



## wwPDB EM Map/Model Validation Report ⓘ

Sep 27, 2016 – 01:44 PM EDT

PDB ID : 5LMS  
EMDB ID: : EMD-4078  
Title : Structure of bacterial 30S-IF1-IF3-mRNA-tRNA translation pre-initiation complex(state-2C)  
Authors : Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.  
Deposited on : 2016-08-01  
Resolution : 5.10 Å(reported)

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

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

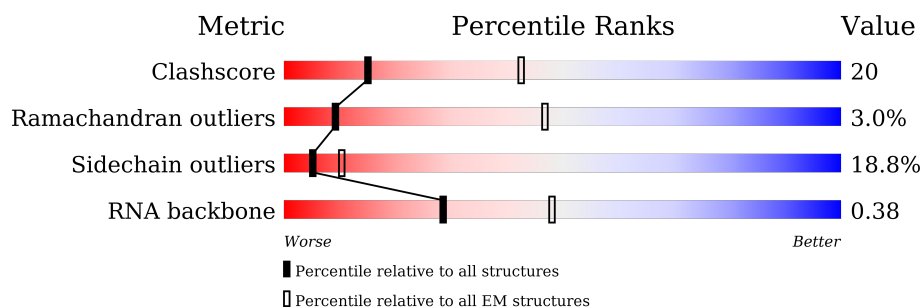
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.10 Å.

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




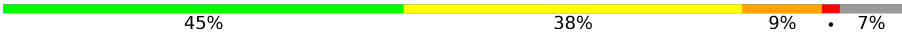






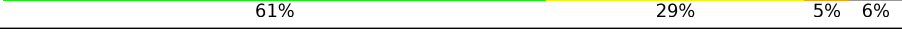

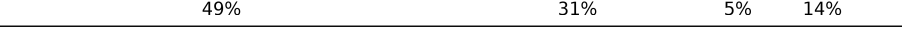
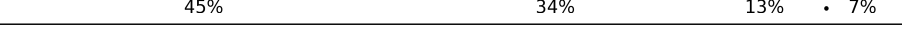

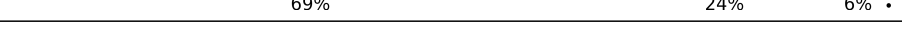



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	A	1522	<div> <div>23%</div> <div>57%</div> <div>18%</div> <div>..</div> </div>
2	B	256	<div> <div>49%</div> <div>35%</div> <div>7%</div> <div>9%</div> </div>
3	C	239	<div> <div>54%</div> <div>29%</div> <div>.</div> <div>14%</div> </div>
4	D	209	<div> <div>53%</div> <div>38%</div> <div>9%</div> </div>
5	E	162	<div> <div>54%</div> <div>32%</div> <div>6%</div> <div>7%</div> </div>
6	F	101	<div> <div>58%</div> <div>38%</div> <div>.</div> </div>
7	G	156	<div> <div>66%</div> <div>29%</div> <div>.</div> </div>
8	H	138	<div> <div>51%</div> <div>41%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	V	27	
22	W	72	
23	X	171	
24	Y	42	
25	Z	77	

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 55648 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1514	Total	C	N	O	P	0	0
			32522	14481	6019	10512	1510		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	234	Total	C	N	O	S	0	0
			1900	1213	341	341	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1612	1016	314	281	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	150	Total	C	N	O	S	0	0
			1146	724	217	201	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	127	Total	C	N	O	0	0
			1010	639	197	174		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			792	498	156	137	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	119	Total	C	N	O	S	0	0
			885	549	168	165	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	118	Total	C	N	O	S	0	0
			937	579	193	163	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0
			823	528	151	142	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	73	Total	C	N	O	0	0
			598	381	118	99		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	80	Total	C	N	O	S	0	0
			647	414	119	112	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 22 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	71	Total	C	N	O	S	0	0
			565	359	102	102	2		

- Molecule 23 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	164	Total	C	N	O	S	0	0
			1336	841	245	241	9		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	20	Total	C	N	O	P	0	0
			439	196	89	134	20		

- Molecule 25 is a RNA chain called tRNAi.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	77	Total	C	N	O	P	S	0	0
			1646	735	297	536	77	1		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

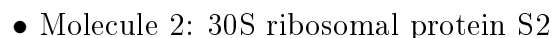
Mol	Chain	Residues	Atoms		AltConf
26	D	1	Total	Zn	0
			1	1	
26	N	1	Total	Zn	0
			1	1	

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
27	W	1	Total	Mg	0
			1	1	
27	Z	1	Total	Mg	0
			1	1	





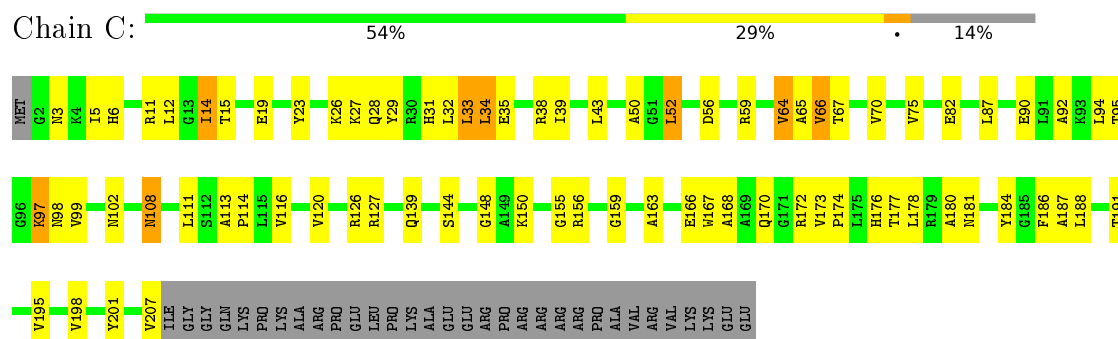


Chain B:  49% 35% 7% 9%

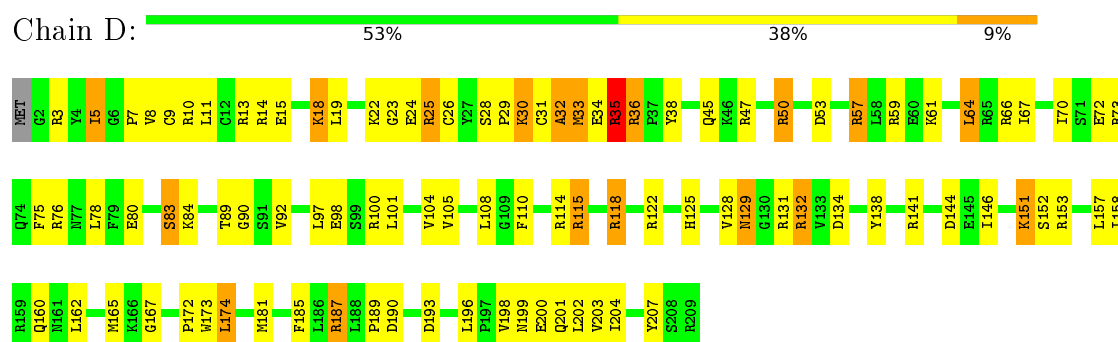


GLU  
VAL  
GLU  
ALA

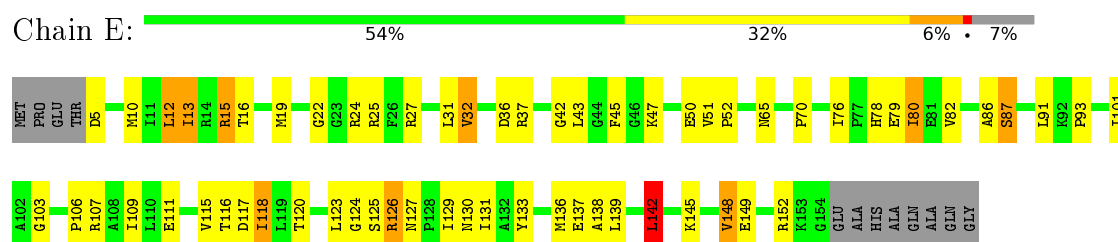
- Molecule 3: 30S ribosomal protein S3



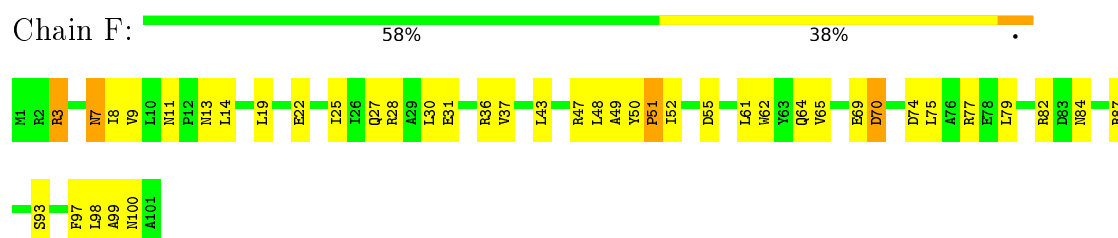
- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5

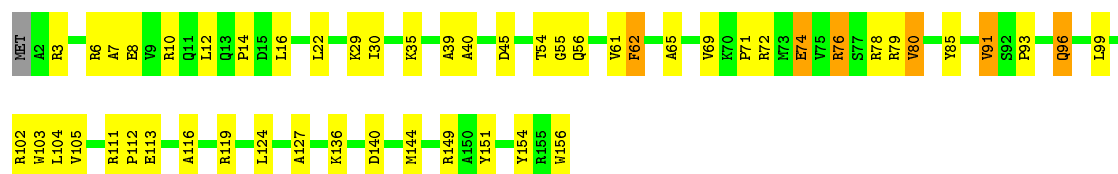


- Molecule 6: 30S ribosomal protein S6



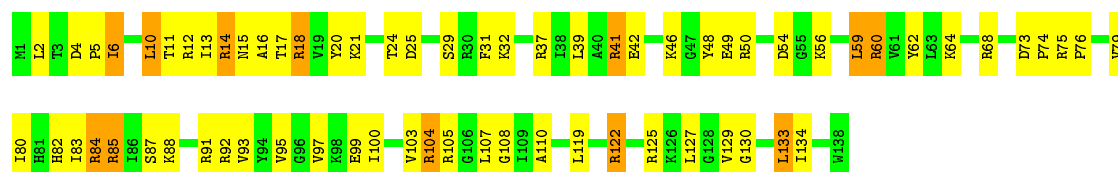
- Molecule 7: 30S ribosomal protein S7





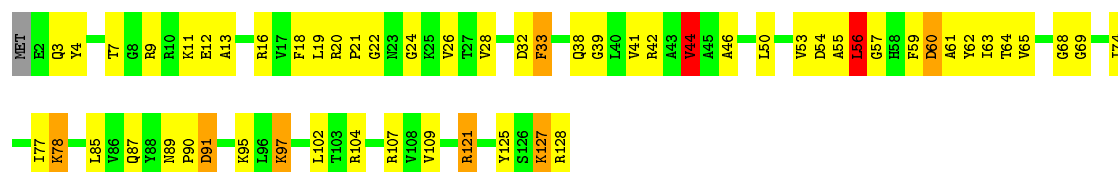
- Molecule 8: 30S ribosomal protein S8

Chain H: 51% 41% 9%



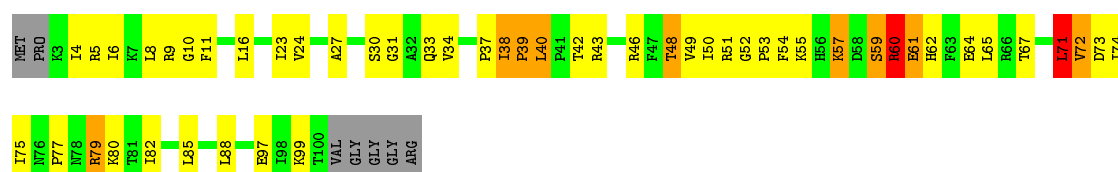
- Molecule 9: 30S ribosomal protein S9

Chain I: 55% 38% 5%



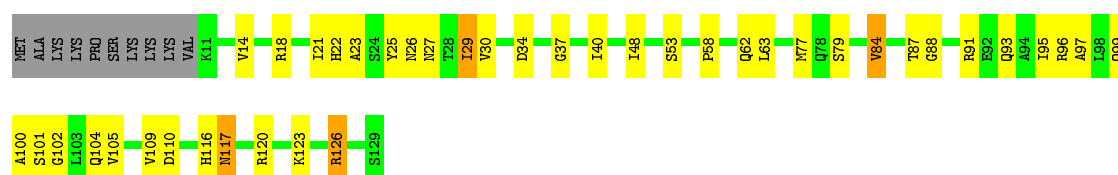
- Molecule 10: 30S ribosomal protein S10

Chain J: 45% 38% 9% 7%



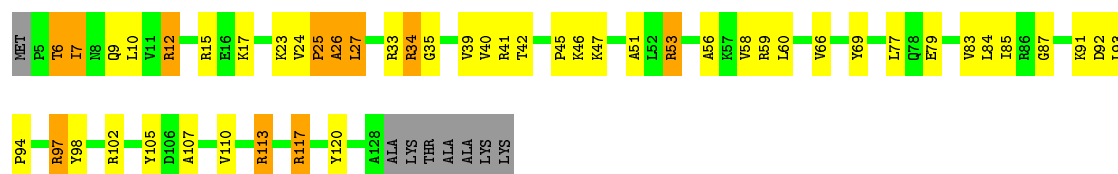
- Molecule 11: 30S ribosomal protein S11

Chain K: 60% 29% 8%



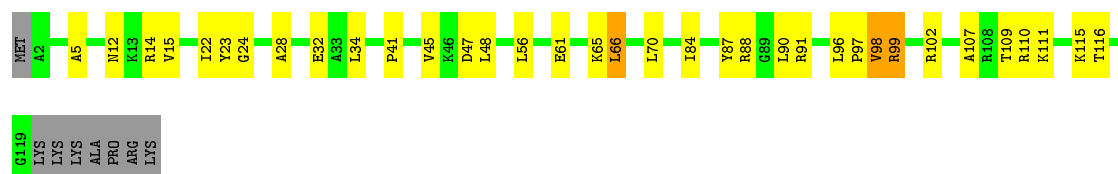
- Molecule 12: 30S ribosomal protein S12

Chain L: 57% 29% 8% 6%



- Molecule 13: 30S ribosomal protein S13

Chain M: 66% 25% 6%



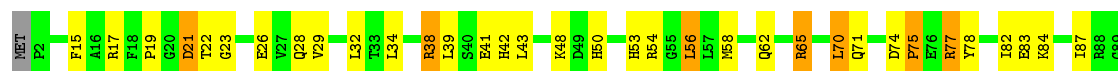
- Molecule 14: 30S ribosomal protein S14 type Z

Chain N: 51% 41% 5% ..



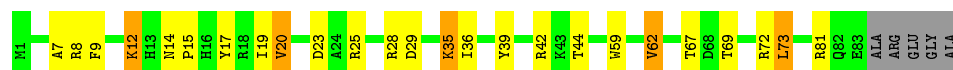
- Molecule 15: 30S ribosomal protein S15

Chain O: 61% 30% 8% .



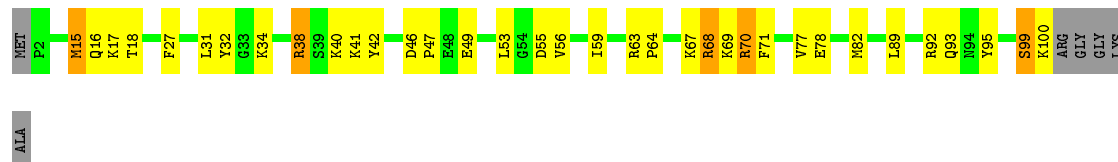
- Molecule 16: 30S ribosomal protein S16

Chain P: 66% 23% 6% 6%



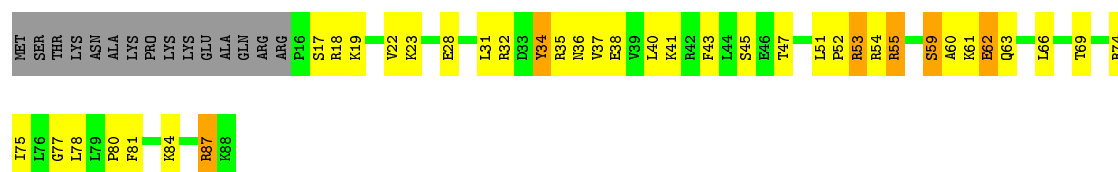
- Molecule 17: 30S ribosomal protein S17

Chain Q: 61% 29% 5% 6%



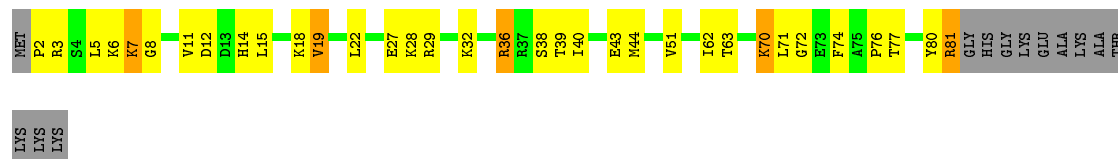
- Molecule 18: 30S ribosomal protein S18

Chain R: 40% 36% 7% 17%



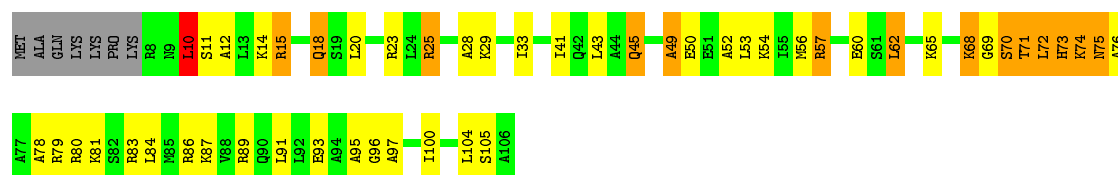
- Molecule 19: 30S ribosomal protein S19

Chain S:



- Molecule 20: 30S ribosomal protein S20

Chain T:



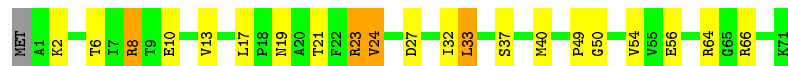
- Molecule 21: 30S ribosomal protein Thx

Chain V:



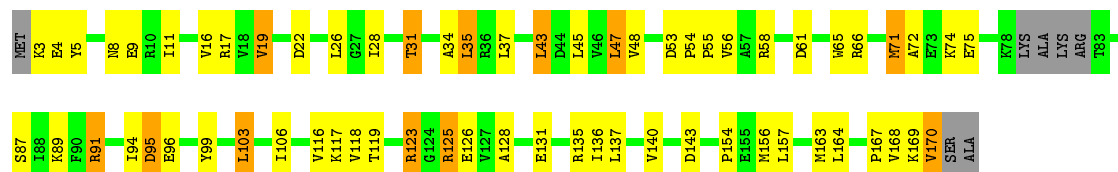
- Molecule 22: Translation initiation factor IF-1

Chain W:

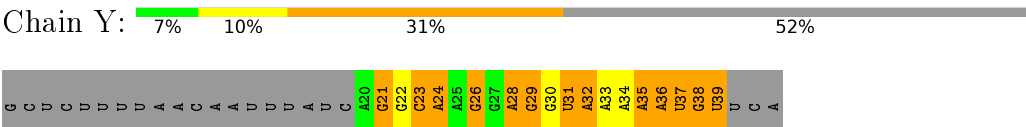


- Molecule 23: Translation initiation factor IF-3

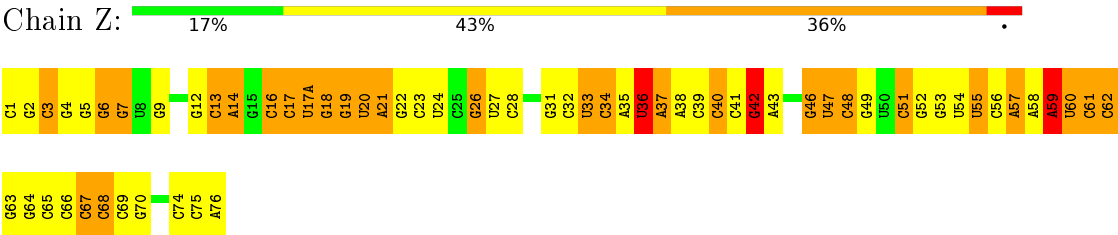
Chain X:



- Molecule 24: mRNA



● Molecule 25: tRNAi



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	7898	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	78000	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, G7M, MG, 4SU, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	A	0.34	1/36394 (0.0%)	0.77	25/56779 (0.0%)
10	J	0.55	0/805	1.35	14/1082 (1.3%)
11	K	0.54	0/900	0.82	0/1213
12	L	0.41	0/986	0.77	0/1320
13	M	0.52	0/947	0.78	0/1270
14	N	0.45	0/501	0.79	0/664
15	O	0.47	0/745	0.88	0/992
16	P	0.46	0/716	0.79	0/963
17	Q	0.41	0/836	0.78	0/1117
18	R	0.52	0/604	0.85	0/801
19	S	0.60	0/661	1.15	3/890 (0.3%)
2	B	0.57	0/1935	0.82	1/2609 (0.0%)
20	T	0.47	0/765	0.93	1/1007 (0.1%)
21	V	0.61	0/212	0.74	0/277
22	W	0.63	0/575	1.05	5/778 (0.6%)
23	X	0.68	0/1354	0.88	3/1813 (0.2%)
24	Y	0.55	0/493	0.82	0/766
25	Z	0.64	1/1719 (0.1%)	0.92	2/2674 (0.1%)
3	C	0.48	0/1636	0.88	5/2205 (0.2%)
4	D	0.49	0/1733	0.90	2/2318 (0.1%)
5	E	0.47	0/1162	0.96	2/1564 (0.1%)
6	F	0.48	0/856	0.82	0/1154
7	G	0.53	0/1276	0.83	0/1709
8	H	0.46	0/1136	0.83	1/1527 (0.1%)
9	I	0.50	0/1029	0.86	1/1379 (0.1%)
All	All	0.43	2/59976 (0.0%)	0.82	65/88871 (0.1%)

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
14	N	0	1
19	S	1	0
23	X	0	1
3	C	1	0
All	All	2	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	42	G	O3'-P	13.26	1.77	1.61
1	A	71	C	O3'-P	-5.43	1.54	1.61

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S	70	LYS	CB-CA-C	23.09	156.58	110.40
10	J	60	ARG	CB-CA-C	-17.82	74.76	110.40
5	E	15	ARG	N-CA-C	-14.56	71.68	111.00
9	I	7	THR	CB-CA-C	-13.77	74.42	111.60
5	E	16	THR	N-CA-CB	-12.45	86.64	110.30
10	J	72	VAL	CB-CA-C	-12.13	88.35	111.40
22	W	33	LEU	CB-CA-C	-11.72	87.94	110.20
10	J	72	VAL	N-CA-C	-11.62	79.64	111.00
10	J	59	SER	N-CA-C	-10.99	81.34	111.00
10	J	73	ASP	N-CA-CB	-10.76	91.23	110.60
22	W	23	ARG	N-CA-C	-10.41	82.89	111.00
10	J	71	LEU	N-CA-C	-10.36	83.03	111.00
3	C	65	ALA	N-CA-C	-10.30	83.19	111.00
3	C	14	ILE	N-CA-C	9.92	137.78	111.00
10	J	59	SER	CB-CA-C	-9.89	91.32	110.10
3	C	65	ALA	CB-CA-C	-9.67	95.60	110.10
4	D	35	ARG	N-CA-CB	-9.33	93.81	110.60
10	J	60	ARG	N-CA-CB	8.70	126.26	110.60
22	W	33	LEU	N-CA-C	-8.68	87.56	111.00
10	J	71	LEU	CB-CA-C	-8.58	93.89	110.20
4	D	34	GLU	N-CA-C	8.51	133.96	111.00
19	S	71	LEU	N-CA-CB	-7.93	94.54	110.40
19	S	70	LYS	N-CA-C	-7.87	89.77	111.00
1	A	1498	U	C2'-C3'-O3'	7.37	125.72	109.50
25	Z	36	U	C2'-C3'-O3'	7.24	125.44	109.50
1	A	1534	A	C2'-C3'-O3'	7.24	125.42	109.50
10	J	61	GLU	N-CA-CB	-6.86	98.26	110.60
1	A	266	G	C2'-C3'-O3'	6.84	124.64	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1301	U	C2'-C3'-O3'	6.83	124.64	113.70
1	A	701	C	C2'-C3'-O3'	6.74	124.48	113.70
1	A	1190	G	C2'-C3'-O3'	6.49	124.09	113.70
20	T	10	LEU	CA-CB-CG	6.47	130.19	115.30
1	A	748	C	C2'-C3'-O3'	6.47	124.05	113.70
1	A	1182	G	C2'-C3'-O3'	6.16	123.56	113.70
1	A	1145	C	C2'-C3'-O3'	6.14	123.52	113.70
1	A	965	A	C2'-C3'-O3'	5.86	123.08	113.70
1	A	1346	A	C2'-C3'-O3'	5.83	123.03	113.70
23	X	103	LEU	CA-CB-CG	5.81	128.65	115.30
1	A	1067	A	C2'-C3'-O3'	5.75	122.90	113.70
1	A	428	G	C2'-C3'-O3'	5.72	122.86	113.70
1	A	812	C	C2'-C3'-O3'	5.71	122.84	113.70
10	J	88	LEU	CA-CB-CG	5.67	128.33	115.30
1	A	509	A	C4'-C3'-O3'	5.58	124.17	113.00
3	C	15	THR	N-CA-CB	-5.58	99.69	110.30
1	A	792	A	C2'-C3'-O3'	5.54	122.56	113.70
1	A	328	C	C2'-C3'-O3'	5.54	122.56	113.70
1	A	281	G	C2'-C3'-O3'	5.49	122.49	113.70
1	A	1065	U	C2'-C3'-O3'	5.47	122.45	113.70
22	W	24	VAL	N-CA-CB	-5.46	99.48	111.50
22	W	23	ARG	CB-CA-C	-5.42	99.57	110.40
1	A	1049	U	C4'-C3'-O3'	5.41	123.82	113.00
25	Z	59	A	N9-C1'-C2'	5.40	121.02	114.00
1	A	960	U	C2'-C3'-O3'	5.39	122.33	113.70
1	A	1001	A	O4'-C4'-C3'	-5.39	98.61	104.00
1	A	559	A	C2'-C3'-O3'	5.37	122.30	113.70
10	J	61	GLU	N-CA-C	-5.34	96.57	111.00
2	B	51	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	1201	A	C2'-C3'-O3'	5.23	122.07	113.70
10	J	71	LEU	CA-CB-CG	5.18	127.22	115.30
8	H	10	LEU	CA-CB-CG	5.17	127.19	115.30
23	X	43	LEU	CA-CB-CG	5.08	126.99	115.30
10	J	60	ARG	N-CA-C	-5.07	97.30	111.00
3	C	66	VAL	N-CA-C	-5.07	97.31	111.00
1	A	575	G	C2'-C3'-O3'	5.05	121.78	113.70
23	X	47	LEU	CA-CB-CG	5.04	126.90	115.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	14	ILE	CA

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Mol	Chain	Res	Type	Atom
19	S	70	LYS	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	13	THR	Peptide
23	X	53	ASP	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	A	32522	0	16436	1209	0
2	B	1900	0	1951	44	0
3	C	1612	0	1677	68	0
4	D	1703	0	1766	59	0
5	E	1146	0	1207	36	0
6	F	843	0	857	25	0
7	G	1257	0	1296	28	0
8	H	1116	0	1177	44	0
9	I	1010	0	1037	34	0
10	J	792	0	835	34	0
11	K	885	0	904	17	0
12	L	970	0	1057	33	0
13	M	937	0	995	17	0
14	N	492	0	530	31	0
15	O	734	0	771	18	0
16	P	700	0	720	15	0
17	Q	823	0	891	20	0
18	R	598	0	670	28	0
19	S	647	0	673	28	0
20	T	763	0	861	31	0
21	V	208	0	221	1	0
22	W	565	0	588	9	0
23	X	1336	0	1389	51	0
24	Y	439	0	219	38	0
25	Z	1646	0	845	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	D	1	0	0	1	0
26	N	1	0	0	0	0
27	W	1	0	0	0	0
27	Z	1	0	0	0	0
All	All	55648	0	39573	1840	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 20.

