.92	0.52
9:E:9:VAL:HG13	9:E:56:HIS:HB2	1.92	0.52
10:F:61:PHE:O	10:F:65:VAL:HG23	2.10	0.52
15:K:84:GLY:O	15:K:112:ARG:NH2	2.36	0.52
16:L:68:ASP:HA	16:L:71:ARG:HH11	1.74	0.52
5:A:107:PHE:HD2	5:A:109:THR:HG23	1.75	0.51
9:E:42:LEU:HD13	9:E:56:HIS:CE1	2.44	0.51
24:T:17:LYS:O	24:T:21:VAL:HG23	2.10	0.51
2:5:35:C:H2'	2:5:36:G:H8	1.74	0.51
2:5:111:A:OP1	2:5:603:U:O2'	2.21	0.51
2:5:394:U:H2'	2:5:395:G:H8	1.74	0.51
2:5:1051:U:O2'	13:I:60:SER:OG	2.22	0.51
2:5:1053:U:H2'	2:5:1054:C:C6	2.44	0.51
9:E:49:ILE:HG23	9:E:83:LEU:HD23	1.92	0.51
11:G:129:ARG:HG2	11:G:129:ARG:HH11	1.75	0.51
12:H:87:ARG:HA	12:H:90:LEU:HD23	1.91	0.51
20:P:58:GLY:HA3	20:P:85:LYS:HD3	1.92	0.51
2:5:136:U:H3	2:5:157:A:H62	1.58	0.51
2:5:1022:G:O2'	2:5:1023:G:O4'	2.28	0.51
2:5:1027:A:H3'	2:5:1028:C:H6	1.75	0.51
2:5:1201:C:OP2	16:L:90:ARG:NH1	2.42	0.51
5:A:293:ARG:HH21	24:T:50:GLN:HG2	1.75	0.51
16:L:101:ARG:HH11	16:L:104:THR:HG22	1.75	0.51
2:5:961:G:N2	3:7:34:G:H5'	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:30:PRO:HA	22:R:48:THR:HG23	1.92	0.51
2:5:492:G:O2'	2:5:494:A:H1'	2.11	0.51
2:5:1000:A:H2'	2:5:1001:A:C8	2.45	0.51
2:5:1496:G:H2'	2:5:1497:U:H6	1.76	0.51
7:C:95:SER:O	7:C:95:SER:OG	2.28	0.51
9:E:96:TYR:O	9:E:100:ILE:HG12	2.10	0.51
9:E:99:SER:O	9:E:105:GLN:NE2	2.42	0.51
16:L:15:ILE:HD13	16:L:34:LEU:HD11	1.93	0.51
2:5:1290:G:N1	2:5:1293:A:OP2	2.42	0.51
9:E:25:GLN:HG2	9:E:35:LEU:HD22	1.93	0.51
2:5:192:A:H2'	2:5:193:G:H8	1.76	0.51
2:5:401:U:H3'	2:5:402:G:H5'	1.93	0.51
2:5:1400:A:H2'	2:5:1401:A:C8	2.45	0.51
5:A:99:ILE:HD13	5:A:233:ALA:HB2	1.93	0.51
10:F:14:ASP:OD2	10:F:17:PHE:N	2.41	0.51
10:F:74:LEU:HD22	10:F:85:GLN:HB2	1.91	0.51
2:5:197:A:O2'	2:5:198:A:O5'	2.28	0.51
13:I:35:VAL:HB	13:I:42:ILE:HD11	1.93	0.51
2:5:896:G:H2'	2:5:897:A:H8	1.75	0.51
2:5:621:C:H2'	2:5:622:A:C8	2.45	0.50
2:5:1220:A:H2'	2:5:1221:A:C8	2.46	0.50
5:A:83:LEU:HD23	5:A:176:LEU:HD11	1.92	0.50
6:B:7:SER:HG	6:B:204:TRP:HE1	1.59	0.50
18:N:29:LEU:O	18:N:33:ILE:HG12	2.10	0.50
19:O:19:ILE:HG22	19:O:36:ILE:HB	1.93	0.50
2:5:813:A:OP1	2:5:1501:G:O2'	2.24	0.50
2:5:821:U:H2'	2:5:822:A:C8	2.46	0.50
4:8:28:A:H2'	4:8:29:U:C6	2.46	0.50
13:I:49:PRO:O	13:I:77:LYS:NZ	2.44	0.50
16:L:120:LYS:HG2	22:R:87:ARG:NE	2.27	0.50
19:O:40:ASN:HB3	19:O:43:LEU:HB2	1.92	0.50
2:5:242:A:C2	2:5:278:A:C5	3.00	0.50
2:5:1332:U:H3	2:5:1338:A:H61	1.58	0.50
5:A:158:ARG:O	5:A:161:LYS:HG2	2.12	0.50
13:I:32:VAL:HG23	13:I:42:ILE:HD12	1.92	0.50
20:P:52:GLU:O	20:P:52:GLU:HG2	2.11	0.50
2:5:169:G:H1	2:5:196:G:H22	1.60	0.50
2:5:295:G:H2'	2:5:296:A:C8	2.47	0.50
2:5:409:G:H22	2:5:425:G:H1'	1.76	0.50
6:B:37:ASP:OD1	6:B:38:GLU:N	2.44	0.50
2:5:123:U:H3	2:5:222:U:H3	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:221:U:H2'	2:5:222:U:C6	2.46	0.50
2:5:305:A:O2'	2:5:605:A:N1	2.39	0.50
2:5:416:U:O2'	2:5:421:G:N2	2.45	0.50
20:P:28:SER:HB3	20:P:41:ARG:HD2	1.93	0.50
2:5:1298:U:H5''	2:5:1337:U:H5'	1.93	0.50
2:5:1366:U:H2'	2:5:1367:G:C8	2.47	0.50
2:5:1509:A:N3	24:T:51:LYS:NZ	2.60	0.50
8:D:67:GLU:OE1	8:D:97:ARG:NH2	2.37	0.50
9:E:40:LEU:HD11	21:Q:54:ILE:HD13	1.93	0.50
9:E:47:TYR:OH	21:Q:94:ARG:O	2.22	0.50
2:5:457:A:H2'	2:5:458:G:C8	2.46	0.50
2:5:458:G:H2'	2:5:459:C:C6	2.47	0.50
4:8:28:A:H2'	4:8:29:U:H6	1.77	0.50
5:A:37:TRP:HB2	5:A:204:THR:HG22	1.94	0.50
12:H:86:VAL:HG13	12:H:100:LEU:HD13	1.94	0.50
13:I:35:VAL:HG22	13:I:93:LEU:HD11	1.94	0.50
13:I:98:ILE:HD12	13:I:99:PRO:O	2.11	0.50
16:L:3:ARG:O	16:L:57:ARG:NH2	2.44	0.50
2:5:520:C:H41	15:K:63:ARG:HH21	1.58	0.49
2:5:1070:G:H2'	2:5:1071:A:C8	2.47	0.49
2:5:1508:C:H2'	2:5:1509:A:C4	2.47	0.49
5:A:182:VAL:HG23	5:A:206:THR:HG22	1.92	0.49
7:C:123:LEU:HD21	7:C:145:LYS:HE2	1.94	0.49
9:E:182:ASN:OD1	9:E:182:ASN:N	2.45	0.49
2:5:18:U:H2'	2:5:19:C:C6	2.47	0.49
2:5:117:U:H2'	2:5:118:C:C6	2.47	0.49
2:5:1288:C:H2'	2:5:1289:U:C6	2.47	0.49
3:7:26:A:H61	3:7:44:G:H1	1.61	0.49
7:C:94:GLU:HG2	7:C:182:PRO:HG2	1.93	0.49
11:G:118:THR:OG1	11:G:119:SER:N	2.45	0.49
3:7:10:G:O2'	3:7:11:U:OP1	2.25	0.49
9:E:165:ASN:OD1	11:G:56:ASN:ND2	2.45	0.49
13:I:72:GLU:HB3	17:M:59:ALA:HB2	1.94	0.49
20:P:80:ILE:HD13	20:P:83:ARG:HH22	1.76	0.49
2:5:197:A:H2'	2:5:198:A:C8	2.48	0.49
2:5:426:U:H5'	7:C:8:PHE:CG	2.48	0.49
9:E:45:LEU:HD11	9:E:49:ILE:HG22	1.95	0.49
16:L:55:ALA:O	16:L:59:VAL:HG23	2.12	0.49
25:Y:52:A:H4'	25:Y:53:A:H5'	1.94	0.49
2:5:974:C:O2	17:M:19:ARG:HD3	2.11	0.49
2:5:1024:U:O2'	2:5:1025:U:OP1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:234:ASP:OD1	5:A:245:MET:N	2.23	0.49
10:F:17:PHE:HB3	10:F:58:LEU:HD22	1.94	0.49
2:5:623:G:H4'	19:O:16:THR:HG21	1.94	0.49
2:5:823:C:H1'	11:G:24:ASN:HD22	1.78	0.49
2:5:991:A:H2'	2:5:992:U:H6	1.77	0.49
2:5:1133:A:N7	2:5:1155:A:N6	2.60	0.49
7:C:69:LYS:HA	7:C:72:ARG:HG3	1.94	0.49
8:D:127:HIS:ND1	8:D:200:LEU:HD21	2.27	0.49
9:E:139:THR:OG1	9:E:140:GLN:N	2.46	0.49
14:J:28:SER:HB3	14:J:34:VAL:HG23	1.94	0.49
17:M:19:ARG:HG3	17:M:19:ARG:HH11	1.76	0.49
19:O:6:LEU:HD22	19:O:17:TYR:HD2	1.78	0.49
2:5:257:U:OP1	23:S:64:ARG:NH1	2.46	0.49
2:5:534:C:H2'	2:5:535:A:C8	2.47	0.49
2:5:966:A:O2'	27:5:1604:SPD:N1	2.45	0.49
3:7:28:C:OP1	22:R:87:ARG:NH1	2.41	0.49
9:E:94:TYR:HB3	21:Q:85:HIS:CD2	2.47	0.49
19:O:23:ASP:HB3	19:O:26:VAL:HG22	1.94	0.49
2:5:252:U:H2'	2:5:253:G:C8	2.48	0.48
2:5:483:U:H2'	2:5:484:A:C8	2.47	0.48
2:5:675:U:H2'	2:5:676:U:C6	2.48	0.48
2:5:725:A:H2'	2:5:726:A:C8	2.48	0.48
2:5:1497:U:H2'	2:5:1498:G:H8	1.78	0.48
7:C:106:PHE:HD1	7:C:157:ALA:HB1	1.78	0.48
12:H:110:LYS:O	12:H:110:LYS:HG2	2.13	0.48
6:B:121:ARG:NH1	6:B:190:GLU:OE2	2.47	0.48
6:B:229:GLN:HG3	6:B:230:PRO:HD2	1.94	0.48
7:C:104:MET:HG2	7:C:106:PHE:HD2	1.78	0.48
2:5:141:A:H2'	2:5:142:G:H8	1.78	0.48
2:5:251:G:OP1	20:P:73:LYS:NZ	2.32	0.48
2:5:1077:U:H2'	2:5:1078:G:H5'	1.96	0.48
6:B:85:ILE:HD12	6:B:231:ASN:CG	2.33	0.48
22:R:36:ARG:HB3	22:R:72:GLY:HA3	1.95	0.48
6:B:160:LEU:HD23	6:B:160:LEU:HA	1.59	0.48
8:D:162:ALA:O	8:D:167:ARG:NE	2.46	0.48
8:D:219:LEU:OXT	11:G:126:LYS:NZ	2.45	0.48
2:5:212:G:H2'	2:5:213:U:C6	2.49	0.48
2:5:356:G:H2'	2:5:357:G:C8	2.48	0.48
2:5:1158:A:O2'	2:5:1159:A:OP1	2.27	0.48
6:B:84:ASN:O	6:B:88:ILE:HG23	2.14	0.48
2:5:18:U:H2'	2:5:19:C:H6	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:55:C:H2'	2:5:348:C:H41	1.79	0.48
2:5:536:U:H2'	2:5:537:A:H8	1.79	0.48
5:A:180:ASP:OD1	5:A:219:ASN:ND2	2.43	0.48
14:J:76:LYS:NZ	14:J:102:GLU:OE1	2.45	0.48
2:5:35:C:H2'	2:5:36:G:C8	2.48	0.48
2:5:403:A:OP1	7:C:111:ARG:HD2	2.13	0.48
2:5:754:U:OP1	2:5:819:G:O2'	2.32	0.48
2:5:977:U:OP2	17:M:23:ARG:NH2	2.47	0.48
13:I:83:VAL:HG23	13:I:84:ASP:H	1.79	0.48
2:5:63:U:O2'	2:5:375:C:O2	2.31	0.48
2:5:169:G:H1	2:5:196:G:N2	2.11	0.48
2:5:633:U:H2'	2:5:634:U:C6	2.49	0.48
16:L:2:ALA:N	16:L:8:ASP:OD1	2.46	0.48
2:5:57:U:H2'	2:5:58:G:C8	2.49	0.48
2:5:374:G:H2'	2:5:375:C:C6	2.48	0.48
2:5:1438:U:H2'	2:5:1439:G:H8	1.77	0.48
4:8:22:G:H2'	4:8:23:A:H8	1.79	0.48
2:5:96:G:H1	2:5:326:C:H41	1.62	0.47
2:5:1351:U:H2'	2:5:1352:A:C8	2.49	0.47
11:G:26:ARG:HG3	11:G:82:PRO:HG3	1.95	0.47
2:5:231:U:H2'	2:5:232:G:H8	1.78	0.47
2:5:1199:U:O2'	2:5:1296:C:OP1	2.33	0.47
6:B:136:ALA:O	6:B:139:GLN:HG2	2.14	0.47
6:B:189:LEU:HD12	6:B:202:LYS:HG2	1.96	0.47
8:D:186:ASN:OD1	8:D:186:ASN:N	2.45	0.47
2:5:117:U:H2'	2:5:118:C:H6	1.79	0.47
2:5:331:C:H2'	2:5:332:A:H8	1.79	0.47