All (1840) 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)
4:D:199:ASN:ND2	4:D:202:LEU:HG	1.25	1.43
3:C:29:TYR:CE1	3:C:33:LEU:HD12	1.67	1.30
1:A:1345:U:N3	1:A:1375:A:N6	1.80	1.28
1:A:72:C:C2'	1:A:73:G:H5'	1.65	1.23
23:X:5:TYR:OH	25:Z:20:U:C6	1.92	1.21
4:D:199:ASN:HD22	4:D:202:LEU:CG	1.54	1.19
3:C:28:GLN:HG2	3:C:31:HIS:CD2	1.77	1.18
1:A:72:C:H2'	1:A:73:G:C5'	1.75	1.17
4:D:199:ASN:ND2	4:D:202:LEU:CG	2.09	1.14
1:A:1022:G:H2'	1:A:1023:G:C8	1.84	1.11
19:S:40:ILE:CD1	19:S:70:LYS:O	1.97	1.11
3:C:29:TYR:HE1	3:C:33:LEU:HD12	0.93	1.09
3:C:29:TYR:HE1	3:C:33:LEU:CD1	1.66	1.08
1:A:1022:G:H2'	1:A:1023:G:H8	0.98	1.08
1:A:1219:U:H2'	1:A:1220:G:C8	1.89	1.06
1:A:1014:A:H5''	19:S:14:HIS:HB3	1.17	1.06
1:A:92:C:H2'	1:A:93:G:H8	1.21	1.04
1:A:1459:C:OP1	20:T:28:ALA:HA	1.57	1.03
20:T:41:ILE:HD13	20:T:87:LYS:HZ3	1.22	1.03
1:A:664:G:N2	1:A:741:G:H1	1.57	1.03
20:T:41:ILE:HD13	20:T:87:LYS:NZ	1.74	1.02
1:A:1219:U:H2'	1:A:1220:G:H8	1.18	1.01
1:A:1256:A:H62	1:A:1278:U:H1'	1.26	1.00
1:A:974:A:H8	1:A:974:A:OP1	1.44	1.00
3:C:28:GLN:OE1	3:C:32:LEU:HD11	1.60	1.00
1:A:600:C:H2'	1:A:601:C:H6	1.27	0.99
1:A:1345:U:H3	1:A:1375:A:N6	1.49	0.99
19:S:40:ILE:HD11	19:S:70:LYS:O	1.57	0.98
1:A:917:G:H2'	1:A:918:A:C8	1.97	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:G:H2'	1:A:712:A:H8	1.30	0.96
1:A:225:C:H2'	1:A:226:G:H8	1.27	0.95
1:A:92:C:H2'	1:A:93:G:C8	2.01	0.94
4:D:199:ASN:HD22	4:D:202:LEU:CD1	1.80	0.94
25:Z:21:A:N7	25:Z:48:C:C4	2.36	0.94
1:A:1539:C:H42	24:Y:26:G:H1	1.14	0.93
1:A:674:G:H2'	1:A:675:A:H8	1.32	0.93
1:A:21:G:H2'	1:A:22:G:C8	2.04	0.93
1:A:80:G:H3'	1:A:81:U:H5''	1.51	0.93
4:D:201:GLN:HE22	5:E:116:THR:HG23	1.34	0.92
19:S:40:ILE:CG1	19:S:70:LYS:O	2.17	0.92
25:Z:51:C:H42	25:Z:63:G:H1	1.17	0.92
1:A:1030:C:H42	1:A:1031:G:H1	1.15	0.91
23:X:17:ARG:CZ	25:Z:56:C:N4	2.34	0.91
1:A:1014:A:C5'	19:S:14:HIS:HB3	2.01	0.91
1:A:79:G:H2'	1:A:80:G:H8	1.34	0.90
3:C:28:GLN:HG2	3:C:31:HIS:HD2	1.35	0.90
19:S:40:ILE:HG13	19:S:70:LYS:O	1.72	0.90
1:A:34:C:H2'	1:A:35:G:C8	2.06	0.90
1:A:745:C:H2'	1:A:746:A:C8	2.06	0.89
1:A:170:U:H2'	1:A:171:A:H8	1.36	0.89
1:A:920:U:H2'	1:A:921:U:C6	2.07	0.89
1:A:125:U:H2'	1:A:126:G:C8	2.08	0.89
1:A:1500:A:OP1	1:A:1508:G:OP1	1.90	0.89
1:A:72:C:H2'	1:A:73:G:H5'	0.90	0.89
8:H:29:SER:HB3	8:H:32:LYS:HG3	1.56	0.88
23:X:72:ALA:HB1	25:Z:14:A:O3'	1.73	0.88
12:L:25:PRO:C	12:L:27:LEU:H	1.75	0.87
23:X:56:VAL:HG21	25:Z:19:G:C5	2.09	0.87
1:A:600:C:H2'	1:A:601:C:C6	2.10	0.87
1:A:999:C:O2	1:A:1043:C:O2	1.91	0.87
23:X:5:TYR:OH	25:Z:20:U:H6	1.41	0.87
1:A:72:C:C2'	1:A:73:G:C5'	2.43	0.87
1:A:1345:U:C2	1:A:1375:A:N6	2.42	0.86
1:A:1264:C:H2'	1:A:1265:G:H8	1.38	0.86
5:E:106:PRO:HA	5:E:109:ILE:HD12	1.55	0.86
1:A:173:U:OP1	1:A:198:G:H4'	1.74	0.86
1:A:736:C:H2'	1:A:737:A:H8	1.40	0.86
12:L:9:GLN:HA	12:L:12:ARG:HE	1.40	0.85
1:A:34:C:H2'	1:A:35:G:H8	1.37	0.85
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:23:C:H2'	25:Z:24:U:C6	2.12	0.84
1:A:1007:C:H42	1:A:1022:G:H1	1.23	0.84
23:X:56:VAL:CG2	25:Z:19:G:C6	2.61	0.84
3:C:92:ALA:O	3:C:95:THR:O	1.94	0.84
1:A:243:A:H4'	1:A:244:U:O5'	1.75	0.84
1:A:743:U:H2'	1:A:744:C:C6	2.11	0.84
1:A:559:A:H4'	1:A:560:U:H5''	1.57	0.84
1:A:1128:C:H4'	9:I:16:ARG:HH22	1.39	0.84
1:A:1040:U:H2'	1:A:1041:A:C8	2.13	0.83
1:A:711:G:H2'	1:A:712:A:C8	2.13	0.83
1:A:1386:G:H2'	1:A:1387:G:H8	1.42	0.83
25:Z:21:A:C8	25:Z:48:C:N4	2.47	0.83
4:D:97:LEU:O	4:D:100:ARG:HB2	1.79	0.83
25:Z:27:U:C2'	25:Z:28:C:H5'	2.08	0.83
1:A:864:A:H2'	1:A:865:A:C8	2.14	0.83
2:B:178:ARG:HE	8:H:74:PRO:HB3	1.44	0.82
3:C:28:GLN:OE1	3:C:32:LEU:CD1	2.26	0.82
6:F:99:ALA:HB2	18:R:31:LEU:HG	1.61	0.82
4:D:199:ASN:HD22	4:D:202:LEU:HG	0.99	0.82
3:C:29:TYR:OH	14:N:54:PRO:HG2	1.79	0.82
23:X:56:VAL:HG21	25:Z:19:G:C6	2.13	0.82
1:A:1151:A:HO2'	1:A:1152:A:H8	1.25	0.81
1:A:256:U:H2'	1:A:257:G:C8	2.15	0.81
1:A:736:C:H2'	1:A:737:A:C8	2.15	0.81
1:A:773:G:H1	1:A:806:C:H42	1.24	0.81
1:A:539:A:H2'	1:A:540:G:H8	1.43	0.81
25:Z:51:C:H2'	25:Z:52:G:O4'	1.81	0.81
1:A:1264:C:H2'	1:A:1265:G:C8	2.15	0.81
1:A:1539:C:N4	24:Y:26:G:H1	1.79	0.80
2:B:61:LEU:HD11	2:B:160:ASP:HB3	1.63	0.80
1:A:1356:G:H2'	1:A:1357:A:C8	2.17	0.80
1:A:155:C:H2'	1:A:156:G:C8	2.17	0.80
10:J:51:ARG:HB2	10:J:59:SER:HB3	1.61	0.80
25:Z:21:A:N7	25:Z:48:C:N4	2.30	0.80
22:W:50:GLY:HA3	23:X:128:ALA:HB3	1.64	0.80
25:Z:68:C:H2'	25:Z:69:C:C6	2.17	0.80
1:A:1457:G:N2	1:A:1458:G:H1'	1.96	0.79
25:Z:22:G:OP2	25:Z:46:G7M:N1	2.15	0.79
1:A:269:C:H2'	1:A:270:A:C8	2.17	0.78
1:A:979:C:H2'	1:A:980:C:O4'	1.81	0.78
1:A:1488:G:H2'	1:A:1489:G:H8	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:TYR:OH	14:N:54:PRO:CG	2.31	0.78
1:A:524:G:C6	1:A:525:C:N4	2.51	0.78
1:A:1020:U:H2'	1:A:1021:G:H8	1.47	0.78
18:R:53:ARG:HH21	18:R:60:ALA:HB2	1.48	0.78
1:A:1407:C:H2'	1:A:1408:A:H8	1.49	0.78
1:A:155:C:H2'	1:A:156:G:H8	1.49	0.78
1:A:170:U:H2'	1:A:171:A:C8	2.19	0.77
13:M:61:GLU:HA	13:M:66:LEU:HD11	1.66	0.77
1:A:1059:C:H2'	1:A:1060:C:C6	2.20	0.77
1:A:1488:G:H2'	1:A:1489:G:C8	2.20	0.77
17:Q:27:PHE:HE1	17:Q:38:ARG:HB2	1.50	0.77
1:A:834:C:H5''	18:R:60:ALA:CB	2.14	0.77
24:Y:36:A:N6	25:Z:37:A:C6	2.51	0.77
1:A:865:A:H2'	1:A:866:C:C6	2.20	0.77
1:A:1311:G:N7	19:S:2:PRO:HA	1.99	0.77
8:H:12:ARG:HA	8:H:15:ASN:HD22	1.50	0.77
1:A:501:C:H2'	1:A:502:G:H8	1.47	0.76
1:A:1127:G:N2	1:A:1144:G:N2	2.33	0.76
16:P:59:TRP:O	16:P:62:VAL:HG23	1.84	0.76
23:X:157:LEU:HB2	25:Z:27:U:OP1	1.86	0.76
1:A:1099:G:C6	1:A:1100:C:N3	2.53	0.76
1:A:967:C:H2'	1:A:968:A:C8	2.20	0.76
4:D:26:CYS:SG	26:D:300:ZN:ZN	1.73	0.76
25:Z:26:G:C5	25:Z:27:U:C5	2.74	0.76
1:A:1039:C:H2'	1:A:1040:U:C6	2.21	0.76
1:A:1097:C:H2'	1:A:1098:C:C6	2.21	0.75
19:S:22:LEU:HD13	19:S:28:LYS:HB3	1.69	0.75
1:A:313:A:H2'	1:A:314:C:C6	2.22	0.75
1:A:544:G:H2'	1:A:545:C:O4'	1.86	0.75
25:Z:54:5MU:H73	25:Z:55:PSU:C2	2.20	0.75
1:A:944:G:O6	1:A:1337:G:H8	1.69	0.75
1:A:539:A:H2'	1:A:540:G:C8	2.21	0.75
1:A:90:U:H2'	1:A:91:C:C6	2.21	0.75
1:A:524:G:C2	1:A:525:C:N3	2.55	0.75
3:C:97:LYS:HB3	3:C:97:LYS:NZ	2.01	0.75
1:A:1396:A:O3'	1:A:1397:C:H5''	1.87	0.74
23:X:65:TRP:CD1	25:Z:17(A):U:N3	2.54	0.74
25:Z:20:U:H5''	25:Z:21:A:OP2	1.88	0.74
25:Z:27:U:H2'	25:Z:28:C:H5'	1.69	0.74
25:Z:27:U:O2'	25:Z:28:C:H5'	1.87	0.74
1:A:1102:A:H2'	1:A:1103:C:C6	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:G:H2'	1:A:675:A:C8	2.21	0.74
4:D:115:ARG:O	4:D:118:ARG:HG2	1.87	0.74
1:A:125:U:H2'	1:A:126:G:H8	1.52	0.74
20:T:70:SER:HA	20:T:73:HIS:CD2	2.23	0.73
1:A:974:A:C8	1:A:974:A:OP1	2.36	0.73
25:Z:21:A:C5	25:Z:48:C:N3	2.56	0.73
2:B:80:ILE:HG21	2:B:212:GLN:HA	1.70	0.73
23:X:17:ARG:CZ	25:Z:56:C:H41	2.02	0.73
1:A:1262:C:H42	1:A:1273:G:H1	1.36	0.73
1:A:1128:C:H4'	9:I:16:ARG:NH2	2.02	0.73
13:M:61:GLU:HA	13:M:66:LEU:CD1	2.17	0.73
1:A:40:C:H2'	1:A:41:G:H8	1.52	0.73
1:A:571:U:H3'	1:A:572:A:H5''	1.68	0.73
23:X:48:VAL:HG21	23:X:58:ARG:HE	1.52	0.73
23:X:17:ARG:NE	25:Z:56:C:N4	2.36	0.73
1:A:1445:C:C2	1:A:1458:G:C2	2.77	0.72
1:A:269:C:H2'	1:A:270:A:H8	1.53	0.72
1:A:1496:C:OP1	23:X:91:ARG:HB2	1.89	0.72
23:X:157:LEU:HD13	25:Z:27:U:C5'	2.20	0.72
1:A:80:G:H3'	1:A:81:U:C5'	2.19	0.72
25:Z:51:C:N4	25:Z:63:G:H1	1.87	0.72
3:C:59:ARG:HH12	3:C:97:LYS:HD3	1.54	0.72
12:L:45:PRO:HG2	12:L:51:ALA:H	1.55	0.72
20:T:83:ARG:HA	20:T:86:ARG:HH11	1.55	0.72
1:A:1314:C:H2'	1:A:1315:U:C6	2.25	0.72
1:A:826:C:O2'	8:H:15:ASN:ND2	2.23	0.72
1:A:1030:C:N4	1:A:1031:G:H1	1.88	0.71
1:A:438:G:N1	1:A:495:A:OP2	2.21	0.71
4:D:199:ASN:HD21	4:D:202:LEU:HG	1.52	0.71
1:A:1338:G:N2	25:Z:42:G:H1'	2.05	0.71
6:F:50:TYR:HB2	6:F:51:PRO:HD2	1.73	0.71
1:A:131:C:H2'	1:A:132:C:C6	2.25	0.71
15:O:15:PHE:CZ	15:O:84:LYS:HB3	2.26	0.71
24:Y:39:U:O4	25:Z:35:A:H1'	1.91	0.71
1:A:1513:A:H2'	1:A:1514:C:C6	2.25	0.71
1:A:312:C:H2'	1:A:313:A:C8	2.26	0.71
10:J:79:ARG:HH11	10:J:79:ARG:HA	1.56	0.71
1:A:72:C:C3'	1:A:73:G:H5'	2.20	0.71
23:X:17:ARG:NH2	23:X:19:VAL:HG22	2.05	0.70
1:A:1389:C:H2'	1:A:1390:U:O4'	1.90	0.70
1:A:1457:G:C4	1:A:1458:G:C8	2.79	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:53:G:H1	25:Z:61:C:H42	1.36	0.70
1:A:1475:G:H2'	1:A:1476:G:H8	1.55	0.70
4:D:201:GLN:NE2	5:E:116:THR:HG23	2.05	0.70
1:A:533:A:O2'	1:A:535:A:OP2	2.10	0.70
25:Z:5:G:H1	25:Z:68:C:H42	1.37	0.70
4:D:201:GLN:HE22	5:E:116:THR:CG2	2.04	0.70
1:A:105:G:H2'	1:A:106:C:C6	2.26	0.70
1:A:868:C:H2'	1:A:869:G:O4'	1.91	0.70
2:B:72:GLY:HA3	2:B:81:VAL:HG21	1.74	0.70
8:H:6:ILE:HB	8:H:85:ARG:HH12	1.57	0.69
10:J:27:ALA:HB2	10:J:85:LEU:HD21	1.74	0.69
11:K:23:ALA:HB1	11:K:88:GLY:H	1.55	0.69
16:P:59:TRP:O	16:P:62:VAL:CG2	2.40	0.69
1:A:255:G:H2'	1:A:256:U:C6	2.27	0.69
1:A:917:G:H2'	1:A:918:A:H8	1.58	0.69
8:H:48:TYR:HD2	8:H:59:LEU:HD21	1.57	0.69
15:O:38:ARG:HB3	15:O:38:ARG:HH11	1.57	0.69
23:X:5:TYR:OH	25:Z:20:U:C5	2.45	0.69
25:Z:21:A:C6	25:Z:48:C:C2	2.80	0.69
1:A:977:A:H1'	1:A:982:U:O4	1.93	0.69
1:A:70:G:C2	1:A:100:C:O2	2.46	0.69
1:A:1124:G:O2'	1:A:1126:U:O4	2.11	0.69
1:A:1463:C:H2'	1:A:1464:G:H8	1.57	0.69
1:A:728:A:H2'	1:A:729:A:C8	2.28	0.69
20:T:50:GLU:HG3	20:T:100:ILE:HB	1.75	0.69
1:A:1457:G:C2	1:A:1458:G:N9	2.60	0.69
1:A:373:A:H2'	1:A:374:A:H8	1.56	0.69
1:A:407:G:H2'	1:A:408:A:H8	1.57	0.69
1:A:442:C:H2'	1:A:443:C:C6	2.28	0.69
1:A:521:G:N2	1:A:522:C:C2	2.60	0.69
1:A:189(A):C:H2'	1:A:189(B):C:C6	2.28	0.68
1:A:614:A:H2'	1:A:615:C:C6	2.27	0.68
1:A:79:G:H2'	1:A:80:G:C8	2.25	0.68
13:M:22:ILE:HG22	13:M:24:GLY:H	1.57	0.68
1:A:1162:C:C2	1:A:1175:G:N2	2.61	0.68
1:A:500:G:H2'	1:A:501:C:C6	2.28	0.68
1:A:1345:U:O4	1:A:1375:A:N1	2.26	0.68
2:B:112:VAL:HG13	2:B:153:ARG:HB3	1.74	0.68
20:T:10:LEU:HD12	20:T:11:SER:H	1.58	0.68
1:A:525:C:H2'	1:A:526:C:C6	2.28	0.68
1:A:745:C:H2'	1:A:746:A:H8	1.54	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:G:H2'	1:A:923:A:C8	2.29	0.68
3:C:29:TYR:CZ	3:C:33:LEU:HD12	2.25	0.68
2:B:68:ILE:HG12	2:B:161:ALA:HB3	1.75	0.68
1:A:70:G:C6	1:A:100:C:N3	2.62	0.68
1:A:778:G:H2'	1:A:779:C:O4'	1.93	0.68
25:Z:67:C:H2'	25:Z:68:C:C6	2.29	0.68
1:A:1124:G:H2'	1:A:1145:C:H5	1.56	0.68
1:A:501:C:H2'	1:A:502:G:C8	2.28	0.68
1:A:571:U:C3'	1:A:572:A:H5''	2.24	0.68
1:A:834:C:H2'	1:A:835:U:C6	2.29	0.68
25:Z:69:C:H2'	25:Z:70:G:C8	2.28	0.68
1:A:1407:C:H2'	1:A:1408:A:C8	2.29	0.67
1:A:287:U:H2'	1:A:288:A:H8	1.59	0.67
1:A:424:G:H2'	1:A:425:G:H8	1.58	0.67
24:Y:32:A:H3'	24:Y:33:A:H5''	1.76	0.67