2:5:409:G:N2	2:5:425:G:H1'	2.30	0.47
2:5:632:A:H2'	2:5:633:U:H6	1.79	0.47
2:5:991:A:H2'	2:5:992:U:C6	2.50	0.47
2:5:1294:U:H2'	2:5:1295:U:C6	2.49	0.47
18:N:4:ASP:OD1	18:N:4:ASP:N	2.46	0.47
2:5:152:U:H2'	2:5:153:A:H8	1.79	0.47
2:5:255:G:H2'	2:5:256:G:C8	2.49	0.47
2:5:472:G:H2'	2:5:473:A:H8	1.79	0.47
2:5:1045:C:H42	25:Y:46:G:N2	2.10	0.47
2:5:1384:A:H2'	2:5:1385:A:C8	2.48	0.47
7:C:90:PHE:O	7:C:93:LEU:HG	2.15	0.47
13:I:32:VAL:HG22	13:I:36:LYS:HD2	1.97	0.47
13:I:56:THR:HG23	13:I:70:GLN:HG3	1.95	0.47
21:Q:65:SER:HB3	21:Q:69:LYS:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:671:G:H2'	2:5:672:A:H8	1.78	0.47
2:5:922:G:H1	2:5:1365:U:H3	1.62	0.47
2:5:70:A:H2'	2:5:71:A:H8	1.78	0.47
2:5:399:C:H5'	7:C:131:THR:HG23	1.97	0.47
2:5:543:C:H5'	7:C:68:ASP:OD2	2.14	0.47
2:5:608:G:C2	2:5:609:G:C8	3.02	0.47
2:5:1032:G:H2'	2:5:1033:U:O4'	2.15	0.47
2:5:1062:C:H2'	2:5:1063:G:H8	1.78	0.47
2:5:1139:A:H2'	2:5:1140:A:C8	2.49	0.47
2:5:1401:A:H2'	2:5:1402:U:C6	2.49	0.47
3:7:44:G:H2'	3:7:45:G:C8	2.50	0.47
16:L:20:THR:HG22	16:L:27:LEU:HA	1.97	0.47
21:Q:39:LYS:HA	21:Q:39:LYS:HD3	1.64	0.47
2:5:369:A:H2'	2:5:370:A:H8	1.79	0.47
2:5:707:G:H2'	2:5:708:A:C8	2.48	0.47
2:5:894:A:H2'	2:5:895:A:C8	2.50	0.47
6:B:167:ARG:HH21	25:Y:48:C:H1'	1.80	0.47
13:I:86:ASN:ND2	13:I:87:GLN:H	2.13	0.47
2:5:271:G:O2'	20:P:18:ASN:ND2	2.45	0.47
2:5:513:G:H2'	2:5:514:U:H6	1.79	0.47
2:5:836:C:H1'	9:E:145:ARG:HG2	1.96	0.47
2:5:892:G:N2	2:5:895:A:OP2	2.47	0.47
2:5:1214:A:H62	2:5:1273:A:N6	2.13	0.47
5:A:30:VAL:HG13	5:A:53:ASN:HB3	1.96	0.47
15:K:55:PRO:HB2	15:K:59:ASN:HB2	1.96	0.47
23:S:21:ASN:HB3	23:S:59:ILE:HG23	1.96	0.47
2:5:70:A:H2'	2:5:71:A:C8	2.50	0.47
2:5:673:A:H2'	2:5:674:U:H6	1.80	0.47
2:5:130:G:H2'	2:5:131:G:C8	2.50	0.46
2:5:152:U:H2'	2:5:153:A:C8	2.50	0.46
2:5:394:U:H2'	2:5:395:G:C8	2.49	0.46
2:5:516:C:H4'	2:5:517:C:H5''	1.95	0.46
11:G:61:GLU:HG2	11:G:65:LYS:HA	1.98	0.46
24:T:36:LEU:H	24:T:41:ARG:HH21	1.63	0.46
2:5:207:C:H2'	2:5:208:A:O4'	2.15	0.46
2:5:681:U:O2	14:J:34:VAL:HG12	2.16	0.46
2:5:933:A:N3	2:5:1351:U:O2'	2.40	0.46
6:B:26:SER:OG	6:B:27:HIS:N	2.49	0.46
2:5:82:C:H2'	2:5:83:U:H6	1.81	0.46
2:5:855:G:HO2'	2:5:868:G:HO2'	1.62	0.46
2:5:1220:A:H2'	2:5:1221:A:H8	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:27:LYS:HE2	7:C:27:LYS:HB2	1.76	0.46
13:I:47:PRO:HA	13:I:78:ARG:HD2	1.97	0.46
2:5:20:C:H2'	2:5:21:U:C6	2.50	0.46
2:5:403:A:H2'	2:5:404:A:C8	2.50	0.46
2:5:1280:A:N6	2:5:1305:G:H1'	2.30	0.46
2:5:1505:G:H2'	2:5:1506:A:C8	2.49	0.46
10:F:87:PRO:HD2	10:F:151:ALA:HA	1.97	0.46
10:F:136:LYS:O	10:F:140:THR:HG22	2.15	0.46
2:5:170:A:O2'	2:5:220:U:OP1	2.22	0.46
2:5:661:G:H5'	21:Q:84:ARG:HH11	1.81	0.46
12:H:93:ASN:OD1	12:H:96:LEU:HD12	2.16	0.46
2:5:137:A:N7	2:5:157:A:N6	2.64	0.46
2:5:157:A:H2'	2:5:158:A:C8	2.50	0.46
2:5:561:A:H2'	2:5:565:G:C8	2.50	0.46
2:5:632:A:H2'	2:5:633:U:C6	2.51	0.46
2:5:853:A:OP2	2:5:863:A:N6	2.42	0.46
2:5:1490:G:H2'	2:5:1491:A:C8	2.51	0.46
10:F:65:VAL:O	10:F:69:MET:HB2	2.16	0.46
16:L:7:ILE:HD12	16:L:7:ILE:H	1.81	0.46
2:5:57:U:H2'	2:5:58:G:H8	1.80	0.46
2:5:498:G:H2'	2:5:499:U:C6	2.50	0.46
2:5:660:A:H2'	2:5:661:G:O4'	2.16	0.46
7:C:179:VAL:HG12	7:C:180:ARG:N	2.31	0.46
9:E:49:ILE:HD13	9:E:84:ARG:NH2	2.29	0.46
16:L:39:ILE:HG12	16:L:52:GLU:HB3	1.97	0.46
2:5:354:U:H2'	2:5:355:A:C8	2.50	0.46
2:5:386:U:H2'	2:5:387:G:C8	2.51	0.46
2:5:862:C:H2'	2:5:863:A:O4'	2.15	0.46
2:5:1024:U:HO2'	2:5:1025:U:P	2.39	0.46
2:5:1225:A:H2'	2:5:1226:A:C8	2.51	0.46
2:5:1496:G:H2'	2:5:1497:U:C6	2.50	0.46
5:A:93:LYS:HE3	5:A:93:LYS:HB2	1.80	0.46
17:M:34:LEU:O	17:M:38:GLY:N	2.49	0.46
19:O:66:THR:HG22	19:O:67:ASP:H	1.80	0.46
2:5:145:G:HO2'	2:5:147:A:H62	1.61	0.46
2:5:147:A:H2'	2:5:148:A:C8	2.51	0.46
2:5:214:U:H2'	2:5:215:C:C6	2.50	0.46
2:5:579:G:N1	2:5:756:A:OP2	2.33	0.46
2:5:765:A:H4'	2:5:1498:G:N2	2.31	0.46
2:5:1316:C:H2'	2:5:1317:A:H8	1.81	0.46
2:5:1405:U:H2'	2:5:1406:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:152:LYS:HB3	8:D:179:TYR:HB2	1.97	0.46
10:F:80:ALA:HA	25:Y:37:G:N2	2.30	0.46
15:K:18:LYS:HB2	15:K:18:LYS:HE2	1.73	0.46
15:K:80:ILE:H	15:K:80:ILE:HD12	1.81	0.46
21:Q:36:ARG:HB2	21:Q:38:LYS:HG2	1.98	0.46
2:5:98:G:H1'	2:5:350:G:H5'	1.98	0.46
2:5:971:A:P	2:5:1332:U:HO2'	2.39	0.46
6:B:71:ALA:O	6:B:109:ILE:HG22	2.16	0.46
7:C:74:LEU:O	7:C:78:VAL:HG12	2.16	0.46
15:K:7:LEU:HD12	15:K:12:ARG:HG2	1.98	0.46
2:5:474:G:H2'	2:5:475:U:C6	2.51	0.45
4:8:40:C:O3'	16:L:119:LYS:NZ	2.49	0.45
9:E:28:THR:HG21	9:E:72:PHE:HA	1.98	0.45
11:G:43:ALA:O	11:G:47:ILE:HG23	2.15	0.45
15:K:57:LYS:HB3	15:K:58:PRO:HD3	1.97	0.45
7:C:14:LEU:HB3	7:C:59:ARG:HE	1.80	0.45
9:E:39:TYR:CE1	9:E:41:GLY:HA2	2.52	0.45
9:E:142:ARG:HB2	9:E:145:ARG:HG3	1.98	0.45
14:J:14:ILE:HG21	14:J:93:PHE:CZ	2.52	0.45
15:K:55:PRO:HB3	15:K:102:ASP:HB3	1.98	0.45
2:5:141:A:H2'	2:5:142:G:C8	2.51	0.45
2:5:397:C:O2'	2:5:619:A:N3	2.49	0.45
2:5:1278:G:N2	2:5:1308:G:O6	2.50	0.45
2:5:1279:G:HO2'	2:5:1280:A:H8	1.60	0.45
14:J:29:ASP:OD1	14:J:30:PRO:HD2	2.15	0.45
2:5:18:U:O2'	2:5:1070:G:H1'	2.17	0.45
2:5:525:G7M:O2'	2:5:533:A:N1	2.39	0.45
2:5:654:U:H2'	2:5:655:G:H8	1.81	0.45
2:5:655:G:H2'	2:5:656:U:H6	1.80	0.45
2:5:1510:C:N4	5:A:291:LEU:HD22	2.31	0.45
3:7:34:G:O6	25:Y:42:U:O4	2.34	0.45
8:D:78:LYS:HG2	8:D:85:ASN:HB2	1.98	0.45
8:D:91:LEU:HD21	8:D:192:ILE:HD12	1.98	0.45
12:H:30:ILE:HG23	12:H:37:PRO:HG3	1.99	0.45
2:5:108:C:H2'	2:5:109:G:H8	1.81	0.45
2:5:260:C:H2'	2:5:261:G:O4'	2.16	0.45
5:A:85:VAL:HG12	5:A:108:ILE:HB	1.99	0.45
7:C:203:LEU:O	7:C:203:LEU:HD23	2.17	0.45
10:F:120:ALA:O	10:F:124:ILE:HG23	2.16	0.45
11:G:125:ASP:OD1	11:G:126:LYS:N	2.49	0.45
2:5:44:C:H4'	19:O:11:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:187:A:H2'	2:5:188:U:C6	2.51	0.45
2:5:195:U:H2'	2:5:196:G:C8	2.47	0.45
2:5:1046:A:N3	6:B:159:ARG:HD3	2.31	0.45
3:7:11:U:H2'	3:7:12:G:H8	1.82	0.45
8:D:187:THR:O	8:D:191:MET:HG3	2.16	0.45
2:5:80:U:H2'	2:5:81:A:C8	2.52	0.45
2:5:920:G:O2'	2:5:922:G:OP1	2.32	0.45
2:5:1121:U:H3'	2:5:1122:U:H5''	1.99	0.45
2:5:1245:A:H2'	2:5:1246:A:C8	2.51	0.45
7:C:85:LEU:HB3	7:C:88:ASN:HB3	1.98	0.45
7:C:99:ASN:O	7:C:103:ARG:HG2	2.16	0.45
9:E:10:ASP:OD2	9:E:52:GLN:HG2	2.17	0.45
2:5:661:G:N2	2:5:723:C:O2'	2.47	0.45
2:5:917:G:H2'	2:5:918:A:C8	2.51	0.45
3:7:23:C:H2'	3:7:24:A:C8	2.52	0.45
11:G:44:ILE:HD12	11:G:138:LEU:HD23	1.99	0.45
15:K:46:VAL:HG22	15:K:92:VAL:HG22	1.99	0.45
2:5:255:G:H2'	2:5:256:G:H8	1.82	0.45
2:5:664:A:H2'	2:5:665:G:C8	2.51	0.45
2:5:871:U:OP1	11:G:92:LYS:HE2	2.17	0.45
2:5:941:A:O2'	2:5:1307:A:N3	2.38	0.45
2:5:1304:U:H2'	2:5:1305:G:O4'	2.17	0.45
11:G:116:ILE:O	11:G:123:MET:N	2.50	0.45
14:J:26:SER:HB3	14:J:34:VAL:HG21	1.98	0.45
2:5:335:C:H2'	2:5:336:U:C6	2.52	0.45
2:5:457:A:H2'	2:5:458:G:H8	1.82	0.45
2:5:596:U:H4'	11:G:98:TYR:CG	2.52	0.45
4:8:44:G:H2'	4:8:45:G:O4'	2.17	0.45
7:C:165:PRO:HB2	7:C:180:ARG:NH2	2.32	0.45
18:N:29:LEU:HD23	18:N:29:LEU:HA	1.87	0.45
2:5:112:U:H2'	2:5:113:C:C6	2.52	0.44
11:G:104:LEU:HD23	11:G:104:LEU:HA	1.80	0.44
19:O:47:LYS:H	19:O:47:LYS:HG3	1.57	0.44
2:5:252:U:H2'	2:5:253:G:H8	1.81	0.44
2:5:471:A:H2'	2:5:472:G:C8	2.52	0.44
2:5:576:A:O2'	2:5:725:A:N3	2.44	0.44
2:5:641:U:C2	2:5:642:A:C8	3.05	0.44
2:5:705:A:H2'	2:5:706:U:C6	2.52	0.44
2:5:1306:A:H2'	2:5:1307:A:O4'	2.17	0.44
7:C:67:THR:HB	7:C:70:GLN:HG3	1.99	0.44
15:K:45:GLY:HA2	15:K:70:LEU:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:47:CYS:HA	15:K:68:VAL:HA	1.98	0.44
2:5:196:G:O2'	2:5:197:A:OP1	2.29	0.44
2:5:766:G:H4'	2:5:1488:A:H4'	1.99	0.44
2:5:999:C:OP1	2:5:1023:G:N2	2.48	0.44
2:5:1156:G:O2'	2:5:1157:G:N7	2.38	0.44
5:A:49:ARG:HG3	5:A:50:LYS:N	2.30	0.44
5:A:192:ASN:HD21	5:A:210:LEU:HA	1.83	0.44
7:C:131:THR:HA	7:C:132:PRO:HD3	1.87	0.44
7:C:149:ILE:HA	7:C:154:VAL:HG21	2.00	0.44
12:H:47:ILE:HA	12:H:50:MET:HE3	1.98	0.44
16:L:48:LEU:HB3	16:L:53:PHE:HE2	1.82	0.44
22:R:76:PRO:O	22:R:76:PRO:HD2	2.17	0.44
2:5:266:A:H2'	2:5:267:C:H6	1.82	0.44
2:5:522:G:H2'	2:5:523:U:C6	2.52	0.44
2:5:682:G:H2'	2:5:683:G:C8	2.53	0.44
2:5:948:U:O4	16:L:103:ARG:NH1	2.50	0.44
2:5:1269:U:H2'	2:5:1270:C:C6	2.52	0.44
2:5:1456:U:H2'	2:5:1457:G:C8	2.52	0.44
9:E:5:ILE:HD12	9:E:62:PHE:CE1	2.53	0.44
9:E:50:LYS:HA	9:E:50:LYS:HD2	1.66	0.44
2:5:331:C:H2'	2:5:332:A:C8	2.52	0.44
2:5:530:A:N6	2:5:1181:G:O2'	2.51	0.44
8:D:219:LEU:HD12	8:D:219:LEU:H	1.82	0.44
11:G:44:ILE:O	11:G:48:LEU:HD12	2.17	0.44
19:O:44:LYS:HG3	19:O:45:GLU:OE2	2.18	0.44
23:S:56:ARG:HH12	23:S:57:LYS:NZ	2.15	0.44
2:5:32:U:O2'	2:5:49:C:N4	2.51	0.44
2:5:386:U:H2'	2:5:387:G:H8	1.83	0.44
2:5:1201:C:P	16:L:90:ARG:HH12	2.41	0.44
6:B:114:LEU:HD23	6:B:114:LEU:H	1.82	0.44
6:B:158:GLY:HA3	6:B:199:ILE:HD13	1.99	0.44
11:G:18:LEU:HD13	11:G:41:LYS:HD2	1.98	0.44
2:5:369:A:H2'	2:5:370:A:C8	2.53	0.44
21:Q:96:LEU:HD23	21:Q:96:LEU:HA	1.87	0.44
2:5:1022:G:H2'	2:5:1023:G:C8	2.53	0.44
2:5:1345:G:OP2	27:5:1601:SPD:N10	2.38	0.44
2:5:1385:A:H2'	2:5:1386:C:H6	1.82	0.44
19:O:86:LYS:HD3	19:O:86:LYS:C	2.38	0.44
2:5:200:G:H2'	2:5:201:G:H8	1.83	0.44
2:5:909:A:O2'	2:5:911:G:H5''	2.18	0.44
13:I:28:THR:O	13:I:32:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:507:A:H5''	7:C:51:ALA:HB2	2.00	0.43
2:5:578:C:H2'	2:5:579:G:O4'	2.18	0.43
2:5:1298:U:H2'	2:5:1299:C:C6	2.53	0.43
6:B:106:ILE:O	6:B:229:GLN:HB3	2.18	0.43
9:E:90:LEU:HD12	9:E:90:LEU:H	1.82	0.43
10:F:129:ASN:O	10:F:129:ASN:ND2	2.40	0.43
16:L:5:LEU:H	16:L:57:ARG:NH2	2.16	0.43
18:N:18:ASP:OD2	18:N:21:SER:HB2	2.17	0.43
25:Y:52:A:H1'	25:Y:53:A:C4	2.53	0.43
2:5:1158:A:HO2'	2:5:1159:A:P	2.41	0.43
8:D:110:GLU:HB2	8:D:113:ASN:OD1	2.18	0.43
10:F:21:LEU:O	10:F:25:ILE:HG22	2.18	0.43
23:S:28:LEU:HD22	23:S:54:LEU:HD12	2.00	0.43
2:5:767:U:H2'	2:5:768:G:H8	1.83	0.43
2:5:1293:A:OP2	22:R:3:ARG:NH1	2.51	0.43
5:A:73:LYS:HE3	5:A:73:LYS:HB3	1.76	0.43
2:5:61:A:N1	2:5:92:G:O2'	2.43	0.43
2:5:250:G:O2'	20:P:19:ALA:O	2.37	0.43
2:5:510:U:H2'	2:5:511:A:H8	1.84	0.43
2:5:675:U:H2'	2:5:676:U:H6	1.82	0.43
2:5:1146:A:H2'	2:5:1147:U:C6	2.53	0.43
10:F:86:VAL:HG11	10:F:154:ARG:HG2	2.01	0.43
10:F:138:ASP:O	10:F:142:LYS:HG2	2.18	0.43
15:K:27:ASN:O	15:K:35:VAL:HA	2.19	0.43
18:N:28:LEU:O	18:N:32:GLN:HG3	2.18	0.43
21:Q:53:LEU:HD23	21:Q:53:LEU:H	1.84	0.43
2:5:335:C:H2'	2:5:336:U:H6	1.84	0.43
2:5:818:A:H2'	2:5:819:G:H8	1.83	0.43
2:5:1110:C:H2'	2:5:1111:G:H8	1.82	0.43
2:5:1111:G:H2'	2:5:1112:U:C6	2.53	0.43
2:5:1288:C:H2'	2:5:1289:U:H6	1.84	0.43
2:5:1510:C:H2'	24:T:58:ASN:HD22	1.84	0.43
5:A:194:LEU:HD23	5:A:194:LEU:HA	1.85	0.43
12:H:26:ASP:O	12:H:27:LYS:HB2	2.18	0.43
18:N:29:LEU:HD11	18:N:59:LYS:HD3	2.00	0.43
19:O:55:ALA:O	19:O:59:LEU:HD23	2.18	0.43
2:5:395:G:H2'	2:5:396:C:C6	2.53	0.43
2:5:918:A:H2'	2:5:919:C:C6	2.54	0.43
2:5:1027:A:H2'	2:5:1028:C:O4'	2.19	0.43
2:5:1321:G:O2'	2:5:1348:G:O6	2.31	0.43
2:5:1387:U:H2'	2:5:1388:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:30:ILE:CG2	12:H:37:PRO:HG3	2.48	0.43
17:M:19:ARG:HG3	17:M:19:ARG:NH1	2.32	0.43
19:O:8:ARG:HB2	19:O:28:ARG:NH1	2.33	0.43
2:5:358:G:OP1	15:K:71:THR:OG1	2.36	0.43
4:8:38:A:C2	16:L:124:LYS:HA	2.53	0.43
2:5:459:C:H2'	2:5:460:A:O4'	2.18	0.43
2:5:725:A:H2'	2:5:726:A:H8	1.83	0.43
2:5:1030:G:C2	2:5:1031:A:C8	3.06	0.43
2:5:1236:A:H62	2:5:1249:G:H21	1.67	0.43
5:A:147:LYS:O	5:A:151:MET:HG3	2.19	0.43
6:B:42:ASN:O	6:B:46:VAL:HG22	2.19	0.43
14:J:76:LYS:HZ3	14:J:102:GLU:HB2	1.84	0.43
2:5:171:A:H2'	2:5:172:C:C6	2.54	0.43
2:5:218:U:H2'	2:5:219:A:H8	1.84	0.43
2:5:471:A:H2'	2:5:472:G:H8	1.83	0.43
2:5:1150:G:H2'	2:5:1151:A:C8	2.52	0.43
7:C:200:TYR:O	7:C:204:VAL:HB	2.19	0.43
15:K:61:ALA:HB3	15:K:63:ARG:NH1	2.33	0.43
18:N:6:ASN:O	18:N:10:LYS:HG3	2.18	0.43
2:5:365:U:H2'	2:5:366:C:C6	2.53	0.43
2:5:503:G:H2'	2:5:504:A:C8	2.53	0.43
5:A:171:ARG:HG2	5:A:172:LEU:H	1.83	0.43
5:A:260:GLN:OE1	5:A:261:LYS:HG2	2.18	0.43
10:F:121:ASN:HA	10:F:124:ILE:HG12	2.01	0.43
2:5:196:G:O2'	2:5:197:A:H5''	2.19	0.42
2:5:622:A:H2'	2:5:623:G:C8	2.54	0.42
2:5:832:G:H2'	2:5:833:G:H8	1.84	0.42
2:5:896:G:H2'	2:5:897:A:C8	2.52	0.42
2:5:1061:U:H2'	2:5:1062:C:H6	1.84	0.42
2:5:1163:A:H2'	2:5:1164:U:O4'	2.18	0.42
5:A:22:LYS:HE2	5:A:254:ILE:HG22	2.01	0.42
5:A:223:GLN:HE22	5:A:277:ILE:HD13	1.83	0.42
7:C:9:LYS:HE2	7:C:9:LYS:HB3	1.68	0.42
9:E:43:LYS:HB3	9:E:43:LYS:HE3	1.83	0.42
13:I:16:LEU:HB3	13:I:24:LEU:HD11	2.00	0.42
15:K:47:CYS:SG	15:K:48:THR:N	2.91	0.42
18:N:9:ILE:HG21	18:N:19:VAL:HG12	2.01	0.42
6:B:230:PRO:HB2	6:B:231:ASN:H	1.65	0.42
10:F:20:THR:O	10:F:24:ARG:HG3	2.18	0.42
13:I:56:THR:CG2	13:I:68:ARG:HD3	2.49	0.42
2:5:633:U:H2'	2:5:634:U:H6	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:825:A:H2'	2:5:826:G:O4'	2.19	0.42
2:5:1061:U:H2'	2:5:1062:C:C6	2.54	0.42
2:5:1123:G:O2'	2:5:1124:U:H6	2.02	0.42
5:A:260:GLN:H	5:A:260:GLN:HG3	1.66	0.42
9:E:86:LEU:HD13	21:Q:95:TYR:CE1	2.54	0.42
2:5:169:G:N2	2:5:170:A:H1'	2.34	0.42
2:5:218:U:C2	2:5:219:A:C8	3.06	0.42
2:5:395:G:H2'	2:5:396:C:H6	1.85	0.42
2:5:441:U:H2'	2:5:442:G:C8	2.54	0.42
2:5:588:U:O3'	11:G:39:LYS:NZ	2.53	0.42
2:5:610:C:H2'	2:5:611:A:H8	1.83	0.42
2:5:625:U:H2'	2:5:626:G:C8	2.53	0.42
2:5:1029:C:H2'	2:5:1030:G:O4'	2.19	0.42
6:B:127:ILE:CD1	6:B:133:LEU:HD13	2.49	0.42
12:H:41:PHE:C	12:H:43:ASN:H	2.22	0.42
14:J:27:ALA:HB3	14:J:36:CYS:SG	2.59	0.42
2:5:571:A:N3	2:5:877:C:O2'	2.48	0.42
2:5:943:C:H2'	2:5:944:A:H8	1.85	0.42
5:A:178:VAL:HG13	5:A:184:GLU:HG3	2.01	0.42
6:B:85:ILE:HD12	6:B:231:ASN:OD1	2.19	0.42
7:C:123:LEU:HB2	7:C:143:ARG:O	2.20	0.42
21:Q:64:LEU:HD23	21:Q:64:LEU:HA	1.79	0.42
25:Y:47:U:H3'	25:Y:48:C:H6	1.85	0.42
2:5:81:A:H2'	2:5:82:C:C6	2.55	0.42
2:5:111:A:H2'	2:5:112:U:O4'	2.19	0.42
2:5:164:C:H2'	2:5:165:A:H8	1.84	0.42
2:5:622:A:H2'	2:5:623:G:H8	1.84	0.42
2:5:1004:U:H2'	2:5:1005:U:C6	2.55	0.42
2:5:1413:G:C6	2:5:1439:G:C6	3.07	0.42
8:D:87:ARG:HG2	8:D:109:LEU:HD22	2.02	0.42
10:F:15:PRO:HB2	12:H:45:LEU:HD11	2.02	0.42
11:G:27:LYS:HD3	11:G:27:LYS:HA	1.83	0.42
13:I:15:LYS:HZ1	13:I:77:LYS:HD2	1.84	0.42
20:P:58:GLY:HA3	20:P:85:LYS:HB3	2.02	0.42
25:Y:54:A:H1'	25:Y:55:A:C8	2.54	0.42
2:5:82:C:H2'	2:5:83:U:C6	2.55	0.42
2:5:661:G:H5'	21:Q:84:ARG:NH1	2.33	0.42
2:5:1118:A:C5	2:5:1119:C:C2	3.07	0.42
2:5:1163:A:O3'	17:M:58:LYS:NZ	2.52	0.42
2:5:1289:U:O2'	2:5:1334:A:N3	2.39	0.42
2:5:189:C:H2'	2:5:190:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:190:A:H2'	2:5:191:A:H8	1.85	0.42
2:5:279:C:H2'	2:5:280:G:H8	1.85	0.42
2:5:1004:U:H2'	2:5:1005:U:H6	1.84	0.42
2:5:1388:A:H2	2:5:1462:G:H22	1.68	0.42
8:D:138:HIS:O	8:D:202:GLN:NE2	2.53	0.42
2:5:913:A:H2'	2:5:914:A:C8	2.55	0.42
2:5:1465:U:H2'	2:5:1466:U:O4'	2.20	0.42