1:A:240:C:H2'	1:A:241:C:H6	1.59	0.67
25:Z:1:C:H2'	25:Z:2:G:H8	1.59	0.67
1:A:1256:A:H62	1:A:1278:U:C1'	2.04	0.67
1:A:183:G:H2'	1:A:184:G:O4'	1.94	0.67
1:A:613:C:H42	1:A:627:G:H1	1.43	0.67
3:C:26:LYS:HD3	14:N:36:PHE:HE1	1.58	0.67
25:Z:21:A:C5	25:Z:48:C:C4	2.81	0.67
10:J:49:VAL:HB	14:N:41:ARG:HB2	1.77	0.67
1:A:999:C:O2'	1:A:1000:U:H5'	1.94	0.67
1:A:1392:G:N2	1:A:1502:A:H8	1.92	0.67
1:A:1534:A:H2'	1:A:1535:C:C6	2.30	0.67
1:A:948:C:H2'	1:A:949:A:H8	1.60	0.67
10:J:38:ILE:HG23	10:J:71:LEU:HB3	1.77	0.67
1:A:1410:G:H2'	1:A:1411:C:C6	2.30	0.67
1:A:1464:G:N2	1:A:1465:C:C2	2.63	0.67
1:A:784:C:C2	1:A:799:G:N2	2.63	0.67
19:S:40:ILE:HD13	19:S:62:ILE:HD11	1.76	0.67
25:Z:6:G:H2'	25:Z:7:G:C8	2.29	0.67
1:A:1059:C:H2'	1:A:1060:C:H6	1.60	0.66
19:S:11:VAL:HA	19:S:38:SER:HB2	1.77	0.66
1:A:1475:G:H2'	1:A:1476:G:C8	2.30	0.66
1:A:683:G:N2	1:A:708:C:C2	2.63	0.66
1:A:671:G:N2	1:A:736:C:C2	2.63	0.66
8:H:12:ARG:HB3	8:H:24:THR:HG21	1.75	0.66
10:J:62:HIS:HB2	14:N:59:ALA:HB3	1.76	0.66
25:Z:26:G:C6	25:Z:27:U:C5	2.83	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:C:C2	1:A:1174:G:N2	2.64	0.66
1:A:728:A:H2'	1:A:729:A:H8	1.60	0.66
1:A:860:A:H3'	1:A:861:G:H8	1.61	0.66
12:L:25:PRO:C	12:L:27:LEU:N	2.48	0.66
23:X:5:TYR:CZ	25:Z:20:U:H6	2.13	0.66
1:A:313:A:H2'	1:A:314:C:H6	1.60	0.66
1:A:546:G:OP2	4:D:72:GLU:HB3	1.95	0.66
15:O:26:GLU:O	15:O:29:VAL:HG12	1.95	0.66
20:T:25:ARG:O	20:T:29:LYS:HG2	1.96	0.66
23:X:106:ILE:HG23	23:X:116:VAL:HG11	1.77	0.66
1:A:1063:C:H2'	1:A:1064:G:C8	2.31	0.66
1:A:1007:C:N3	1:A:1022:G:N2	2.44	0.66
1:A:1046:A:H3'	1:A:1047:G:H8	1.61	0.66
1:A:1525:G:H2'	1:A:1526:G:H8	1.61	0.66
20:T:41:ILE:CD1	20:T:87:LYS:NZ	2.56	0.66
1:A:773:G:H1	1:A:806:C:N4	1.92	0.65
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.61	0.65
1:A:955:U:H2'	1:A:956:U:O4'	1.96	0.65
2:B:223:ILE:HG21	2:B:230:VAL:HB	1.78	0.65
23:X:56:VAL:HG22	25:Z:19:G:C6	2.31	0.65
1:A:1030:C:C2	1:A:1032:G:N2	2.64	0.65
1:A:1395:C:H2'	1:A:1396:A:C8	2.32	0.65
1:A:1511:G:H2'	1:A:1512:U:C6	2.31	0.65
1:A:737:A:H2'	1:A:738:C:C6	2.31	0.65
1:A:234:C:H2'	1:A:235:C:C6	2.31	0.65
1:A:834:C:H2'	1:A:835:U:H6	1.61	0.65
1:A:834:C:H5''	18:R:60:ALA:HB2	1.77	0.65
1:A:670:G:H1	1:A:736:C:H42	1.43	0.65
1:A:225:C:H2'	1:A:226:G:C8	2.20	0.65
25:Z:59:A:H2'	25:Z:60:U:O4'	1.95	0.65
1:A:849:C:H2'	1:A:850:U:O4'	1.95	0.65
8:H:64:LYS:HB3	8:H:79:VAL:HG11	1.79	0.65
16:P:81:ARG:HH11	16:P:81:ARG:HB2	1.62	0.65
1:A:1198:G:H2'	1:A:1199:U:O4'	1.96	0.65
1:A:256:U:H2'	1:A:257:G:H8	1.61	0.65
1:A:880:C:H2'	1:A:881:G:H8	1.61	0.65
12:L:24:VAL:HG12	12:L:26:ALA:H	1.63	0.65
1:A:1221:G:H5''	1:A:1321:C:O2	1.98	0.64
3:C:28:GLN:O	3:C:31:HIS:HD2	1.80	0.64
1:A:1137:C:H4'	1:A:1138:G:C2	2.32	0.64
6:F:27:GLN:HA	6:F:30:LEU:HD12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:30:G:H2'	24:Y:31:U:H5''	1.79	0.64
25:Z:23:C:H2'	25:Z:24:U:H6	1.60	0.64
1:A:1143:G:H2'	1:A:1144:G:C8	2.32	0.64
2:B:59:GLU:HG3	2:B:225:ALA:HB2	1.79	0.64
1:A:1071:C:H2'	1:A:1072:G:H8	1.62	0.64
1:A:1305:G:HO2'	1:A:1306:A:H8	1.44	0.64
1:A:1415:G:N2	1:A:1486:G:H1'	2.12	0.64
1:A:911:U:H2'	1:A:912:C:C6	2.33	0.64
3:C:64:VAL:HB	3:C:99:VAL:HG23	1.79	0.64
1:A:132:C:C2	1:A:231:G:N2	2.66	0.64
1:A:677:U:H3	1:A:713:G:H22	1.44	0.64
5:E:145:LYS:HA	8:H:107:LEU:HD21	1.80	0.64
1:A:1157:A:H4'	1:A:1158:C:O5'	1.96	0.64
1:A:324:G:N2	1:A:326:G:H3'	2.12	0.64
1:A:329:A:H4'	1:A:330:C:OP1	1.96	0.64
9:I:53:VAL:HG12	9:I:95:LYS:HB3	1.79	0.64
1:A:1166:G:N2	1:A:1170:A:OP2	2.31	0.64
1:A:1283:G:N2	1:A:1284:C:C2	2.65	0.64
7:G:65:ALA:O	7:G:69:VAL:HG23	1.98	0.64
1:A:1392:G:H21	1:A:1502:A:H8	1.43	0.64
1:A:1201:A:H4'	1:A:1202:G:H5''	1.78	0.64
1:A:481:G:O2'	1:A:483:C:N4	2.31	0.64
3:C:148:GLY:HA3	3:C:172:ARG:O	1.97	0.64
1:A:1005:A:O4'	1:A:1036:G:N2	2.31	0.63
1:A:1312:G:N2	1:A:1326:C:C2	2.66	0.63
1:A:1464:G:N1	1:A:1465:C:C4	2.66	0.63
1:A:1507:A:H2'	1:A:1508:G:H8	1.63	0.63
1:A:299:G:H2'	1:A:300:A:C8	2.33	0.63
17:Q:92:ARG:O	17:Q:95:TYR:HB2	1.97	0.63
1:A:1274:G:H2'	1:A:1275:A:H8	1.62	0.63
5:E:31:LEU:HD23	5:E:45:PHE:HD1	1.63	0.63
1:A:1530:G:H2'	1:A:1531:A:H8	1.63	0.63
1:A:925:G:H1	1:A:1391:U:H3	1.46	0.63
1:A:971:G:H1'	1:A:1365:G:O2'	1.98	0.63
6:F:49:ALA:CB	18:R:80:PRO:HA	2.27	0.63
1:A:1252:A:H2'	1:A:1253:G:O4'	1.97	0.63
1:A:537:G:H5''	12:L:113:ARG:HH12	1.63	0.63
1:A:1151:A:O2'	1:A:1152:A:H8	1.81	0.63
1:A:1244:C:H2'	1:A:1245:A:H8	1.64	0.63
1:A:1464:G:C2	1:A:1465:C:C4	2.87	0.63
1:A:1007:C:C2	1:A:1023:G:N1	2.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:C:O2'	1:A:470:C:N4	2.32	0.63
1:A:715:A:H2'	1:A:716:A:C8	2.34	0.63
1:A:1067:A:O5'	1:A:1067:A:H8	1.82	0.63
25:Z:68:C:H2'	25:Z:69:C:H6	1.61	0.63
4:D:24:GLU:O	4:D:25:ARG:HB3	1.99	0.62
1:A:1509:C:H2'	1:A:1510:U:O4'	1.99	0.62
1:A:243:A:H2	1:A:245:C:H2'	1.62	0.62
1:A:370:C:C2	1:A:392:G:N2	2.67	0.62
1:A:407:G:H2'	1:A:408:A:C8	2.34	0.62
1:A:994:A:C2	14:N:5:ALA:HA	2.34	0.62
1:A:1039:C:H2'	1:A:1040:U:H6	1.62	0.62
1:A:1457:G:H21	1:A:1458:G:H1'	1.62	0.62
1:A:522:C:H41	12:L:53:ARG:HH22	1.47	0.62
1:A:29:G:N2	1:A:555:C:C2	2.67	0.62
1:A:738:C:H2'	1:A:739:C:C6	2.35	0.62
1:A:987:G:H1	1:A:1218:C:H42	1.47	0.62
1:A:1386:G:H2'	1:A:1387:G:C8	2.29	0.62
1:A:785:G:H8	1:A:785:G:H5''	1.64	0.62
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.81	0.62
17:Q:27:PHE:CE1	17:Q:38:ARG:HB2	2.33	0.62
1:A:42:G:H2'	1:A:43:C:O4'	1.99	0.62
1:A:1382:C:H2'	1:A:1383:C:C6	2.35	0.62
1:A:189(K):U:H2'	1:A:189(L):G:C8	2.35	0.62
17:Q:15:MET:HB3	17:Q:18:THR:HB	1.80	0.62
1:A:1217:C:N4	1:A:1218:C:N4	2.47	0.62
1:A:1432:G:O2'	1:A:1468:A:N6	2.33	0.62
1:A:1493:A:H4'	1:A:1494:G:H5'	1.81	0.62
1:A:17:U:H2'	1:A:18:C:C6	2.34	0.62
1:A:296:U:H2'	1:A:297:G:C8	2.35	0.62
1:A:895:G:H1	1:A:904:C:H42	1.48	0.62
4:D:18:LYS:HA	4:D:33:MET:HG3	1.81	0.62
1:A:639:G:H2'	1:A:640:A:H8	1.65	0.62
1:A:1536:C:H42	24:Y:29:G:H1	1.46	0.62
1:A:40:C:H2'	1:A:41:G:C8	2.33	0.62
1:A:834:C:H5''	18:R:60:ALA:HB3	1.82	0.62
1:A:1119:C:H2'	1:A:1120:G:H8	1.65	0.61
1:A:778:G:C6	1:A:779:C:N3	2.68	0.61
1:A:1240:U:OP1	7:G:116:ALA:HB2	2.00	0.61
1:A:131:C:H2'	1:A:132:C:H6	1.64	0.61
1:A:240:C:H2'	1:A:241:C:C6	2.35	0.61
1:A:401:C:H2'	1:A:402:G:H8	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:LYS:HB2	3:C:173:VAL:HG21	1.81	0.61
1:A:1127:G:N2	1:A:1144:G:H22	1.97	0.61
1:A:1311:G:N7	19:S:2:PRO:CA	2.63	0.61
1:A:1391:U:H2'	1:A:1392:G:C8	2.35	0.61
20:T:65:LYS:O	20:T:68:LYS:HB3	2.00	0.61
1:A:1000:U:C6	1:A:1000:U:H3'	2.36	0.61
14:N:41:ARG:HG3	14:N:42:ILE:N	2.14	0.61
1:A:372:C:H4'	1:A:373:A:O5'	2.01	0.61
1:A:927:G:H1	1:A:1390:U:H3	1.48	0.61
1:A:1367:C:H4'	10:J:48:THR:HG21	1.83	0.61
1:A:1536:C:N4	24:Y:29:G:H1	1.98	0.61
1:A:19:C:H2'	1:A:20:U:C6	2.36	0.61
1:A:69:G:H1	1:A:100:C:N4	1.99	0.61
1:A:1457:G:C2	1:A:1458:G:C8	2.89	0.61
1:A:391:G:H2'	1:A:392:G:O4'	2.01	0.61
1:A:770:C:H2'	1:A:771:G:H8	1.65	0.61
13:M:34:LEU:HD13	13:M:41:PRO:HG3	1.82	0.61
1:A:1020:U:H2'	1:A:1021:G:C8	2.33	0.61
1:A:1266:G:N2	1:A:1270:C:C2	2.69	0.61
1:A:392:G:H2'	1:A:393:A:C8	2.36	0.61
1:A:398:C:H2'	1:A:399:G:H8	1.66	0.61
9:I:4:TYR:HE2	9:I:21:PRO:HG3	1.66	0.61
20:T:83:ARG:HA	20:T:86:ARG:NH1	2.15	0.61
1:A:1323:G:H2'	1:A:1324:A:C8	2.36	0.61
1:A:1530:G:H2'	1:A:1531:A:C8	2.36	0.61
20:T:73:HIS:HB3	20:T:74:LYS:HE3	1.82	0.61
23:X:47:LEU:HA	23:X:56:VAL:O	2.01	0.61
1:A:1244:C:H2'	1:A:1245:A:C8	2.37	0.60
1:A:1342:C:H2'	1:A:1343:G:H8	1.66	0.60
5:E:127:ASN:O	5:E:131:ILE:HG12	2.01	0.60
11:K:99:GLN:HA	11:K:105:VAL:HG21	1.83	0.60
14:N:37:PHE:HB3	14:N:39:LEU:HB2	1.83	0.60
1:A:1369:C:H2'	1:A:1370:G:C8	2.36	0.60
1:A:417:C:N4	1:A:418:C:N4	2.49	0.60
1:A:521:G:N1	1:A:522:C:C4	2.69	0.60
1:A:824:C:H2'	1:A:825:G:H8	1.65	0.60
3:C:29:TYR:CE1	3:C:33:LEU:CD1	2.54	0.60
10:J:50:ILE:HA	10:J:60:ARG:HA	1.84	0.60
1:A:785:G:C8	1:A:785:G:H5''	2.36	0.60
2:B:8:LYS:HD2	2:B:9:GLU:H	1.66	0.60
1:A:1447:A:H4'	1:A:1452:C:OP2	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:G:H2'	1:A:629:G:C8	2.37	0.60
1:A:720:C:H2'	1:A:721:G:C8	2.36	0.60
19:S:12:ASP:HB3	19:S:14:HIS:CD2	2.36	0.60
1:A:1084:G:H2'	1:A:1085:U:C6	2.37	0.60
1:A:1525:G:H2'	1:A:1526:G:C8	2.36	0.60
1:A:725:G:N2	1:A:726:C:C2	2.70	0.60
1:A:939:G:C6	1:A:940:C:N4	2.69	0.60
11:K:100:ALA:O	11:K:102:GLY:N	2.33	0.60
25:Z:26:G:C5	25:Z:27:U:H5	2.20	0.60
1:A:1412:C:H2'	1:A:1413:A:C8	2.37	0.60
1:A:664:G:H22	1:A:741:G:H1	0.74	0.60
1:A:926:G:H2'	1:A:1505:G:N3	2.16	0.60
6:F:49:ALA:HB3	6:F:50:TYR:HD1	1.67	0.60
7:G:16:LEU:HB3	9:I:44:VAL:HG23	1.83	0.60
1:A:1105:A:H2'	1:A:1106:G:H8	1.67	0.60
12:L:45:PRO:HG3	12:L:53:ARG:HD3	1.83	0.60
15:O:34:LEU:O	15:O:38:ARG:HG2	2.02	0.60
1:A:1537:U:O2	24:Y:28:A:N1	2.35	0.60
1:A:455:C:C6	1:A:455:C:O5'	2.55	0.60
1:A:690:G:OP2	11:K:27:ASN:HB3	2.02	0.60
8:H:104:ARG:HB2	8:H:108:GLY:H	1.66	0.60
23:X:157:LEU:HD13	25:Z:27:U:H5'	1.84	0.60
1:A:1218:C:H2'	1:A:1219:U:C6	2.37	0.60
2:B:187:LEU:HD11	2:B:214:ILE:HD12	1.83	0.60
7:G:40:ALA:HB3	9:I:41:VAL:HG21	1.83	0.60
1:A:20:U:H2'	1:A:21:G:O4'	2.02	0.59
1:A:1081:G:H8	1:A:1081:G:H5''	1.68	0.59
1:A:588:G:N2	1:A:589:C:C2	2.70	0.59
1:A:924:C:H2'	1:A:925:G:C8	2.38	0.59
23:X:16:VAL:HG12	23:X:55:PRO:HB2	1.84	0.59
1:A:113:G:H1'	1:A:354:G:H5''	1.84	0.59
25:Z:41:C:H2'	25:Z:42:G:O4'	2.01	0.59
1:A:1342:C:H2'	1:A:1343:G:C8	2.38	0.59
1:A:939:G:C2	1:A:940:C:N3	2.71	0.59
1:A:986:A:H2'	1:A:987:G:O4'	2.02	0.59
4:D:30:LYS:C	4:D:32:ALA:H	2.04	0.59
1:A:1255:G:C6	1:A:1279:A:C8	2.90	0.59
1:A:1443:G:N2	1:A:1444:C:C2	2.71	0.59
1:A:246:A:O2'	17:Q:99:SER:HB2	2.02	0.59
1:A:334:C:H2'	1:A:335:C:C6	2.38	0.59
1:A:442:C:H2'	1:A:443:C:H6	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:A:H2'	1:A:33:A:C8	2.37	0.59
9:I:19:LEU:HD22	9:I:59:PHE:HB3	1.85	0.59
11:K:87:THR:HG21	24:Y:28:A:O2'	2.03	0.59
1:A:1106:G:N2	1:A:1107:C:C2	2.70	0.59
1:A:1126:U:OP1	1:A:1280:A:C8	2.56	0.59
1:A:24:U:H2'	1:A:25:C:C6	2.38	0.59
3:C:187:ALA:HB3	3:C:198:VAL:HB	1.83	0.59
1:A:1040:U:H2'	1:A:1041:A:H8	1.63	0.59
1:A:1395:C:H2'	1:A:1396:A:H8	1.68	0.59
6:F:7:ASN:ND2	18:R:34:TYR:HE1	2.00	0.59
20:T:41:ILE:HD13	20:T:87:LYS:HZ2	1.64	0.59
22:W:33:LEU:O	22:W:64:ARG:HA	2.03	0.59
1:A:529:G:H5'	1:A:530:G:OP2	2.02	0.59
1:A:838:G:N2	1:A:849:C:C2	2.71	0.59
1:A:953:G:H2'	1:A:954:G:O4'	2.02	0.59
2:B:201:ILE:HG21	2:B:214:ILE:HG21	1.85	0.59
8:H:91:ARG:HD3	12:L:7:ILE:HD12	1.84	0.59