10:F:110:ARG:HG2	10:F:112:GLU:CG	2.46	0.42
19:O:1:MET:HG3	19:O:24:SER:HB3	2.01	0.42
25:Y:53:A:H2	25:Y:54:A:H2'	1.85	0.42
2:5:115:A:C2	2:5:186:A:H1'	2.55	0.42
2:5:416:U:O4	2:5:418:U:O2'	2.33	0.42
2:5:441:U:H2'	2:5:442:G:H8	1.85	0.42
2:5:470:U:H2'	2:5:471:A:H8	1.84	0.42
2:5:625:U:H2'	2:5:626:G:H8	1.84	0.42
2:5:998:G:N3	2:5:998:G:H2'	2.35	0.42
2:5:1022:G:O2'	2:5:1023:G:O5'	2.38	0.42
2:5:1456:U:H2'	2:5:1457:G:H8	1.85	0.42
16:L:15:ILE:O	16:L:19:LEU:HD23	2.20	0.42
24:T:3:LYS:H	24:T:3:LYS:HG3	1.71	0.42
2:5:684:A:C2	2:5:701:A:C5	3.08	0.41
2:5:1410:A:H2'	2:5:1411:A:H8	1.83	0.41
2:5:93:A:H62	23:S:10:ARG:HG2	1.85	0.41
2:5:403:A:H2'	2:5:404:A:H8	1.84	0.41
2:5:680:G:H21	14:J:33:ASN:H	1.68	0.41
2:5:1227:A:H2'	2:5:1228:C:O4'	2.20	0.41
20:P:27:GLU:HG2	20:P:42:HIS:CD2	2.55	0.41
23:S:68:LEU:HD23	23:S:68:LEU:HA	1.84	0.41
2:5:562:U:OP2	15:K:12:ARG:NH2	2.37	0.41
2:5:664:A:H2'	2:5:665:G:H8	1.85	0.41
2:5:885:U:H2'	2:5:886:A:H8	1.85	0.41
2:5:1026:A:N3	2:5:1026:A:H2'	2.35	0.41
2:5:1157:G:H4'	2:5:1158:A:H5'	2.01	0.41
4:8:42:U:H2'	4:8:43:U:O4'	2.20	0.41
5:A:88:LYS:HG2	5:A:89:ASN:H	1.85	0.41
2:5:23:G:H2'	2:5:24:C:H6	1.85	0.41
2:5:661:G:O2'	2:5:722:G:O2'	2.38	0.41
2:5:1027:A:H3'	2:5:1028:C:C6	2.54	0.41
2:5:1248:U:H2'	2:5:1249:G:O4'	2.20	0.41
2:5:1343:G:OP1	13:I:70:GLN:NE2	2.53	0.41
7:C:101:VAL:O	7:C:104:MET:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:17:TYR:N	19:O:17:TYR:CD1	2.89	0.41
2:5:328:G:OP1	23:S:7:ASN:ND2	2.53	0.41
2:5:469:C:O2'	19:O:80:LYS:HE2	2.21	0.41
2:5:1028:C:O2'	2:5:1029:C:H6	2.04	0.41
5:A:136:LYS:HE3	5:A:136:LYS:HB2	1.83	0.41
8:D:160:ILE:HG22	8:D:162:ALA:H	1.85	0.41
11:G:73:ASN:OD1	11:G:73:ASN:N	2.54	0.41
12:H:82:ARG:NH1	12:H:105:LEU:HD22	2.35	0.41
13:I:44:GLY:HA2	13:I:45:PRO:HD3	1.86	0.41
2:5:1347:U:H2'	2:5:1348:G:O4'	2.21	0.41
5:A:124:SER:HA	5:A:127:ILE:HG12	2.03	0.41
7:C:155:LYS:O	7:C:159:GLU:HG2	2.20	0.41
9:E:127:ASN:OD1	9:E:127:ASN:N	2.53	0.41
11:G:41:LYS:O	11:G:44:ILE:HG22	2.20	0.41
16:L:79:HIS:HE1	22:R:65:ASP:OD2	2.03	0.41
18:N:68:LYS:HG3	18:N:75:TYR:CD2	2.56	0.41
22:R:69:HIS:HB2	22:R:74:PHE:CZ	2.55	0.41
2:5:931:C:C4	2:5:932:A:N7	2.89	0.41
2:5:1024:U:H1'	2:5:1025:U:OP2	2.21	0.41
2:5:1389:U:H2'	2:5:1390:G:H8	1.85	0.41
2:5:1408:A:H2'	2:5:1409:A:C8	2.56	0.41
7:C:18:LEU:HD12	7:C:18:LEU:H	1.85	0.41
7:C:106:PHE:CD1	7:C:157:ALA:HB1	2.55	0.41
15:K:16:LYS:HE3	15:K:16:LYS:HB3	1.92	0.41
23:S:20:ASN:O	23:S:24:GLN:HG2	2.21	0.41
2:5:90:G:OP2	23:S:17:ARG:NH2	2.54	0.41
2:5:1211:A:H2'	2:5:1212:C:C6	2.56	0.41
2:5:1298:U:H2'	2:5:1299:C:H6	1.85	0.41
5:A:232:LEU:O	5:A:236:VAL:HG23	2.20	0.41
10:F:82:SER:OG	10:F:83:ASN:N	2.52	0.41
14:J:23:THR:HG21	14:J:56:ALA:HA	2.03	0.41
14:J:43:MET:HA	14:J:43:MET:CE	2.51	0.41
19:O:67:ASP:OD1	19:O:67:ASP:N	2.52	0.41
23:S:39:ILE:HD13	23:S:79:THR:HG21	2.02	0.41
2:5:426:U:H3'	7:C:8:PHE:CD1	2.56	0.41
2:5:542:G:OP1	7:C:58:GLN:NE2	2.54	0.41
2:5:613:C:H2'	2:5:614:U:C6	2.56	0.41
2:5:680:G:N2	14:J:33:ASN:H	2.19	0.41
2:5:1451:A:H2'	2:5:1452:C:C6	2.56	0.41
2:5:1482:A:H2'	2:5:1483:C:C6	2.56	0.41
3:7:25:U:C2	3:7:26:A:C8	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:61:GLN:NE2	5:A:217:ALA:HA	2.35	0.41
8:D:67:GLU:H	8:D:67:GLU:HG3	1.65	0.41
10:F:32:ASP:OD1	10:F:32:ASP:O	2.39	0.41
12:H:89:LEU:HD23	12:H:89:LEU:HA	1.82	0.41
15:K:52:THR:HG22	15:K:64:LYS:HD3	2.03	0.41
16:L:5:LEU:H	16:L:57:ARG:HH21	1.69	0.41
18:N:36:LEU:HA	18:N:36:LEU:HD23	1.83	0.41
19:O:34:ALA:HB3	19:O:58:TRP:HE1	1.86	0.41
2:5:23:G:H4'	2:5:879:G:C8	2.56	0.41
2:5:536:U:H2'	2:5:537:A:C8	2.54	0.41
2:5:737:U:OP1	18:N:35:GLN:NE2	2.53	0.41
2:5:838:A:O2'	9:E:111:LYS:HD2	2.21	0.41
2:5:920:G:C2	2:5:922:G:C8	3.09	0.41
2:5:943:C:OP1	16:L:106:ALA:HA	2.20	0.41
3:7:10:G:HO2'	3:7:11:U:P	2.43	0.41
7:C:170:ASN:O	7:C:173:THR:OG1	2.36	0.41
12:H:86:VAL:O	12:H:90:LEU:HD22	2.21	0.41
22:R:28:LYS:H	22:R:28:LYS:HG2	1.68	0.41
2:5:976:U:H2'	2:5:977:U:C5	2.56	0.40
2:5:1215:U:H4'	10:F:37:LEU:HD21	2.03	0.40
7:C:134:ILE:H	7:C:134:ILE:HG12	1.64	0.40
9:E:101:ASN:HD22	9:E:104:LYS:HG3	1.86	0.40
11:G:90:ILE:HG22	11:G:97:ILE:HG13	2.03	0.40
14:J:98:LEU:H	14:J:98:LEU:HD12	1.86	0.40
21:Q:57:LEU:HD11	21:Q:98:LEU:HD23	2.03	0.40
1:3:1931:C:H2'	1:3:1932:C:C6	2.55	0.40
2:5:120:A:H61	19:O:25:ARG:NH1	2.19	0.40
2:5:354:U:C2	2:5:355:A:C8	3.09	0.40
2:5:355:A:H2'	2:5:356:G:H8	1.86	0.40
2:5:372:G:H4'	19:O:5:ARG:HH11	1.86	0.40
2:5:473:A:C4	2:5:474:G:C8	3.10	0.40
2:5:1151:A:H2'	2:5:1152:G:C8	2.56	0.40
2:5:1300:C:H2'	2:5:1301:U:H6	1.85	0.40
5:A:44:PHE:CE2	5:A:214:ILE:HG21	2.55	0.40
7:C:19:LEU:HD13	7:C:188:PRO:HG2	2.03	0.40
7:C:186:GLU:O	7:C:188:PRO:HD3	2.21	0.40
13:I:97:LYS:HA	13:I:97:LYS:HD2	1.95	0.40
19:O:47:LYS:HE3	19:O:47:LYS:HB2	1.84	0.40
2:5:33:A:H2'	2:5:34:A:C8	2.56	0.40
2:5:320:G:N1	2:5:323:A:OP2	2.54	0.40
2:5:708:A:H2'	2:5:709:A:C8	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:49:ARG:CG	5:A:50:LYS:H	2.30	0.40
5:A:177:ILE:HG12	5:A:199:VAL:CG2	2.50	0.40
5:A:208:PRO:HA	5:A:214:ILE:HD11	2.03	0.40
17:M:39:VAL:HG13	17:M:43:CYS:HB2	2.03	0.40
21:Q:78:ASN:N	21:Q:78:ASN:OD1	2.54	0.40
2:5:177:G:N2	2:5:188:U:O2	2.40	0.40
2:5:348:C:H4'	2:5:350:G:OP1	2.22	0.40
2:5:836:C:H3'	2:5:837:G:C8	2.55	0.40
2:5:1115:G:H1'	2:5:1116:U:H5	1.86	0.40
2:5:1280:A:H61	2:5:1305:G:H1'	1.87	0.40
4:8:30:G:N3	4:8:31:A:C8	2.89	0.40
5:A:171:ARG:HG2	5:A:172:LEU:N	2.36	0.40
9:E:65:ASP:OD1	9:E:66:ASN:N	2.48	0.40
19:O:39:LEU:HD23	19:O:40:ASN:N	2.36	0.40
23:S:40:ASN:ND2	23:S:42:ASP:HB2	2.36	0.40
2:5:68:C:H2'	2:5:69:G:C8	2.57	0.40
2:5:248:U:O2	2:5:271:G:N2	2.55	0.40
2:5:352:A:H2'	2:5:353:G:O4'	2.20	0.40
2:5:858:A:H2'	2:5:859:A:C8	2.57	0.40
2:5:1006:A:N6	2:5:1016:A:N6	2.70	0.40
2:5:1125:C:H2'	2:5:1126:U:C6	2.57	0.40
2:5:1487:U:H2'	2:5:1488:A:C8	2.56	0.40
5:A:282:LEU:HA	5:A:282:LEU:HD23	1.86	0.40
6:B:44:PHE:HE2	6:B:92:ILE:HD11	1.87	0.40
6:B:71:ALA:C	6:B:109:ILE:HG22	2.42	0.40
9:E:7:LEU:HD12	9:E:85:GLU:HB3	2.04	0.40
10:F:76:VAL:HG13	10:F:83:ASN:HB3	2.02	0.40
19:O:64:LYS:HA	19:O:64:LYS:HD3	1.83	0.40
20:P:8:VAL:O	20:P:9:LEU:HD23	2.22	0.40
20:P:43:LYS:HG2	20:P:45:TYR:CE1	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	
5	A	262/294 (89%)	240 (92%)	22 (8%)	0	100	100
6	B	230/273 (84%)	215 (94%)	13 (6%)	2 (1%)	14	49
7	C	202/205 (98%)	171 (85%)	30 (15%)	1 (0%)	25	60
8	D	153/219 (70%)	148 (97%)	5 (3%)	0	100	100
9	E	182/215 (85%)	161 (88%)	20 (11%)	1 (0%)	25	60
10	F	153/155 (99%)	139 (91%)	13 (8%)	1 (1%)	19	54
11	G	139/142 (98%)	134 (96%)	5 (4%)	0	100	100
12	H	127/132 (96%)	114 (90%)	12 (9%)	1 (1%)	16	51
13	I	102/108 (94%)	90 (88%)	12 (12%)	0	100	100
14	J	112/121 (93%)	104 (93%)	8 (7%)	0	100	100
15	K	133/139 (96%)	122 (92%)	9 (7%)	2 (2%)	8	38
16	L	121/124 (98%)	112 (93%)	9 (7%)	0	100	100
17	M	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
18	N	83/86 (96%)	80 (96%)	3 (4%)	0	100	100
19	O	85/94 (90%)	82 (96%)	2 (2%)	1 (1%)	11	43
20	P	83/85 (98%)	73 (88%)	9 (11%)	1 (1%)	11	43
21	Q	69/104 (66%)	64 (93%)	5 (7%)	0	100	100
22	R	84/87 (97%)	80 (95%)	4 (5%)	0	100	100
23	S	77/87 (88%)	75 (97%)	2 (3%)	0	100	100
24	T	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
26	x	41/97 (42%)	30 (73%)	10 (24%)	1 (2%)	5	29
All	All	2553/2888 (88%)	2345 (92%)	197 (8%)	11 (0%)	32	64