25:Z:7:G:H1	25:Z:66:C:H42	1.51	0.59
1:A:1124:G:H2'	1:A:1145:C:C5	2.38	0.58
1:A:1463:C:H2'	1:A:1464:G:C8	2.38	0.58
1:A:616:G:H2'	1:A:617:G:H8	1.68	0.58
1:A:601:C:H42	1:A:637:G:H1	1.51	0.58
8:H:49:GLU:HG3	8:H:60:ARG:HB2	1.85	0.58
1:A:1249:C:H6	1:A:1249:C:H5''	1.68	0.58
1:A:1507:A:H2'	1:A:1508:G:C8	2.39	0.58
1:A:146:G:N2	1:A:177:C:C2	2.72	0.58
1:A:312:C:H2'	1:A:313:A:H8	1.65	0.58
11:K:21:ILE:HG12	11:K:30:VAL:HG22	1.83	0.58
1:A:1443:G:C6	1:A:1444:C:N4	2.71	0.58
1:A:514:C:H2'	1:A:515:G:H8	1.68	0.58
1:A:551:U:H2'	1:A:552:U:C6	2.38	0.58
1:A:1016:A:H2'	1:A:1017:G:O4'	2.02	0.58
1:A:518:C:H4'	1:A:519:C:O5'	2.02	0.58
1:A:189(A):C:H2'	1:A:189(B):C:H6	1.69	0.58
3:C:59:ARG:NH1	3:C:97:LYS:HD3	2.18	0.58
1:A:1305:G:N2	1:A:1331:G:H1'	2.19	0.58
1:A:504:C:C2	1:A:542:G:N2	2.71	0.58
4:D:201:GLN:NE2	5:E:116:THR:CG2	2.65	0.58
23:X:9:GLU:HA	23:X:35:LEU:HD11	1.85	0.58
1:A:553:A:H2'	1:A:554:C:C6	2.38	0.58
1:A:584:G:H2'	1:A:585:G:H8	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1112:C:N3	3:C:177:THR:HA	2.19	0.58
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.84	0.58
25:Z:53:G:H1	25:Z:61:C:N4	2.02	0.58
1:A:1201:A:H4'	1:A:1202:G:C5'	2.34	0.58
1:A:1293:G:H2'	1:A:1294:G:C8	2.38	0.58
1:A:1466:C:H2'	1:A:1467:G:O4'	2.04	0.58
1:A:643:C:H2'	1:A:644:G:H8	1.67	0.58
3:C:97:LYS:HB3	3:C:97:LYS:HZ3	1.68	0.58
4:D:31:CYS:C	4:D:33:MET:H	2.05	0.58
1:A:334:C:H2'	1:A:335:C:H6	1.68	0.58
1:A:955:U:H6	1:A:955:U:O5'	1.87	0.58
1:A:500:G:C6	1:A:501:C:N4	2.72	0.58
1:A:969:A:H2'	1:A:970:C:O4'	2.01	0.58
1:A:124:G:H2'	1:A:125:U:O4'	2.03	0.57
1:A:750:G:N3	15:O:23:GLY:HA3	2.19	0.57
1:A:836:G:H2'	1:A:837:G:C8	2.38	0.57
9:I:11:LYS:HE2	9:I:109:VAL:HG23	1.85	0.57
1:A:397:A:N3	1:A:397:A:H3'	2.19	0.57
1:A:652:U:O4	1:A:752:G:O2'	2.17	0.57
1:A:1119:C:H2'	1:A:1120:G:C8	2.39	0.57
1:A:417:C:N4	1:A:418:C:H41	2.02	0.57
1:A:767:A:H2'	1:A:768:A:O4'	2.05	0.57
1:A:1258:G:C6	1:A:1259:C:N4	2.73	0.57
1:A:148:G:H2'	1:A:149:A:C8	2.39	0.57
1:A:165:C:H2'	1:A:166:G:H8	1.68	0.57
1:A:987:G:H2'	1:A:988:G:C8	2.38	0.57
1:A:1113:C:O4'	3:C:178:LEU:HG	2.04	0.57
23:X:17:ARG:NH2	25:Z:56:C:N4	2.52	0.57
1:A:1485:U:H2'	1:A:1486:G:H8	1.69	0.57
4:D:98:GLU:O	4:D:104:VAL:HG23	2.05	0.57
1:A:61:G:H2'	1:A:62:U:O4'	2.05	0.57
7:G:65:ALA:HA	7:G:127:ALA:HB1	1.87	0.57
23:X:168:VAL:HG12	23:X:169:LYS:HG3	1.87	0.57
1:A:1041:A:H2'	1:A:1042:G:H8	1.70	0.57
1:A:426:G:H2'	1:A:427:U:O4'	2.04	0.57
1:A:649:G:H2'	1:A:650:G:O4'	2.05	0.57
1:A:69:G:H1	1:A:100:C:H42	1.51	0.57
1:A:1345:U:N3	1:A:1375:A:C6	2.63	0.57
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.20	0.57
11:K:123:LYS:HA	11:K:126:ARG:HB2	1.87	0.57
1:A:122:G:C6	1:A:123:C:C4	2.93	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:G:H2'	1:A:233:C:C6	2.40	0.57
1:A:504:C:N3	1:A:542:G:C2	2.73	0.57
10:J:53:PRO:HA	14:N:41:ARG:NH2	2.20	0.57
1:A:1081:G:C8	1:A:1081:G:H5''	2.40	0.56
1:A:1512:U:H2'	1:A:1513:A:H8	1.69	0.56
1:A:541:G:H2'	1:A:542:G:O4'	2.05	0.56
1:A:616:G:H2'	1:A:617:G:C8	2.40	0.56
2:B:44:LEU:HA	2:B:47:THR:HB	1.87	0.56
1:A:663:A:H5''	18:R:61:LYS:HE3	1.86	0.56
23:X:157:LEU:CD1	25:Z:27:U:OP1	2.53	0.56
1:A:1004:A:H5''	1:A:1025:U:C5	2.41	0.56
1:A:1163:C:N3	1:A:1174:G:C2	2.74	0.56
1:A:1241:G:N2	1:A:1242:C:C2	2.73	0.56
10:J:79:ARG:HH12	10:J:82:ILE:HB	1.70	0.56
1:A:1081:G:H2'	1:A:1082:G:H8	1.71	0.56
1:A:129(A):G:H1	1:A:189(D):C:H2'	1.71	0.56
7:G:71:PRO:HG3	7:G:103:TRP:HZ3	1.69	0.56
12:L:60:LEU:HD11	12:L:85:ILE:HD12	1.86	0.56
1:A:1521:G:H2'	1:A:1522:U:C6	2.40	0.56
1:A:1190:G:H5'	3:C:176:HIS:CE1	2.40	0.56
24:Y:36:A:N6	25:Z:37:A:N6	2.53	0.56
1:A:408:A:H2'	1:A:409:G:C8	2.40	0.56
25:Z:22:G:H8	25:Z:22:G:P	2.28	0.56
1:A:165:C:H2'	1:A:166:G:C8	2.40	0.56
1:A:821:G:H2'	1:A:822:C:C6	2.41	0.56
4:D:101:LEU:HB2	4:D:138:TYR:HB3	1.88	0.56
1:A:1076:C:C2	1:A:1082:G:N2	2.73	0.56
1:A:10:A:H2'	1:A:11:G:C8	2.40	0.56
1:A:571:U:O5'	1:A:571:U:H6	1.89	0.56
1:A:671:G:C2	1:A:736:C:N3	2.74	0.56
1:A:755:G:N2	1:A:756:C:C2	2.74	0.56
1:A:781:A:N6	1:A:802:A:H1'	2.20	0.56
1:A:830:G:H2'	1:A:831:U:O4'	2.06	0.56
1:A:64:G:H4'	1:A:65:U:H5''	1.88	0.56
1:A:687:A:H2	1:A:700:G:N3	2.04	0.56
1:A:824:C:H2'	1:A:825:G:C8	2.41	0.56
1:A:874:G:N2	1:A:875:C:C2	2.73	0.56
1:A:837:G:H1	1:A:849:C:H42	1.52	0.56
1:A:877:C:H2'	1:A:878:G:H8	1.70	0.56
3:C:29:TYR:OH	14:N:54:PRO:HD2	2.05	0.56
6:F:11:ASN:HD21	6:F:13:ASN:HD22	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:G:H2'	1:A:276:G:H8	1.70	0.56
1:A:377:G:H1	1:A:386:C:H42	1.54	0.56
1:A:893:C:H2'	1:A:894:G:O4'	2.05	0.56
8:H:122:ARG:HB3	8:H:122:ARG:HH11	1.71	0.56
1:A:1103:C:H2'	1:A:1104:G:O4'	2.06	0.56
1:A:21:G:H2'	1:A:22:G:H8	1.64	0.56
1:A:613:C:H2'	1:A:614:A:H8	1.70	0.56
11:K:22:HIS:HB3	11:K:29:ILE:HG22	1.88	0.56
23:X:56:VAL:HG11	25:Z:19:G:N7	2.21	0.56
1:A:939:G:H1	1:A:1344:C:H42	1.54	0.55
1:A:1401:G:H2'	1:A:1402:C:O4'	2.07	0.55
1:A:258:G:N2	1:A:269:C:C2	2.74	0.55
1:A:548:G:C6	1:A:549:C:N4	2.75	0.55
1:A:613:C:H2'	1:A:614:A:C8	2.40	0.55
1:A:835:U:OP1	18:R:61:LYS:HB2	2.06	0.55
9:I:22:GLY:HA3	9:I:60:ASP:HB2	1.87	0.55
1:A:926:G:N2	24:Y:35:A:H5'	2.22	0.55
1:A:1412:C:H2'	1:A:1413:A:H8	1.69	0.55
1:A:377:G:H1	1:A:386:C:N4	2.04	0.55
1:A:1001(A):G:N1	1:A:1002:G:C6	2.74	0.55
1:A:1380:U:C4	7:G:3:ARG:HG2	2.41	0.55
1:A:317:G:C2	1:A:337:C:C2	2.95	0.55
1:A:584:G:H2'	1:A:585:G:C8	2.42	0.55
1:A:69:G:H2'	1:A:70:G:H8	1.70	0.55
23:X:17:ARG:HH22	23:X:19:VAL:HG22	1.69	0.55
1:A:987:G:H1	1:A:1218:C:N4	2.04	0.55
1:A:1257:U:H4'	1:A:1258:G:O5'	2.06	0.55
1:A:601:C:C2	1:A:638:G:N2	2.75	0.55
1:A:860:A:H3'	1:A:861:G:C8	2.41	0.55
1:A:1409:C:H2'	1:A:1410:G:C8	2.42	0.55
1:A:864:A:C2'	1:A:865:A:C8	2.87	0.55
1:A:948:C:H2'	1:A:949:A:C8	2.41	0.55
23:X:5:TYR:HH	25:Z:20:U:H6	0.60	0.55
1:A:1126:U:H5'	1:A:1280:A:O2'	2.07	0.55
4:D:23:GLY:H	4:D:26:CYS:HB2	1.71	0.55
24:Y:38:G:O6	25:Z:34:C:N3	2.40	0.55
1:A:1102:A:H2'	1:A:1103:C:H6	1.72	0.55
1:A:1225:A:N3	1:A:1225:A:H2'	2.21	0.55
4:D:157:LEU:HA	4:D:160:GLN:HE21	1.72	0.55
1:A:296:U:H2'	1:A:297:G:H8	1.72	0.55
3:C:29:TYR:HH	14:N:54:PRO:HG2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:C:H2'	1:A:175:C:C6	2.42	0.55
1:A:424:G:H2'	1:A:425:G:C8	2.40	0.55
4:D:187:ARG:HB2	4:D:187:ARG:NH1	2.22	0.55
19:S:81:ARG:HB2	19:S:81:ARG:HH11	1.70	0.55
20:T:41:ILE:CD1	20:T:87:LYS:HZ2	2.18	0.55
25:Z:49:G:C2	25:Z:66:C:C2	2.95	0.55
1:A:1068:G:N2	1:A:1069:C:C2	2.75	0.54
1:A:1115:C:H2'	1:A:1116:C:C6	2.41	0.54
1:A:1262:C:N4	1:A:1273:G:H1	2.02	0.54
1:A:1256:A:N6	1:A:1278:U:C2	2.75	0.54
1:A:105:G:C6	1:A:106:C:N4	2.76	0.54
1:A:1512:U:H2'	1:A:1513:A:C8	2.42	0.54
1:A:502:G:H2'	1:A:503:C:O4'	2.07	0.54
1:A:591:U:H2'	1:A:592:G:C8	2.42	0.54
1:A:105:G:C5	1:A:106:C:C4	2.95	0.54
1:A:216:G:C2	1:A:217:C:N3	2.75	0.54
1:A:354:G:N2	1:A:355:C:C2	2.75	0.54
19:S:22:LEU:HD22	19:S:28:LYS:HD2	1.88	0.54
1:A:983:A:H2	1:A:1222:G:H22	1.53	0.54
1:A:687:A:C2	1:A:700:G:N3	2.75	0.54
1:A:1129:C:H1'	1:A:1132:C:H5	1.72	0.54
1:A:1353:G:N2	1:A:1354:C:C2	2.76	0.54
1:A:532:A:H2'	1:A:532:A:N3	2.22	0.54
1:A:880:C:H2'	1:A:881:G:C8	2.42	0.54
25:Z:5:G:H1	25:Z:68:C:N4	2.05	0.54
1:A:1271:G:C6	1:A:1272:G:C5	2.96	0.54
1:A:998:G:N2	1:A:999:C:C2	2.75	0.54
1:A:1504:G:P	1:A:1504:G:H3'	2.48	0.54
1:A:45:U:H2'	1:A:46:G:C8	2.43	0.54
1:A:613:C:N4	1:A:627:G:H1	2.05	0.54
1:A:1111:A:N6	3:C:176:HIS:O	2.41	0.54
4:D:8:VAL:HG13	4:D:9:CYS:H	1.72	0.54
1:A:568:G:C6	1:A:569:C:N4	2.76	0.54
9:I:28:VAL:HA	9:I:63:ILE:O	2.08	0.54
1:A:1189:C:H5'	14:N:58:LYS:HZ3	1.73	0.54
24:Y:23:C:H2'	24:Y:24:A:O4'	2.07	0.54
1:A:1128:C:H1'	1:A:1146:A:H61	1.73	0.54
1:A:988:G:C6	1:A:989:C:N3	2.76	0.54
20:T:14:LYS:HE2	20:T:18:GLN:HE22	1.73	0.54
1:A:1097:C:H2'	1:A:1098:C:H6	1.71	0.54
1:A:1115:C:H2'	1:A:1116:C:H6	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1248:A:C6	1:A:1249:C:N4	2.76	0.54
1:A:976:G:H22	1:A:1363:C:H5''	1.73	0.54
1:A:275:G:H2'	1:A:276:G:C8	2.42	0.54
1:A:72:C:C3'	1:A:73:G:C5'	2.81	0.54
1:A:742:G:H2'	1:A:743:U:O4'	2.08	0.54
23:X:89:LYS:HA	23:X:119:THR:O	2.07	0.54
24:Y:28:A:N6	24:Y:29:G:N1	2.56	0.54
1:A:926:G:H22	24:Y:35:A:H5'	1.73	0.54
25:Z:12:G:C6	25:Z:13:C:N3	2.76	0.54
1:A:1283:G:N1	1:A:1284:C:C4	2.76	0.53
1:A:243:A:C2	1:A:245:C:H2'	2.42	0.53
1:A:730:G:N2	1:A:765:G:H5''	2.23	0.53
25:Z:37:A:H3'	25:Z:38:A:H8	1.72	0.53
25:Z:38:A:H2'	25:Z:39:C:O4'	2.08	0.53
1:A:1415:G:H22	1:A:1486:G:H1'	1.73	0.53
1:A:257:G:H1	1:A:269:C:H42	1.56	0.53
1:A:300:A:H2'	1:A:301:G:O4'	2.08	0.53
1:A:731:G:N2	1:A:732:C:C2	2.77	0.53
1:A:562:C:H41	1:A:884:U:H2'	1.73	0.53
8:H:14:ARG:HG3	8:H:83:ILE:HG22	1.91	0.53
11:K:25:TYR:HB2	11:K:26:ASN:ND2	2.23	0.53
23:X:56:VAL:HG13	25:Z:19:G:O6	2.08	0.53
25:Z:69:C:H2'	25:Z:70:G:H8	1.71	0.53
1:A:1101:A:H4'	1:A:1102:A:O5'	2.07	0.53
1:A:1424:C:H42	1:A:1476:G:H1	1.56	0.53
1:A:661:G:C2	1:A:745:C:N3	2.77	0.53
10:J:39:PRO:O	10:J:40:LEU:HB2	2.07	0.53
1:A:1347:G:HO2'	1:A:1348:U:P	2.32	0.53
1:A:822:C:H2'	1:A:823:G:H8	1.74	0.53
3:C:39:ILE:HD11	3:C:95:THR:HG21	1.90	0.53
1:A:132:C:N3	1:A:231:G:C2	2.76	0.53
1:A:18:C:O5'	1:A:18:C:H6	1.92	0.53
1:A:60:A:H4'	1:A:61:G:O5'	2.09	0.53
13:M:88:ARG:HA	13:M:98:VAL:HG11	1.91	0.53
1:A:1081:G:H2'	1:A:1082:G:C8	2.43	0.53
1:A:333:G:N2	1:A:334:C:C2	2.76	0.53
4:D:90:GLY:HA2	4:D:204:ILE:HD11	1.89	0.53
18:R:51:LEU:HD13	18:R:55:ARG:HD2	1.91	0.53
25:Z:22:G:OP2	25:Z:46:G7M:N2	2.42	0.53
4:D:132:ARG:HD3	4:D:151:LYS:NZ	2.24	0.53
1:A:1258:G:C2	1:A:1259:C:N3	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1443:G:C2	1:A:1444:C:C4	2.97	0.53
1:A:335:C:H2'	1:A:336:C:C6	2.44	0.53
1:A:687:A:H4'	1:A:688:G:O5'	2.09	0.53
22:W:6:THR:HB	22:W:56:GLU:HG2	1.90	0.53
1:A:258:G:C2	1:A:269:C:N3	2.77	0.53
1:A:761:G:C2	1:A:762:C:C2	2.96	0.53
3:C:56:ASP:HB2	3:C:67:THR:HB	1.90	0.53
6:F:49:ALA:HB2	18:R:80:PRO:HA	1.89	0.53
1:A:1141:C:H2'	1:A:1142:G:H8	1.73	0.53
1:A:129(A):G:O2'	1:A:130:A:OP2	2.24	0.53
1:A:580:U:H2'	1:A:581:G:O4'	2.08	0.53
6:F:48:LEU:HD13	6:F:52:ILE:HD12	1.91	0.53
3:C:29:TYR:OH	14:N:54:PRO:CD	2.55	0.53
23:X:137:LEU:HD13	23:X:163:MET:HG3	1.91	0.53
1:A:455:C:H6	1:A:455:C:O5'	1.91	0.52
1:A:557:G:H2'	1:A:558:G:C8	2.43	0.52
1:A:66:G:N2	1:A:67:C:C2	2.77	0.52
10:J:30:SER:HB2	10:J:80:LYS:O	2.08	0.52
1:A:278:G:N7	17:Q:92:ARG:NH1	2.57	0.52
1:A:1392:G:N2	1:A:1502:A:C8	2.75	0.52
1:A:559:A:O2'	1:A:560:U:OP2	2.23	0.52