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	230	PRO
20	P	54	LEU
15	K	56	LYS
7	C	81	GLN
6	B	231	ASN
10	F	12	LEU
9	E	169	VAL

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Mol	Chain	Res	Type
19	O	44	LYS
26	x	58	ARG
12	H	94	PRO
15	K	57	LYS

### 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	
5	A	238/262 (91%)	228 (96%)	10 (4%)	25	58
6	B	195/232 (84%)	195 (100%)	0	100	100
7	C	182/183 (100%)	174 (96%)	8 (4%)	24	57
8	D	125/178 (70%)	123 (98%)	2 (2%)	58	79
9	E	165/196 (84%)	160 (97%)	5 (3%)	36	66
10	F	132/132 (100%)	125 (95%)	7 (5%)	19	52
11	G	123/124 (99%)	122 (99%)	1 (1%)	79	90
12	H	112/115 (97%)	111 (99%)	1 (1%)	75	89
13	I	97/99 (98%)	95 (98%)	2 (2%)	48	74
14	J	91/97 (94%)	88 (97%)	3 (3%)	33	64
15	K	117/120 (98%)	111 (95%)	6 (5%)	20	53
16	L	104/105 (99%)	98 (94%)	6 (6%)	17	49
17	M	47/48 (98%)	46 (98%)	1 (2%)	48	74
18	N	77/78 (99%)	73 (95%)	4 (5%)	19	52
19	O	76/82 (93%)	73 (96%)	3 (4%)	27	60
20	P	75/75 (100%)	73 (97%)	2 (3%)	40	69
21	Q	62/94 (66%)	61 (98%)	1 (2%)	58	79
22	R	76/77 (99%)	74 (97%)	2 (3%)	41	70
23	S	71/77 (92%)	71 (100%)	0	100	100
24	T	55/56 (98%)	52 (94%)	3 (6%)	18	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	x	35/86 (41%)	34 (97%)	1 (3%)	37 67
All	All	2255/2516 (90%)	2187 (97%)	68 (3%)	37 66