1:A:1256:A:H8	3:C:27:LYS:NZ	2.08	0.52
17:Q:56:VAL:HG13	17:Q:77:VAL:HB	1.91	0.52
1:A:41:G:H1	1:A:401:C:H42	1.56	0.52
1:A:502:G:C2	1:A:503:C:C2	2.97	0.52
1:A:790:A:H2'	1:A:791:G:C8	2.45	0.52
1:A:855:G:N1	1:A:856:C:C2	2.78	0.52
1:A:1008:C:N3	1:A:1022:G:N2	2.57	0.52
1:A:1464:G:N2	1:A:1465:C:N3	2.58	0.52
1:A:216:G:C6	1:A:217:C:N4	2.77	0.52
1:A:298:A:H2'	1:A:299:G:C8	2.45	0.52
1:A:1194:U:H4'	5:E:22:GLY:HA3	1.92	0.52
12:L:6:THR:O	12:L:9:GLN:HB3	2.10	0.52
23:X:157:LEU:HD13	25:Z:27:U:OP1	2.10	0.52
1:A:1018:C:H2'	1:A:1019:C:C6	2.44	0.52
1:A:1048:G:H2'	1:A:1050:G:C8	2.44	0.52
1:A:1132:C:H2'	1:A:1133:G:C8	2.45	0.52
1:A:1241:G:C6	1:A:1242:C:N4	2.78	0.52
1:A:1355:G:H2'	1:A:1356:G:C8	2.44	0.52
1:A:566:G:O3'	1:A:567:G:H5'	2.08	0.52
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:3:GLN:HG3	9:I:20:ARG:HG3	1.91	0.52
1:A:199:G:N2	1:A:219:C:C2	2.78	0.52
1:A:729:A:H2'	1:A:730:G:H8	1.75	0.52
1:A:967:C:C4	1:A:968:A:C6	2.98	0.52
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.92	0.52
1:A:1198:G:C5	1:A:1199:U:C4	2.98	0.52
1:A:53:A:H2'	1:A:54:C:O4'	2.09	0.52
15:O:19:PRO:C	15:O:21:ASP:H	2.13	0.52
1:A:918:A:H2'	1:A:919:A:C8	2.44	0.52
8:H:6:ILE:N	8:H:6:ILE:HD13	2.24	0.52
23:X:157:LEU:HD13	25:Z:27:U:H5''	1.91	0.52
1:A:1518:A:H2'	1:A:1519:A:C8	2.45	0.52
1:A:44:G:H2'	1:A:45:U:O4'	2.10	0.52
6:F:37:VAL:HA	6:F:65:VAL:HG12	1.92	0.52
11:K:62:GLN:HG3	11:K:97:ALA:HB2	1.92	0.52
1:A:110:C:H2'	1:A:111:G:O4'	2.09	0.52
1:A:1502:A:H2'	1:A:1504:G:C8	2.44	0.52
1:A:21:G:H21	1:A:914:A:H62	1.58	0.52
1:A:70:G:N1	1:A:100:C:C2	2.78	0.52
1:A:829:G:C8	1:A:829:G:H5''	2.45	0.52
9:I:26:VAL:HG22	9:I:61:ALA:HB3	1.92	0.52
1:A:1500:A:H5''	1:A:1508:G:H5''	1.92	0.51
1:A:333:G:C6	1:A:334:C:N4	2.79	0.51
1:A:633:G:H2'	1:A:634:C:H6	1.75	0.51
1:A:663:A:H2'	1:A:664:G:O4'	2.09	0.51
1:A:774:G:N2	1:A:806:C:C2	2.77	0.51
6:F:30:LEU:HD22	6:F:65:VAL:HG11	1.92	0.51
10:J:6:ILE:HA	10:J:97:GLU:O	2.09	0.51
1:A:1347:G:C2'	1:A:1373:G:H1	2.23	0.51
1:A:1375:A:N3	1:A:1375:A:H2'	2.24	0.51
1:A:662:G:H2'	1:A:663:A:C8	2.46	0.51
1:A:983:A:H2	1:A:1222:G:N2	2.07	0.51
8:H:14:ARG:O	8:H:18:ARG:HD2	2.10	0.51
9:I:24:GLY:HA3	9:I:57:GLY:HA2	1.91	0.51
12:L:51:ALA:HB3	12:L:53:ARG:HE	1.75	0.51
1:A:143:A:H2	1:A:220:G:H1	1.58	0.51
1:A:1457:G:C2	1:A:1458:G:C1'	2.93	0.51
1:A:590:C:C2	1:A:650:G:N2	2.78	0.51
9:I:4:TYR:CE2	9:I:21:PRO:HG3	2.45	0.51
13:M:97:PRO:HA	13:M:110:ARG:NH1	2.25	0.51
18:R:51:LEU:HB3	18:R:55:ARG:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001(A):G:N2	1:A:1040:U:C2	2.77	0.51
1:A:983:A:C2	1:A:1222:G:N2	2.77	0.51
1:A:1536:C:H2'	1:A:1537:U:C6	2.46	0.51
1:A:416:G:H1	1:A:427:U:H3	1.58	0.51
1:A:520:A:H62	1:A:529:G:H21	1.58	0.51
1:A:499:A:C6	1:A:547:A:C8	2.98	0.51
1:A:548:G:N2	1:A:549:C:C2	2.78	0.51
1:A:554:C:H2'	1:A:555:C:C6	2.45	0.51
1:A:696:A:H8	1:A:696:A:O5'	1.92	0.51
1:A:725:G:N1	1:A:726:C:C4	2.79	0.51
1:A:784:C:N3	1:A:799:G:C2	2.79	0.51
1:A:105:G:C5	1:A:106:C:N4	2.79	0.51
1:A:233:C:H2'	1:A:234:C:C6	2.46	0.51
1:A:24:U:H2'	1:A:25:C:H6	1.76	0.51
1:A:985:C:H2'	1:A:986:A:C8	2.46	0.51
1:A:988:G:N1	1:A:989:C:C2	2.79	0.51
10:J:46:ARG:HH12	10:J:64:GLU:HB3	1.74	0.51
1:A:564:C:P	12:L:15:ARG:HH21	2.32	0.51
1:A:101:A:O2'	1:A:102:G:H5'	2.10	0.51
1:A:1305:G:O2'	1:A:1306:A:H8	1.92	0.51
1:A:186:C:H5'	20:T:78:ALA:HB1	1.92	0.51
1:A:22:G:C2	1:A:23:C:C2	2.99	0.51
1:A:624:C:H2'	1:A:625:G:H8	1.75	0.51
4:D:3:ARG:HB2	4:D:5:ILE:HD12	1.92	0.51
1:A:1120:G:H2'	1:A:1121:U:C6	2.46	0.51
1:A:1457:G:N3	1:A:1458:G:C8	2.79	0.51
1:A:22:G:C6	1:A:23:C:C4	2.99	0.51
4:D:61:LYS:HA	4:D:203:VAL:HG22	1.91	0.51
12:L:83:VAL:HG22	12:L:84:LEU:H	1.75	0.51
14:N:50:LYS:HD2	14:N:52:GLN:NE2	2.25	0.51
18:R:53:ARG:NH2	18:R:60:ALA:HB2	2.21	0.51
23:X:137:LEU:HB3	23:X:163:MET:SD	2.51	0.51
24:Y:36:A:H2'	24:Y:37:U:C6	2.45	0.51
1:A:1007:C:O2	1:A:1023:G:C2	2.64	0.51
1:A:1190:G:H5'	3:C:176:HIS:NE2	2.25	0.51
1:A:238:G:H2'	1:A:239:U:O4'	2.11	0.51
1:A:604:G:H2'	1:A:605:U:O4'	2.10	0.51
1:A:590:C:N3	1:A:650:G:C2	2.79	0.51
1:A:1008:C:H2'	1:A:1009:G:O4'	2.11	0.51
1:A:138:G:H2'	1:A:139:G:O4'	2.11	0.51
1:A:984:C:N3	1:A:1222:G:C2	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:ARG:NH2	3:C:207:VAL:HG21	2.26	0.51
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.93	0.51
8:H:79:VAL:HG13	8:H:80:ILE:HG13	1.93	0.51
17:Q:40:LYS:HB3	17:Q:42:TYR:HE1	1.76	0.51
6:F:7:ASN:ND2	18:R:34:TYR:CE1	2.79	0.51
1:A:500:G:C2	1:A:501:C:N3	2.79	0.51
1:A:772:U:H3	1:A:807:A:H61	1.59	0.51
3:C:23:TYR:HE2	10:J:9:ARG:HD3	1.76	0.51
15:O:62:GLN:HA	15:O:65:ARG:HD3	1.93	0.51
24:Y:22:G:C6	24:Y:23:C:N3	2.79	0.51
24:Y:36:A:C6	25:Z:37:A:C6	2.99	0.51
1:A:1041:A:H2'	1:A:1042:G:C8	2.46	0.50
1:A:975:A:N6	1:A:1366:C:O2'	2.39	0.50
1:A:344:A:H4'	1:A:345:C:OP2	2.10	0.50
1:A:413:G:O2'	1:A:428:G:N2	2.44	0.50
1:A:748:C:H1'	1:A:749:C:C5	2.46	0.50
1:A:903:G:H2'	1:A:904:C:C6	2.46	0.50
2:B:167:PRO:HG3	2:B:186:ALA:HB1	1.93	0.50
5:E:139:LEU:HA	5:E:142:LEU:HD12	1.92	0.50
7:G:93:PRO:O	7:G:96:GLN:HG2	2.10	0.50
3:C:6:HIS:HB3	14:N:49:HIS:HB3	1.93	0.50
1:A:122:G:C2	1:A:123:C:C2	2.99	0.50
1:A:1534:A:H2'	1:A:1535:C:H6	1.75	0.50
1:A:457:C:H2'	1:A:458:C:H6	1.76	0.50
1:A:524:G:C2	1:A:525:C:C4	2.98	0.50
1:A:1328:C:H5''	13:M:28:ALA:HB3	1.93	0.50
1:A:1023:G:H2'	1:A:1023:G:N3	2.26	0.50
1:A:976:G:N2	1:A:1363:C:H5''	2.27	0.50
1:A:502:G:C6	1:A:503:C:C4	3.00	0.50
1:A:591:U:H2'	1:A:592:G:H8	1.76	0.50
2:B:124:SER:HB2	2:B:125:PRO:HD2	1.93	0.50
1:A:1243:C:H2'	1:A:1244:C:O4'	2.12	0.50
1:A:471:G:O2'	1:A:472:A:H5'	2.11	0.50
1:A:886:G:C6	1:A:887:G:C5	2.98	0.50
1:A:910:C:H4'	1:A:1413:A:H4'	1.93	0.50
3:C:113:ALA:N	3:C:114:PRO:CD	2.74	0.50
24:Y:30:G:H3'	24:Y:31:U:H5''	1.94	0.50
25:Z:27:U:H2'	25:Z:28:C:C5'	2.41	0.50
1:A:1004:A:N7	1:A:1037:C:N3	2.59	0.50
1:A:1148:U:H2'	1:A:1149:C:O4'	2.12	0.50
1:A:141:A:H2'	1:A:142:G:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:C:H2'	1:A:370:C:C6	2.46	0.50
1:A:554:C:C2	1:A:555:C:C5	3.00	0.50
1:A:778:G:N1	1:A:779:C:C2	2.80	0.50
1:A:1240:U:P	7:G:116:ALA:H	2.34	0.50
1:A:1374:A:C5	1:A:1375:A:C8	3.00	0.50
1:A:1457:G:H2'	1:A:1458:G:O4'	2.12	0.50
1:A:303:A:H2'	1:A:304:U:C6	2.47	0.50
4:D:185:PHE:HZ	4:D:189:PRO:HD3	1.77	0.50
4:D:64:LEU:HA	4:D:67:ILE:HD12	1.94	0.50
9:I:42:ARG:O	9:I:74:ILE:HG21	2.12	0.50
18:R:40:LEU:HA	18:R:43:PHE:HD2	1.76	0.50
1:A:1001:A:H2'	1:A:1001(A):G:C8	2.47	0.50
1:A:1071:C:H2'	1:A:1072:G:C8	2.45	0.50
1:A:1338:G:H21	25:Z:42:G:H1'	1.76	0.50
1:A:358:U:H2'	1:A:359:U:C6	2.46	0.50
1:A:441:A:H5''	1:A:441:A:H8	1.77	0.50
1:A:992:U:H1'	1:A:993:G:C2	2.46	0.50
6:F:3:ARG:HB3	6:F:93:SER:HB2	1.93	0.50
10:J:50:ILE:HG23	10:J:59:SER:HB2	1.94	0.50
20:T:43:LEU:HB3	20:T:52:ALA:HB2	1.94	0.50
1:A:1007:C:N3	1:A:1023:G:C6	2.80	0.50
1:A:855:G:C6	1:A:856:C:C4	2.99	0.50
1:A:370:C:N3	1:A:392:G:C2	2.80	0.50
1:A:798:G:H2'	1:A:799:G:O4'	2.12	0.50
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.94	0.50
8:H:82:HIS:NE2	8:H:84:ARG:HB2	2.27	0.50
1:A:100:C:H2'	1:A:101:A:C8	2.47	0.49
1:A:1293:G:H2'	1:A:1294:G:H8	1.76	0.49
1:A:1346:A:C8	1:A:1348:U:C2	3.00	0.49
1:A:255:G:H2'	1:A:256:U:H6	1.75	0.49
1:A:721:G:H4'	1:A:722:A:O4'	2.12	0.49
1:A:858:G:H5''	1:A:869:G:O6	2.12	0.49
1:A:902:G:H2'	1:A:903:G:H8	1.77	0.49
1:A:1346:A:H2'	7:G:10:ARG:HH22	1.76	0.49
7:G:30:ILE:HG22	7:G:39:ALA:HB1	1.94	0.49
8:H:14:ARG:NH2	8:H:83:ILE:O	2.45	0.49
12:L:84:LEU:HB2	12:L:105:TYR:HD2	1.77	0.49
25:Z:32:OMC:N3	25:Z:38:A:N6	2.60	0.49
25:Z:67:C:C2	25:Z:68:C:C5	3.00	0.49
1:A:200:G:C6	1:A:201:C:N3	2.80	0.49
1:A:399:G:C6	1:A:400:C:N4	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:A:C4	1:A:609:A:C8	3.00	0.49
1:A:761:G:C6	1:A:762:C:C4	3.01	0.49
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.93	0.49
1:A:1025:U:H2'	1:A:1026:G:C8	2.47	0.49
1:A:1399:C:C2	1:A:1502:A:N6	2.81	0.49
1:A:33:A:H2'	1:A:34:C:C6	2.48	0.49
1:A:504:C:C2	1:A:542:G:C2	3.00	0.49
1:A:623:C:H2'	1:A:624:C:O4'	2.12	0.49
1:A:855:G:C2	1:A:856:C:C2	3.01	0.49
1:A:861:G:N2	1:A:862:C:C2	2.79	0.49
15:O:82:ILE:HA	15:O:87:ILE:HD12	1.93	0.49
1:A:1060:C:H2'	1:A:1061:G:H8	1.78	0.49
1:A:460:G:H1'	1:A:472:A:H61	1.78	0.49
1:A:550:G:H2'	1:A:551:U:C6	2.46	0.49
1:A:767:A:H2'	1:A:768:A:C8	2.48	0.49
1:A:823:G:N2	1:A:824:C:C2	2.80	0.49
1:A:825:G:H1	1:A:875:C:H42	1.61	0.49
3:C:116:VAL:O	3:C:120:VAL:HG23	2.12	0.49
8:H:12:ARG:HA	8:H:15:ASN:ND2	2.22	0.49
9:I:55:ALA:HB1	9:I:59:PHE:HD2	1.77	0.49
17:Q:38:ARG:HE	17:Q:38:ARG:HA	1.77	0.49
1:A:1000:U:C3'	1:A:1000:U:C6	2.96	0.49
1:A:1114:C:C2	1:A:1187:G:C2	3.01	0.49
1:A:939:G:H1'	1:A:1375:A:C2	2.48	0.49
1:A:621:A:C6	1:A:622:A:C6	3.01	0.49
1:A:738:C:H5''	6:F:69:GLU:HB3	1.95	0.49
8:H:87:SER:HB2	8:H:133:LEU:O	2.13	0.49
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.95	0.49
1:A:1351:U:H2'	1:A:1352:C:H6	1.76	0.49
13:M:45:VAL:HA	13:M:48:LEU:HD12	1.94	0.49
1:A:1189:C:H5'	14:N:58:LYS:NZ	2.28	0.49
1:A:1276:G:H2'	1:A:1277:C:O4'	2.12	0.49
1:A:1347:G:C4	1:A:1373:G:C6	3.01	0.49
1:A:303:A:H2'	1:A:304:U:H6	1.77	0.49
1:A:511:C:HO2'	1:A:512:U:H6	1.58	0.49
1:A:769:G:N2	1:A:770:C:C2	2.81	0.49
16:P:12:LYS:C	16:P:14:ASN:H	2.16	0.49
25:Z:22:G:N2	25:Z:23:C:C2	2.80	0.49
1:A:954:G:H21	1:A:1227:A:H62	1.60	0.49
1:A:1281:U:H3	10:J:5:ARG:HH12	1.59	0.49
1:A:1347:G:H8	9:I:107:ARG:O	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1371:G:H2'	1:A:1372:U:H6	1.77	0.49
1:A:1464:G:N1	1:A:1465:C:N4	2.61	0.49
1:A:1484:C:H2'	1:A:1485:U:O4'	2.13	0.49
1:A:636:U:H2'	1:A:637:G:C8	2.48	0.49
4:D:8:VAL:HG13	4:D:9:CYS:N	2.27	0.49
7:G:54:THR:O	7:G:56:GLN:N	2.44	0.49
11:K:79:SER:HA	11:K:104:GLN:HB3	1.95	0.49
1:A:1464:G:C2	1:A:1465:C:N3	2.81	0.49
1:A:232:G:H2'	1:A:233:C:H6	1.77	0.49
1:A:460:G:H1'	1:A:472:A:N6	2.28	0.49
1:A:514:C:H2'	1:A:515:G:C8	2.48	0.49
1:A:734:G:C2	1:A:735:C:C2	3.01	0.49
1:A:974:A:H4'	1:A:975:A:H3'	1.93	0.49
22:W:10:GLU:HG2	22:W:54:VAL:HG22	1.95	0.49
1:A:1057:G:H2'	1:A:1058:G:H8	1.78	0.49
1:A:236:G:C2	1:A:237:C:C2	3.01	0.49
1:A:610:G:C4	1:A:611:A:C8	3.01	0.49
1:A:67:C:H2'	1:A:68:G:C8	2.48	0.49
1:A:883:C:H2'	1:A:884:U:C6	2.48	0.49
2:B:63:MET:HG3	2:B:64:ARG:HH11	1.78	0.49
20:T:89:ARG:O	20:T:93:GLU:HG2	2.13	0.49
1:A:1001:A:C6	1:A:1001(A):G:C6	3.01	0.48
1:A:1233:G:C6	1:A:1234:C:N4	2.81	0.48
1:A:1347:G:C2'	1:A:1348:U:OP2	2.61	0.48
1:A:187:C:N3	20:T:105:SER:HB2	2.28	0.48