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	16	GLU
5	A	26	MET
5	A	37	TRP
5	A	140	ASN
5	A	162	PHE
5	A	179	ASP
5	A	229	MET
5	A	242	MET
5	A	249	LYS
5	A	260	GLN
7	C	18	LEU
7	C	71	PHE
7	C	82	ARG
7	C	89	LEU
7	C	97	LEU
7	C	102	TYR
7	C	164	SER
7	C	172	LYS
8	D	103	TYR
8	D	113	ASN
9	E	33	GLU
9	E	134	SER
9	E	166	PHE
9	E	175	ARG
9	E	178	PHE
10	F	19	ASN
10	F	67	ASN
10	F	121	ASN
10	F	128	ASN
10	F	129	ASN
10	F	138	ASP
10	F	155	TRP
11	G	73	ASN
12	H	50	MET
13	I	18	SER
13	I	21	SER

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Mol	Chain	Res	Type
14	J	17	SER
14	J	19	SER
14	J	48	SER
15	K	14	LYS
15	K	18	LYS
15	K	47	CYS
15	K	53	MET
15	K	60	SER
15	K	94	LEU
16	L	21	TYR
16	L	28	SER
16	L	42	ASP
16	L	70	ARG
16	L	79	HIS
16	L	93	LYS
17	M	61	TRP
18	N	13	GLN
18	N	15	HIS
18	N	18	ASP
18	N	38	ASP
19	O	9	MET
19	O	48	CYS
19	O	51	ASP
20	P	49	ASN
20	P	56	LYS
21	Q	78	ASN
22	R	59	ASN
22	R	64	ASP
24	T	7	LYS
24	T	19	LYS
24	T	53	ARG
26	x	61	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	192	ASN
6	B	231	ASN
7	C	61	GLN
8	D	193	HIS
9	E	17	GLN
9	E	25	GLN