1:A:355:C:H2'	1:A:356:A:O4'	2.13	0.48
1:A:443:C:C2	1:A:492:G:C2	3.00	0.48
1:A:427:U:O2'	1:A:541:G:OP1	2.30	0.48
1:A:682:G:H2'	1:A:683:G:O4'	2.13	0.48
1:A:942:G:C2	1:A:1342:C:O2	2.66	0.48
1:A:962:C:H2'	1:A:963:G:O4'	2.13	0.48
5:E:103:GLY:O	5:E:106:PRO:HD2	2.12	0.48
6:F:97:PHE:HB2	18:R:32:ARG:CZ	2.43	0.48
10:J:65:LEU:HD23	14:N:56:VAL:HG22	1.95	0.48
18:R:37:VAL:HG21	18:R:78:LEU:HD22	1.95	0.48
1:A:1087:G:H2'	1:A:1088:G:H8	1.77	0.48
1:A:1222:G:OP2	1:A:1322:C:C5	2.66	0.48
1:A:253:U:H2'	1:A:254:G:H8	1.78	0.48
1:A:373:A:H2'	1:A:374:A:C8	2.44	0.48
1:A:987:G:H2'	1:A:988:G:H8	1.76	0.48
3:C:29:TYR:C	3:C:29:TYR:CD1	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:8:ARG:HD3	22:W:56:GLU:HG3	1.96	0.48
1:A:1063:C:H2'	1:A:1064:G:N7	2.29	0.48
1:A:1074:G:C6	1:A:1075:C:C4	3.02	0.48
1:A:146:G:H2'	1:A:147:G:H8	1.78	0.48
1:A:1502:A:H2'	1:A:1504:G:N7	2.27	0.48
1:A:473:G:OP1	16:P:81:ARG:NH1	2.46	0.48
1:A:632:A:H2'	1:A:633:G:O4'	2.13	0.48
1:A:639:G:H2'	1:A:640:A:C8	2.48	0.48
1:A:778:G:C6	1:A:779:C:C4	3.02	0.48
16:P:81:ARG:NH1	16:P:81:ARG:HB2	2.27	0.48
1:A:309:G:H2'	1:A:310:G:H8	1.77	0.48
1:A:874:G:N1	1:A:875:C:C4	2.81	0.48
1:A:942:G:C6	1:A:1342:C:N3	2.81	0.48
6:F:75:LEU:O	6:F:79:LEU:HG	2.13	0.48
1:A:522:C:H41	12:L:53:ARG:NH2	2.10	0.48
24:Y:36:A:H61	25:Z:37:A:N6	2.10	0.48
1:A:1457:G:C2	1:A:1458:G:H1'	2.48	0.48
1:A:392:G:H2'	1:A:393:A:H8	1.74	0.48
1:A:633:G:H2'	1:A:634:C:C6	2.49	0.48
1:A:792:A:C6	1:A:794:A:C6	3.02	0.48
8:H:103:VAL:HG21	8:H:110:ALA:HB2	1.96	0.48
1:A:881:G:P	12:L:12:ARG:HH22	2.36	0.48
1:A:1241:G:C2	1:A:1242:C:C4	3.01	0.48
1:A:1245:A:H2'	1:A:1246:C:C6	2.48	0.48
1:A:1366:C:H2'	1:A:1367:C:C6	2.49	0.48
1:A:555:C:H2'	1:A:556:C:C6	2.48	0.48
12:L:102:ARG:HB2	12:L:120:TYR:O	2.13	0.48
23:X:9:GLU:HG2	23:X:35:LEU:CD2	2.43	0.48
1:A:1164:G:N2	1:A:1165:C:C2	2.81	0.48
1:A:1369:C:H2'	1:A:1370:G:O4'	2.14	0.48
1:A:1464:G:C6	1:A:1465:C:N4	2.82	0.48
1:A:1487:G:H2'	1:A:1488:G:C8	2.48	0.48
1:A:512:U:H2'	1:A:513:C:C6	2.49	0.48
2:B:29:ALA:HA	2:B:32:ILE:HD12	1.96	0.48
12:L:9:GLN:HG3	12:L:12:ARG:HH21	1.79	0.48
25:Z:22:G:H8	25:Z:22:G:O5'	1.96	0.48
1:A:199:G:C2	1:A:219:C:N3	2.81	0.48
1:A:7:G:H5'	1:A:298:A:O4'	2.13	0.48
1:A:653:A:C4	8:H:56:LYS:HG2	2.48	0.48
23:X:157:LEU:HD22	25:Z:27:U:H5''	1.94	0.48
1:A:47:C:C6	1:A:365:U:H2'	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:G:H2'	1:A:549:C:C6	2.49	0.48
4:D:83:SER:HA	4:D:89:THR:CG2	2.44	0.48
7:G:65:ALA:HB1	7:G:127:ALA:CB	2.43	0.48
17:Q:64:PRO:HA	17:Q:70:ARG:HG3	1.95	0.48
20:T:45:GLN:HA	20:T:91:LEU:HD22	1.95	0.48
24:Y:36:A:C6	25:Z:37:A:N1	2.82	0.48
1:A:1351:U:H2'	1:A:1352:C:C6	2.48	0.48
1:A:1481:U:H2'	1:A:1482:G:O4'	2.14	0.48
1:A:289:G:N2	1:A:290:C:C2	2.82	0.48
1:A:575:G:H4'	1:A:576:G:O5'	2.13	0.48
5:E:148:VAL:O	5:E:152:ARG:HG2	2.13	0.48
20:T:53:LEU:HD21	20:T:104:LEU:HD12	1.96	0.48
1:A:1078:U:H2'	1:A:1079:G:O4'	2.13	0.47
1:A:1162:C:C2	1:A:1175:G:C2	3.02	0.47
1:A:289:G:C6	1:A:290:C:N4	2.82	0.47
1:A:919:A:H2'	1:A:920:U:C6	2.49	0.47
9:I:33:PHE:HZ	9:I:46:ALA:HB3	1.79	0.47
23:X:94:ILE:HG22	23:X:136:ILE:HD13	1.96	0.47
1:A:1099:G:C2	1:A:1100:C:O2	2.67	0.47
1:A:1053:G:C2	1:A:1199:U:C4	3.02	0.47
1:A:230:G:O2'	16:P:25:ARG:NH2	2.47	0.47
7:G:22:LEU:HB3	7:G:62:PHE:HZ	1.78	0.47
1:A:1286:A:H2'	1:A:1287:A:H4'	1.96	0.47
1:A:384:G:H2'	1:A:385:C:C6	2.49	0.47
4:D:64:LEU:HD12	4:D:198:VAL:HG21	1.97	0.47
6:F:7:ASN:ND2	6:F:62:TRP:HD1	2.13	0.47
13:M:23:TYR:HE1	13:M:70:LEU:HB3	1.80	0.47
25:Z:18:G:HO2'	25:Z:57:A:H2	1.56	0.47
1:A:1074:G:C2	1:A:1075:C:C2	3.02	0.47
1:A:1312:G:H2'	1:A:1313:U:C6	2.49	0.47
1:A:1355:G:H2'	1:A:1356:G:H8	1.79	0.47
1:A:829:G:H8	1:A:829:G:H5''	1.78	0.47
7:G:65:ALA:CB	7:G:127:ALA:HB3	2.44	0.47
20:T:54:LYS:HA	20:T:57:ARG:HD3	1.96	0.47
23:X:71:MET:O	23:X:75:GLU:HG2	2.15	0.47
24:Y:21:G:H2'	24:Y:22:G:H8	1.78	0.47
1:A:1419:G:C2	1:A:1420:C:C2	3.02	0.47
1:A:513:C:H2'	1:A:514:C:C6	2.50	0.47
1:A:629:G:H2'	1:A:630:G:O4'	2.15	0.47
1:A:690:G:H2'	1:A:691:G:O4'	2.14	0.47
1:A:878:G:H2'	1:A:879:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:A:H5'	5:E:101:ILE:HG22	1.97	0.47
4:D:29:PRO:HB3	4:D:35:ARG:CZ	2.44	0.47
4:D:80:GLU:HB3	4:D:84:LYS:NZ	2.30	0.47
8:H:88:LYS:HB2	8:H:91:ARG:HB3	1.97	0.47
9:I:46:ALA:HA	9:I:78:LYS:HB2	1.97	0.47
12:L:7:ILE:HA	12:L:10:LEU:HD12	1.96	0.47
1:A:1106:G:N1	1:A:1107:C:C4	2.82	0.47
1:A:41:G:H2'	1:A:42:G:C8	2.49	0.47
4:D:200:GLU:HG2	4:D:201:GLN:N	2.29	0.47
1:A:750:G:H1'	15:O:23:GLY:H	1.80	0.47
13:M:84:ILE:HD12	19:S:74:PHE:HE1	1.80	0.47
1:A:1046:A:H3'	1:A:1047:G:C8	2.45	0.47
1:A:1057:G:H2'	1:A:1058:G:C8	2.49	0.47
1:A:1370:G:C2	1:A:1371:G:N7	2.83	0.47
1:A:562:C:N4	1:A:884:U:H2'	2.29	0.47
5:E:76:ILE:HG13	5:E:142:LEU:HD21	1.96	0.47
1:A:1470:G:H2'	1:A:1471:G:O4'	2.15	0.47
22:W:37:SER:HB3	22:W:40:MET:HG3	1.97	0.47
23:X:56:VAL:CG1	25:Z:19:G:O6	2.62	0.47
24:Y:21:G:H2'	24:Y:22:G:C8	2.49	0.47
1:A:1387:G:C6	1:A:1388:C:N4	2.83	0.47
1:A:1457:G:C5	1:A:1458:G:C8	3.03	0.47
1:A:448:A:OP2	1:A:485:G:N2	2.48	0.47
1:A:670:G:H1	1:A:736:C:N4	2.09	0.47
2:B:185:ILE:HG13	2:B:199:TYR:HB2	1.97	0.47
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.50	0.47
1:A:967:C:O2'	9:I:128:ARG:NH2	2.47	0.47
20:T:12:ALA:O	20:T:15:ARG:HB2	2.15	0.47
1:A:1129:C:N4	1:A:1134:G:N7	2.62	0.47
1:A:568:G:H2'	1:A:569:C:C6	2.49	0.47
1:A:673:G:H2'	1:A:674:G:C8	2.49	0.47
1:A:895:G:H1	1:A:904:C:N4	2.10	0.47
1:A:979:C:H41	1:A:1360:A:N6	2.13	0.47
15:O:74:ASP:HA	15:O:75:PRO:HD3	1.84	0.47
1:A:1328:C:H2'	1:A:1329:A:H8	1.79	0.47
1:A:1334:G:O5'	1:A:1334:G:H8	1.98	0.47
1:A:351:G:H4'	1:A:352:C:OP1	2.15	0.47
1:A:473:G:H5''	16:P:81:ARG:NH2	2.30	0.47
1:A:588:G:N1	1:A:589:C:C4	2.83	0.47
4:D:9:CYS:SG	4:D:22:LYS:HG2	2.55	0.47
5:E:115:VAL:HG11	5:E:118:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:107:ALA:HB3	13:M:111:LYS:HD2	1.97	0.47
13:M:91:ARG:HG3	13:M:98:VAL:HG13	1.96	0.47
25:Z:22:G:OP2	25:Z:46:G7M:C2	2.63	0.47
1:A:1347:G:O2'	1:A:1348:U:P	2.73	0.46
1:A:235:C:H2'	1:A:236:G:H8	1.81	0.46
1:A:316:G:H1	1:A:337:C:H42	1.61	0.46
1:A:739:C:O2'	15:O:42:HIS:ND1	2.43	0.46
1:A:743:U:H2'	1:A:744:C:H6	1.77	0.46
12:L:53:ARG:HH11	12:L:53:ARG:HG2	1.80	0.46
20:T:33:ILE:HG13	20:T:62:LEU:HD22	1.96	0.46
1:A:1067:A:H1'	1:A:1068:G:O4'	2.14	0.46
1:A:1075:C:H4'	1:A:1101:A:N6	2.30	0.46
1:A:1099:G:C6	1:A:1100:C:C2	3.03	0.46
1:A:1251:A:H2'	1:A:1252:A:C8	2.49	0.46
1:A:1309:G:C6	1:A:1329:A:C6	3.03	0.46
1:A:27:G:H2'	1:A:28:G:O4'	2.14	0.46
1:A:319:G:N2	1:A:320:C:C2	2.83	0.46
1:A:486:U:C2	1:A:487:A:C8	3.04	0.46
1:A:761:G:H2'	1:A:762:C:C6	2.50	0.46
1:A:778:G:C2	1:A:779:C:C2	3.03	0.46
1:A:864:A:C3'	1:A:865:A:C8	2.98	0.46
1:A:865:A:P	1:A:865:A:H8	2.38	0.46
1:A:947:G:H2'	1:A:948:C:C6	2.50	0.46
3:C:184:TYR:HE1	3:C:186:PHE:HB2	1.80	0.46
5:E:70:PRO:HG2	5:E:142:LEU:HD22	1.97	0.46
7:G:78:ARG:NH1	7:G:154:TYR:HB3	2.30	0.46
15:O:77:ARG:HG2	15:O:77:ARG:HH11	1.79	0.46
19:S:36:ARG:HB2	19:S:72:GLY:HA3	1.97	0.46
1:A:1419:G:C6	1:A:1420:C:C4	3.03	0.46
1:A:17:U:H2'	1:A:18:C:C5	2.50	0.46
1:A:500:G:C2	1:A:501:C:C2	3.04	0.46
1:A:509:A:H4'	1:A:510:A:OP1	2.15	0.46
2:B:209:ARG:HD3	2:B:239:VAL:HG11	1.97	0.46
7:G:65:ALA:CB	7:G:127:ALA:CB	2.94	0.46
1:A:112:G:H1	1:A:315:A:H61	1.63	0.46
1:A:116:A:H2'	1:A:117:G:H8	1.80	0.46
1:A:1256:A:C8	3:C:27:LYS:NZ	2.78	0.46
1:A:1312:G:C2	1:A:1326:C:C2	3.03	0.46
1:A:599:C:H4'	8:H:130:GLY:C	2.36	0.46
1:A:734:G:C6	1:A:735:C:C4	3.03	0.46
1:A:661:G:N2	1:A:745:C:C2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.97	0.46
3:C:26:LYS:HD3	14:N:36:PHE:CE1	2.46	0.46
8:H:46:LYS:HB3	8:H:62:TYR:HB3	1.97	0.46
9:I:50:LEU:HB3	9:I:56:LEU:H	1.79	0.46
1:A:1178:G:OP2	9:I:97:LYS:HD2	2.15	0.46
1:A:146:G:H2'	1:A:147:G:C8	2.50	0.46
1:A:320:C:H2'	1:A:321:A:O4'	2.15	0.46
1:A:398:C:H2'	1:A:399:G:C8	2.48	0.46
1:A:416:G:C6	1:A:417:C:C4	3.03	0.46
1:A:834:C:C2	1:A:853:G:C2	3.04	0.46
5:E:80:ILE:HG23	8:H:104:ARG:HH12	1.81	0.46
16:P:8:ARG:HE	16:P:15:PRO:HB3	1.80	0.46
25:Z:33:U:C6	25:Z:35:A:OP2	2.68	0.46
1:A:1288:A:N1	1:A:1371:G:H1'	2.31	0.46
1:A:1306:A:N6	1:A:1331:G:O4'	2.49	0.46
1:A:603:U:H2'	1:A:604:G:H8	1.80	0.46
1:A:914:A:H2'	1:A:915:A:H8	1.80	0.46
8:H:10:LEU:HA	8:H:13:ILE:HD12	1.97	0.46
9:I:89:ASN:C	9:I:91:ASP:H	2.19	0.46
16:P:19:ILE:O	16:P:36:ILE:HG13	2.16	0.46
25:Z:64:G:C6	25:Z:65:C:C4	3.03	0.46
1:A:1087:G:H2'	1:A:1088:G:C8	2.51	0.46
1:A:1298:C:OP1	1:A:1299:A:C8	2.69	0.46
1:A:682:G:H1	1:A:708:C:H42	1.64	0.46
1:A:90:U:H2'	1:A:91:C:C5	2.49	0.46
1:A:942:G:N1	1:A:1342:C:C2	2.82	0.46
24:Y:39:U:O4	25:Z:35:A:C1'	2.63	0.46
25:Z:64:G:C2	25:Z:65:C:C2	3.04	0.46
1:A:1076:C:N3	1:A:1082:G:C2	2.84	0.46
1:A:1297:C:H1'	1:A:1298:C:H5	1.79	0.46
1:A:1537:U:N3	24:Y:28:A:N6	2.63	0.46
1:A:36:C:H4'	12:L:117:ARG:HH21	1.81	0.46
1:A:519:C:H2'	1:A:520:A:O4'	2.16	0.46
1:A:527:G:N2	1:A:528:C:C2	2.84	0.46
1:A:800:G:H2'	1:A:801:U:C5	2.51	0.46
1:A:799:G:H3'	1:A:800:G:H8	1.80	0.46
1:A:918:A:N6	1:A:919:A:N6	2.64	0.46
1:A:920:U:H2'	1:A:921:U:H6	1.71	0.46
14:N:50:LYS:HD2	14:N:52:GLN:HE21	1.81	0.46
1:A:1017:G:C2	1:A:1018:C:C2	3.03	0.46
1:A:1274:G:H2'	1:A:1275:A:C8	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1493:A:H4'	1:A:1494:G:C5'	2.45	0.46
1:A:1517:G:H2'	1:A:1518:A:O4'	2.15	0.46
1:A:321:A:H2'	1:A:322:C:C6	2.51	0.46
1:A:402:G:N2	1:A:403:C:C2	2.83	0.46
4:D:158:ILE:HD12	4:D:158:ILE:H	1.80	0.46
4:D:67:ILE:HG21	4:D:196:LEU:HD13	1.97	0.46
3:C:23:TYR:HD1	10:J:11:PHE:HZ	1.64	0.46
10:J:6:ILE:HD11	10:J:23:ILE:HG21	1.97	0.46
15:O:50:HIS:O	15:O:53:HIS:HB3	2.16	0.46
20:T:71:THR:HB	20:T:72:LEU:HG	1.97	0.46
24:Y:28:A:C6	24:Y:29:G:C6	3.04	0.46
1:A:105:G:C2	1:A:106:C:C2	3.04	0.46
1:A:1187:G:H2'	1:A:1188:A:C8	2.51	0.46
1:A:1430:C:C2	1:A:1471:G:N2	2.83	0.46
1:A:257:G:H1	1:A:269:C:N4	2.13	0.46
1:A:522:C:OP2	12:L:69:TYR:OH	2.29	0.46
1:A:524:G:H2'	1:A:525:C:C6	2.51	0.46
1:A:524:G:C5	1:A:525:C:N4	2.84	0.46
1:A:544:G:C2	1:A:545:C:C2	3.04	0.46
1:A:999:C:N3	1:A:1043:C:N3	2.63	0.46
2:B:196:LEU:HG	8:H:74:PRO:HG3	1.97	0.46
2:B:15:VAL:HG11	2:B:209:ARG:HB3	1.98	0.46
8:H:82:HIS:CE1	8:H:84:ARG:HB2	2.51	0.46
1:A:1539:C:N3	24:Y:26:G:N2	2.47	0.45
1:A:456:C:C2	1:A:476:G:N2	2.84	0.45
1:A:939:G:H2'	1:A:940:C:C6	2.51	0.45
8:H:13:ILE:O	8:H:17:THR:HG23	2.16	0.45
25:Z:52:G:C2	25:Z:63:G:C2	3.04	0.45
1:A:1303:C:H42	1:A:1334:G:H1	1.63	0.45
1:A:447:G:H3'	1:A:485:G:H22	1.81	0.45