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Mol	Chain	Res	Type
13	I	86	ASN
16	L	100	GLN
26	x	98	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	23/2907 (0%)	1 (4%)	0
2	5	1503/1520 (98%)	234 (15%)	6 (0%)
25	Y	20/21 (95%)	11 (55%)	1 (5%)
3	7	28/75 (37%)	2 (7%)	1 (3%)
4	8	28/76 (36%)	4 (14%)	0
All	All	1602/4599 (34%)	252 (15%)	8 (0%)

All (252) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	1920	A
2	5	6	C
2	5	10	G
2	5	40	G
2	5	48	C
2	5	49	C
2	5	52	A
2	5	61	A
2	5	86	A
2	5	106	C
2	5	114	C
2	5	115	A
2	5	117	U
2	5	130	G
2	5	149	G
2	5	154	G
2	5	163	G
2	5	167	A
2	5	173	U
2	5	176	G
2	5	180	C
2	5	182	C
2	5	185	G
2	5	186	A

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Mol	Chain	Res	Type
2	5	189	C
2	5	190	A
2	5	197	A
2	5	198	A
2	5	199	A
2	5	220	U
2	5	222	U
2	5	223	G
2	5	239	A
2	5	241	C
2	5	243	G
2	5	247	G
2	5	262	G
2	5	263	C
2	5	269	A
2	5	275	A
2	5	276	U
2	5	285	G
2	5	301	G
2	5	302	A
2	5	324	C
2	5	325	A
2	5	326	C
2	5	328	G
2	5	341	C
2	5	342	G
2	5	344	G
2	5	347	G
2	5	348	C
2	5	350	G
2	5	363	U
2	5	368	C
2	5	369	A
2	5	370	A
2	5	374	G
2	5	380	G
2	5	394	U
2	5	408	U
2	5	416	U
2	5	418	U
2	5	419	A
2	5	422	A

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Mol	Chain	Res	Type
2	5	425	G
2	5	426	U
2	5	447	G
2	5	449	A
2	5	450	U
2	5	452	A
2	5	461	G
2	5	464	A
2	5	468	G
2	5	471	A
2	5	475	U
2	5	476	U
2	5	481	U
2	5	482	G
2	5	489	U
2	5	493	A
2	5	494	A
2	5	495	U
2	5	507	A
2	5	510	U
2	5	516	C
2	5	517	C
2	5	522	G
2	5	525	G7M
2	5	530	A
2	5	545	A
2	5	557	A
2	5	560	U
2	5	562	U
2	5	571	A
2	5	574	C
2	5	575	A
2	5	579	G
2	5	586	G
2	5	594	A
2	5	595	G
2	5	628	A
2	5	646	A
2	5	650	A
2	5	661	G
2	5	662	G
2	5	700	G

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Mol	Chain	Res	Type
2	5	715	A
2	5	719	G
2	5	720	U
2	5	721	G
2	5	728	G
2	5	745	U
2	5	752	G
2	5	768	G
2	5	790	U
2	5	791	A
2	5	807	C
2	5	811	A
2	5	812	A
2	5	814	C
2	5	818	A
2	5	825	A
2	5	829	G
2	5	836	C
2	5	867	A
2	5	883	A
2	5	908	A
2	5	910	C
2	5	911	G
2	5	921	G
2	5	922	G
2	5	929	C
2	5	930	A
2	5	955	U
2	5	964	A
2	5	970	A
2	5	971	A
2	5	972	A
2	5	987	U
2	5	988	G
2	5	994	C
2	5	995	U
2	5	996	U
2	5	997	G
2	5	998	G
2	5	999	C
2	5	1000	A
2	5	1002	A

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Mol	Chain	Res	Type
2	5	1007	U
2	5	1009	G
2	5	1015	U
2	5	1018	U
2	5	1020	G
2	5	1022	G
2	5	1023	G
2	5	1024	U
2	5	1025	U
2	5	1027	A
2	5	1029	C
2	5	1030	G
2	5	1032	G
2	5	1034	G
2	5	1036	C
2	5	1044	G
2	5	1056	U
2	5	1072	G
2	5	1078	G
2	5	1085	G
2	5	1086	U
2	5	1092	A
2	5	1118	A
2	5	1121	U
2	5	1122	U
2	5	1123	G
2	5	1124	U
2	5	1134	C
2	5	1135	U
2	5	1141	U
2	5	1142	G
2	5	1144	A
2	5	1146	A
2	5	1158	A
2	5	1159	A
2	5	1171	A
2	5	1172	A
2	5	1188	A
2	5	1189	U
2	5	1202	A
2	5	1203	A
2	5	1231	U

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Mol	Chain	Res	Type
2	5	1232	C
2	5	1233	G
2	5	1235	C
2	5	1255	A
2	5	1260	U
2	5	1271	U
2	5	1274	G
2	5	1276	U
2	5	1279	G
2	5	1291	C
2	5	1294	U
2	5	1296	C
2	5	1297	G
2	5	1306	A
2	5	1312	G
2	5	1320	A
2	5	1321	G
2	5	1337	U
2	5	1338	A
2	5	1345	G
2	5	1356	U
2	5	1372	C
2	5	1373	A
2	5	1397	G
2	5	1417	U
2	5	1426	U
2	5	1427	U
2	5	1428	A
2	5	1429	G
2	5	1466	U
2	5	1467	A
2	5	1469	G
2	5	1472	G
2	5	1478	A
2	5	1480	G
2	5	1481	U
2	5	1482	A
2	5	1492	G
2	5	1504	G
2	5	1505	G
2	5	1509	A
2	5	1510	C

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Mol	Chain	Res	Type
2	5	1511	C
3	7	11	U
3	7	46	U
4	8	10	G
4	8	30	G
4	8	41	A
4	8	46	G
25	Y	36	U
25	Y	37	G
25	Y	40	G
25	Y	47	U
25	Y	49	U
25	Y	50	U
25	Y	51	C
25	Y	52	A
25	Y	53	A
25	Y	54	A
25	Y	55	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	5	196	G
2	5	197	A
2	5	994	C
2	5	1024	U
2	5	1123	G
2	5	1158	A
3	7	10	G
25	Y	51	C

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

5 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
2	G7M	5	525	2	20,26,27	4.04	10 (50%)	17,39,42	1.02	1 (5%)
2	5MC	5	1375	2	18,22,23	4.02	7 (38%)	26,32,35	1.03	2 (7%)
2	B8T	5	1377	2	19,22,23	3.24	8 (42%)	26,31,34	0.84	1 (3%)
2	MA6	5	1494	2	18,26,27	1.08	2 (11%)	19,38,41	3.41	3 (15%)
2	MA6	5	1493	2	18,26,27	1.06	2 (11%)	19,38,41	3.40	3 (15%)

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
2	G7M	5	525	2	-	2/3/25/26	0/3/3/3
2	5MC	5	1375	2	-	2/7/25/26	0/2/2/2
2	B8T	5	1377	2	-	2/7/27/28	0/2/2/2
2	MA6	5	1494	2	-	2/7/29/30	0/3/3/3
2	MA6	5	1493	2	-	0/7/29/30	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	525	G7M	C8-N7	10.07	1.51	1.33
2	5	1375	5MC	C6-C5	9.87	1.50	1.34
2	5	525	G7M	C8-N9	9.85	1.51	1.33
2	5	1375	5MC	C4-N3	7.42	1.46	1.34
2	5	1377	B8T	C4-N3	7.11	1.45	1.32
2	5	1375	5MC	C2-N3	6.90	1.50	1.36
2	5	1377	B8T	C2-N3	6.39	1.49	1.36
2	5	1377	B8T	C6-C5	6.07	1.49	1.35
2	5	525	G7M	C2-N3	5.77	1.47	1.33
2	5	1375	5MC	C4-N4	5.70	1.48	1.34
2	5	1375	5MC	C6-N1	5.46	1.47	1.38
2	5	525	G7M	C6-N1	4.80	1.45	1.37
2	5	525	G7M	C2-N2	4.70	1.45	1.34
2	5	1377	B8T	C4-N4	4.67	1.45	1.35
2	5	1375	5MC	C2-N1	4.59	1.49	1.40
2	5	1377	B8T	C2-N1	4.11	1.48	1.40
2	5	525	G7M	C4-N3	4.10	1.47	1.37
2	5	1377	B8T	C5-C4	3.83	1.49	1.40
2	5	525	G7M	C2-N1	3.67	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1377	B8T	C6-N1	3.02	1.45	1.38
2	5	1377	B8T	O2-C2	-2.72	1.18	1.23
2	5	525	G7M	C5-C6	2.67	1.52	1.45
2	5	1494	MA6	C2-N3	2.53	1.36	1.32
2	5	1493	MA6	C2-N3	2.45	1.36	1.32
2	5	1493	MA6	C5-C4	-2.41	1.34	1.40
2	5	1494	MA6	C5-C4	-2.41	1.34	1.40
2	5	1375	5MC	O2-C2	-2.32	1.19	1.23
2	5	525	G7M	O6-C6	-2.27	1.18	1.23
2	5	525	G7M	C5-C4	2.22	1.43	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1493	MA6	N1-C6-N6	-12.42	103.98	117.06
2	5	1494	MA6	N1-C6-N6	-12.35	104.06	117.06
2	5	1494	MA6	N3-C2-N1	-5.58	119.96	128.68
2	5	1494	MA6	C1'-N9-C4	5.50	136.30	126.64
2	5	1493	MA6	C1'-N9-C4	5.44	136.19	126.64
2	5	1493	MA6	N3-C2-N1	-5.38	120.27	128.68
2	5	1375	5MC	C5-C6-N1	-3.22	120.02	123.34
2	5	525	G7M	C2-N1-C6	-2.84	119.86	125.10
2	5	1377	B8T	C6-C5-C4	2.40	119.90	116.96
2	5	1375	5MC	CM5-C5-C6	-2.07	120.08	122.85

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	5	525	G7M	O4'-C4'-C5'-O5'
2	5	525	G7M	C3'-C4'-C5'-O5'
2	5	1494	MA6	O4'-C4'-C5'-O5'
2	5	1377	B8T	O4'-C4'-C5'-O5'
2	5	1494	MA6	C3'-C4'-C5'-O5'
2	5	1377	B8T	C3'-C4'-C5'-O5'
2	5	1375	5MC	O4'-C4'-C5'-O5'
2	5	1375	5MC	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	5	525	G7M	1	0
2	5	1493	MA6	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 105 are monoatomic - leaving 5 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	$\# Z  > 2$
27	SPD	5	1604	-	9,9,9	0.32	0	8,8,8	0.88	0
28	PUT	5	1605	-	5,5,5	0.24	0	4,4,4	0.52	0
29	N2P	5	1603	-	6,6,6	0.24	0	5,5,5	0.64	0
27	SPD	5	1601	-	9,9,9	0.32	0	8,8,8	0.91	0
28	PUT	5	1602	-	5,5,5	0.24	0	4,4,4	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SPD	5	1604	-	-	0/7/7/7	-
28	PUT	5	1605	-	-	0/3/3/3	-
29	N2P	5	1603	-	-	0/4/4/4	-
27	SPD	5	1601	-	-	1/7/7/7	-
28	PUT	5	1602	-	-	0/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	5	1601	SPD	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	5	1604	SPD	1	0
27	5	1601	SPD	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.