1:A:765:G:N1	1:A:812:C:H2'	2.31	0.45
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.98	0.45
1:A:1190:G:OP1	3:C:5:ILE:HG13	2.16	0.45
4:D:50:ARG:HH21	5:E:10:MET:HB3	1.82	0.45
5:E:50:GLU:HG2	5:E:52:PRO:HD2	1.98	0.45
6:F:22:GLU:HA	6:F:25:ILE:HD12	1.96	0.45
8:H:48:TYR:HA	8:H:60:ARG:O	2.15	0.45
1:A:1241:G:N1	1:A:1242:C:C4	2.85	0.45
1:A:1387:G:H2'	1:A:1388:C:C6	2.50	0.45
1:A:200:G:C2	1:A:201:C:O2	2.70	0.45
1:A:250:A:H4'	1:A:251:G:O5'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:G:H2'	1:A:559:A:C2	2.52	0.45
5:E:51:VAL:HG12	5:E:52:PRO:HD3	1.97	0.45
9:I:9:ARG:HD2	9:I:104:ARG:HH21	1.81	0.45
11:K:84:VAL:HG11	11:K:95:ILE:HD11	1.98	0.45
24:Y:37:U:H2'	24:Y:38:G:C8	2.52	0.45
25:Z:21:A:N6	25:Z:46:G7M:O2'	2.50	0.45
1:A:1147:C:O2	9:I:16:ARG:NH1	2.50	0.45
1:A:1324:A:H2'	1:A:1325:C:O4'	2.16	0.45
1:A:1517:G:H2'	1:A:1518:A:C8	2.52	0.45
1:A:276:G:H2'	1:A:277:C:C6	2.51	0.45
1:A:323:U:O5'	1:A:323:U:H6	2.00	0.45
1:A:41:G:H1	1:A:401:C:N4	2.14	0.45
1:A:447:G:H2'	1:A:485:G:N2	2.31	0.45
1:A:51:A:H4'	1:A:52:G:O5'	2.16	0.45
1:A:577:G:C2	1:A:578:C:C2	3.04	0.45
1:A:70:G:C2	1:A:100:C:C2	3.04	0.45
1:A:724:G:H8	1:A:724:G:O5'	2.00	0.45
1:A:76:C:N4	1:A:77:G:O6	2.49	0.45
4:D:76:ARG:HD2	4:D:207:TYR:CE1	2.51	0.45
5:E:37:ARG:HH12	5:E:111:GLU:HB3	1.80	0.45
1:A:363:A:OP2	12:L:34:ARG:HG3	2.16	0.45
1:A:1311:G:N7	19:S:2:PRO:N	2.64	0.45
23:X:34:ALA:HB1	23:X:45:LEU:HD11	1.99	0.45
25:Z:37:A:H3'	25:Z:38:A:C8	2.51	0.45
1:A:1168:A:H2'	1:A:1169:A:C8	2.52	0.45
1:A:391:G:C6	1:A:392:G:C5	3.05	0.45
1:A:1002:G:O6	1:A:1039:C:N3	2.49	0.45
1:A:1162:C:N3	1:A:1175:G:C2	2.84	0.45
1:A:941:G:H1	1:A:1342:C:H42	1.65	0.45
1:A:1508:G:H2'	1:A:1509:C:C6	2.52	0.45
1:A:198:G:H2'	1:A:199:G:O4'	2.17	0.45
1:A:43:C:H2'	1:A:44:G:H8	1.81	0.45
1:A:626:U:H2'	1:A:627:G:C8	2.51	0.45
2:B:96:ARG:CG	2:B:98:LEU:HG	2.47	0.45
7:G:124:LEU:HD23	7:G:124:LEU:HA	1.90	0.45
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.17	0.45
25:Z:7:G:P	25:Z:16:C:H42	2.40	0.45
25:Z:21:A:N6	25:Z:48:C:C6	2.85	0.45
1:A:1219:U:OP1	14:N:19:ARG:NH2	2.49	0.45
1:A:242:C:C2	1:A:285:G:N2	2.85	0.45
1:A:544:G:C6	1:A:545:C:C4	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:C:H1'	1:A:749:C:H5	1.81	0.45
1:A:909:A:H2'	1:A:910:C:O4'	2.16	0.45
2:B:130:ARG:NH2	3:C:207:VAL:CG2	2.80	0.45
5:E:117:ASP:O	5:E:118:ILE:HG23	2.16	0.45
6:F:100:ASN:HD22	18:R:23:LYS:HG2	1.81	0.45
17:Q:67:LYS:O	17:Q:68:ARG:HG3	2.15	0.45
25:Z:47:U:H4'	25:Z:48:C:O5'	2.17	0.45
25:Z:67:C:H2'	25:Z:68:C:H6	1.81	0.45
1:A:1217:C:H2'	1:A:1218:C:O4'	2.15	0.45
1:A:450:G:N7	1:A:481:G:C6	2.85	0.45
1:A:72:C:C2'	1:A:73:G:H5''	2.43	0.45
1:A:874:G:C2	1:A:875:C:C2	3.05	0.45
5:E:148:VAL:HG11	8:H:107:LEU:CD2	2.47	0.45
17:Q:59:ILE:HG22	17:Q:71:PHE:HB3	1.98	0.45
18:R:59:SER:HB3	18:R:62:GLU:HB2	1.98	0.45
23:X:99:TYR:HE1	23:X:140:VAL:HG22	1.82	0.45
1:A:1001(A):G:C6	1:A:1002:G:O6	2.70	0.45
1:A:1096:C:H2'	1:A:1097:C:C6	2.52	0.45
1:A:1266:G:C2	1:A:1270:C:N3	2.85	0.45
1:A:129(A):G:O2'	1:A:189(F):U:H5''	2.17	0.45
1:A:190:U:H2'	1:A:191:G:C8	2.52	0.45
1:A:416:G:C2	1:A:417:C:C2	3.04	0.45
1:A:998:G:N1	1:A:999:C:C4	2.85	0.45
8:H:41:ARG:HG2	8:H:42:GLU:N	2.31	0.45
10:J:33:GLN:HB3	10:J:75:ILE:HD12	1.98	0.45
17:Q:92:ARG:HA	17:Q:95:TYR:CD2	2.51	0.45
1:A:1255:G:O2'	1:A:1258:G:H1'	2.17	0.45
1:A:1492:A:H3'	1:A:1493:A:H3'	1.99	0.45
1:A:1510:U:H2'	1:A:1511:G:C8	2.52	0.45
1:A:519:C:H4'	22:W:66:ARG:CZ	2.47	0.45
1:A:838:G:C2	1:A:849:C:C2	3.04	0.45
3:C:52:LEU:HA	3:C:70:VAL:HG12	1.99	0.45
10:J:79:ARG:NH1	10:J:82:ILE:HB	2.32	0.45
23:X:66:ARG:HD2	23:X:66:ARG:HA	1.93	0.45
1:A:1305:G:H22	1:A:1331:G:H1'	1.81	0.44
1:A:166:G:N1	1:A:167:G:C6	2.84	0.44
1:A:417:C:H42	1:A:418:C:N4	2.15	0.44
12:L:93:LEU:HA	12:L:94:PRO:HD3	1.79	0.44
1:A:1110:A:H2'	1:A:1111:A:O4'	2.17	0.44
1:A:1184:G:O5'	1:A:1184:G:H8	1.99	0.44
1:A:1508:G:C2	1:A:1509:C:C2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:G:N1	1:A:165:C:C2	2.85	0.44
1:A:189:G:C2	1:A:189(A):C:C2	3.05	0.44
1:A:262:A:H5''	20:T:76:ALA:HB2	2.00	0.44
1:A:394:G:N2	1:A:395:C:C2	2.85	0.44
1:A:557:G:C6	1:A:558:G:N1	2.85	0.44
1:A:947:G:C2	1:A:948:C:C2	3.05	0.44
3:C:67:THR:HA	3:C:102:ASN:HB2	1.99	0.44
5:E:145:LYS:O	5:E:148:VAL:HG12	2.16	0.44
10:J:50:ILE:HG22	10:J:52:GLY:H	1.80	0.44
1:A:1061:G:H1	1:A:1195:C:H42	1.66	0.44
1:A:1233:G:N2	1:A:1234:C:C2	2.86	0.44
1:A:354:G:C6	1:A:355:C:N4	2.85	0.44
1:A:491:G:H2'	1:A:492:G:H8	1.82	0.44
1:A:545:C:O2'	1:A:549:C:H5''	2.16	0.44
1:A:778:G:C6	1:A:779:C:C2	3.06	0.44
1:A:973:G:H3'	1:A:974:A:H5''	2.00	0.44
2:B:15:VAL:HG21	2:B:209:ARG:HG2	1.98	0.44
5:E:10:MET:HA	5:E:32:VAL:HG23	1.98	0.44
15:O:70:LEU:O	15:O:74:ASP:N	2.50	0.44
19:S:19:VAL:HG21	19:S:44:MET:HG2	1.99	0.44
25:Z:62:C:H2'	25:Z:63:G:C8	2.53	0.44
1:A:1263:C:N4	1:A:1264:C:N4	2.66	0.44
1:A:1339:A:H1'	25:Z:41:C:O2'	2.17	0.44
1:A:1468:A:H2'	1:A:1469:G:O4'	2.18	0.44
1:A:1536:C:N3	24:Y:29:G:N2	2.61	0.44
1:A:157:G:C6	1:A:165:C:N3	2.85	0.44
1:A:146:G:C2	1:A:177:C:N3	2.85	0.44
1:A:35:G:C6	1:A:36:C:N4	2.85	0.44
1:A:568:G:N2	1:A:569:C:C2	2.85	0.44
1:A:618:C:H4'	16:P:42:ARG:HH22	1.82	0.44
1:A:785:G:C5'	1:A:785:G:C8	3.00	0.44
10:J:43:ARG:HD3	10:J:43:ARG:HA	1.78	0.44
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.99	0.44
22:W:17:LEU:HB2	22:W:21:THR:O	2.18	0.44
1:A:149:A:H2'	1:A:150:C:C6	2.52	0.44
1:A:537:G:H2'	1:A:538:G:O4'	2.16	0.44
1:A:573:A:H2'	1:A:574:A:O4'	2.17	0.44
1:A:774:G:C2	1:A:806:C:C2	3.05	0.44
1:A:13:U:N3	1:A:915:A:N6	2.65	0.44
1:A:977:A:H3'	1:A:977:A:N3	2.32	0.44
2:B:127:ILE:H	2:B:127:ILE:HG13	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:77:LEU:HD13	12:L:107:ALA:HB2	1.99	0.44
20:T:49:ALA:O	20:T:53:LEU:HB2	2.18	0.44
24:Y:35:A:H4'	24:Y:36:A:OP2	2.16	0.44
25:Z:1:C:H2'	25:Z:2:G:C8	2.46	0.44
25:Z:20:U:O2	25:Z:20:U:H3'	2.16	0.44
1:A:119:A:H2'	1:A:240:C:H41	1.82	0.44
1:A:1048:G:H1	1:A:1209:C:N4	2.16	0.44
1:A:548:G:C2	1:A:549:C:C4	3.05	0.44
1:A:764:C:H2'	1:A:765:G:O4'	2.17	0.44
13:M:87:TYR:HD1	19:S:76:PRO:HB3	1.83	0.44
19:S:51:VAL:HG11	19:S:72:GLY:HA2	1.99	0.44
9:I:127:LYS:HG3	25:Z:32:OMC:OP2	2.18	0.44
1:A:1216:G:N2	1:A:1217:C:C2	2.85	0.44
1:A:189(B):C:H2'	1:A:189(C):C:C6	2.53	0.44
1:A:363:A:H2'	1:A:364:A:C8	2.53	0.44
1:A:554:C:H2'	1:A:555:C:H6	1.83	0.44
1:A:939:G:H1	1:A:1344:C:N4	2.13	0.44
2:B:19:HIS:CD2	2:B:20:GLU:HG2	2.53	0.44
2:B:221:LEU:HD12	2:B:221:LEU:HA	1.76	0.44
14:N:42:ILE:H	14:N:42:ILE:HD12	1.83	0.44
25:Z:7:G:C6	25:Z:49:G:N7	2.86	0.44
1:A:1029:C:H2'	1:A:1030:C:C6	2.53	0.44
1:A:999:C:C2	1:A:1043:C:O2	2.69	0.44
1:A:1142:G:H2'	1:A:1143:G:O4'	2.17	0.44
1:A:1222:G:OP2	1:A:1322:C:H5	2.01	0.44
1:A:276:G:C2	1:A:277:C:C2	3.05	0.44
1:A:41:G:H2'	1:A:42:G:H8	1.83	0.44
1:A:729:A:H2'	1:A:730:G:C8	2.53	0.44
1:A:44:G:OP2	16:P:12:LYS:HD2	2.18	0.44
1:A:994:A:N7	1:A:1216:G:H4'	2.33	0.44
1:A:500:G:H2'	1:A:501:C:H6	1.82	0.44
1:A:683:G:C2	1:A:708:C:N3	2.86	0.44
1:A:769:G:C2	1:A:770:C:C2	3.05	0.44
1:A:881:G:C2	1:A:882:C:C2	3.06	0.44
2:B:112:VAL:HG23	2:B:149:LEU:HD23	1.99	0.44
2:B:90:MET:HA	2:B:91:PRO:HD2	1.78	0.44
5:E:12:LEU:HD13	5:E:13:ILE:H	1.83	0.44
5:E:43:LEU:HD22	5:E:136:MET:HG3	2.00	0.44
1:A:1000:U:H6	1:A:1000:U:H3'	1.79	0.43
1:A:1048:G:H2'	1:A:1050:G:H8	1.81	0.43
1:A:189(B):C:C2	1:A:189(J):G:N2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:C:C2	1:A:286:G:N2	2.86	0.43
1:A:568:G:C2	1:A:569:C:N3	2.86	0.43
3:C:155:GLY:HA2	3:C:163:ALA:HB1	1.99	0.43
7:G:80:VAL:HG23	7:G:85:TYR:CD2	2.53	0.43
10:J:50:ILE:HG12	10:J:57:LYS:HA	2.00	0.43
10:J:51:ARG:HA	14:N:45:ARG:HD2	2.00	0.43
11:K:109:VAL:HG13	18:R:84:LYS:HB3	1.99	0.43
1:A:1347:G:O2'	1:A:1348:U:OP2	2.32	0.43
1:A:1504:G:H4'	1:A:1505:G:O5'	2.18	0.43
1:A:31:G:O2'	1:A:48:C:N4	2.52	0.43
1:A:903:G:C2	1:A:904:C:C2	3.05	0.43
1:A:947:G:H2'	1:A:948:C:O4'	2.18	0.43
4:D:108:LEU:HB3	4:D:110:PHE:CD1	2.54	0.43
1:A:1423:G:N2	1:A:1424:C:C2	2.86	0.43
1:A:1520:G:H2'	1:A:1521:G:C8	2.53	0.43
1:A:189:G:C6	1:A:189(A):C:C4	3.07	0.43
1:A:585:G:C2	1:A:586:C:C2	3.06	0.43
1:A:861:G:N1	1:A:862:C:C4	2.86	0.43
1:A:872:A:C8	1:A:874:G:C8	3.07	0.43
2:B:16:HIS:NE2	2:B:214:ILE:HD11	2.33	0.43
15:O:15:PHE:CE2	15:O:84:LYS:HB3	2.52	0.43
17:Q:46:ASP:HA	17:Q:47:PRO:HD2	1.90	0.43
18:R:53:ARG:HH21	18:R:60:ALA:CB	2.23	0.43
1:A:1263:C:C4	1:A:1264:C:N4	2.86	0.43
1:A:19:C:H5''	5:E:86:ALA:HB3	1.99	0.43
1:A:28:G:C2	1:A:556:C:N3	2.86	0.43
1:A:378:G:C6	1:A:379:C:N4	2.87	0.43
1:A:89:C:H2'	1:A:90:U:O4'	2.18	0.43
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.99	0.43
5:E:76:ILE:HG22	5:E:93:PRO:HB3	2.00	0.43
3:C:19:GLU:HB2	14:N:52:GLN:HA	2.00	0.43
25:Z:28:C:C2	25:Z:43:A:C2	3.06	0.43
1:A:1009:G:C6	1:A:1021:G:C5	3.07	0.43
1:A:1311:G:OP2	19:S:3:ARG:HG3	2.19	0.43
1:A:157:G:C2	1:A:165:C:O2	2.72	0.43
1:A:333:G:C2	1:A:334:C:C4	3.06	0.43
1:A:340:U:H2'	1:A:341:C:C6	2.53	0.43
1:A:548:G:C2	1:A:549:C:N3	2.86	0.43
1:A:893:C:O5'	1:A:893:C:H6	2.02	0.43
3:C:50:ALA:HB2	3:C:75:VAL:HB	1.99	0.43
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:C:H2'	1:A:458:C:C6	2.53	0.43
1:A:601:C:C2	1:A:638:G:C2	3.07	0.43
1:A:823:G:C2	1:A:824:C:C2	3.07	0.43
3:C:56:ASP:O	3:C:66:VAL:HA	2.19	0.43
1:A:564:C:C2	17:Q:31:LEU:HD11	2.53	0.43
1:A:1095:U:C4	1:A:1096:C:C4	3.06	0.43
1:A:1445:C:N3	1:A:1458:G:C2	2.86	0.43
1:A:306:G:C2	1:A:307:C:C2	3.06	0.43
16:P:20:VAL:HG23	16:P:35:LYS:HA	2.00	0.43
1:A:1024:G:O3'	1:A:1025:U:H4'	2.16	0.43
1:A:127:G:C2	1:A:235:C:N3	2.86	0.43
1:A:1302:U:H3'	1:A:1303:C:H5''	2.01	0.43
1:A:1402:C:H2'	1:A:1403:C:O4'	2.19	0.43
1:A:21:G:C2	1:A:22:G:C5	3.07	0.43
1:A:279:A:N3	1:A:281:G:N2	2.67	0.43
1:A:410:G:OP2	4:D:25:ARG:NE	2.44	0.43
1:A:542:G:N2	1:A:543:C:C2	2.87	0.43
1:A:821:G:C2	1:A:822:C:C2	3.07	0.43
2:B:17:PHE:HD1	2:B:18:GLY:H	1.67	0.43
2:B:79:ASP:HB3	2:B:238:LEU:HD23	2.01	0.43
12:L:23:LYS:O	12:L:97:ARG:NH1	2.51	0.43
15:O:53:HIS:HA	15:O:56:LEU:HD23	1.99	0.43
18:R:52:PRO:HD2	18:R:55:ARG:HB2	2.00	0.43
25:Z:22:G:N1	25:Z:23:C:C4	2.87	0.43
1:A:1198:G:H2'	1:A:1199:U:C6	2.54	0.43
1:A:1281:U:H4'	1:A:1282:C:OP2	2.19	0.43
1:A:1298:C:H4'	1:A:1299:A:C4	2.54	0.43
1:A:1305:G:C5'	21:V:4:GLY:HA3	2.49	0.43
1:A:1353:G:C6	1:A:1354:C:N4	2.87	0.43
1:A:1502:A:C2	1:A:1504:G:C4	3.06	0.43
1:A:287:U:H2'	1:A:288:A:C8	2.47	0.43
1:A:306:G:C6	1:A:307:C:C4	3.07	0.43
1:A:320:C:H2'	1:A:321:A:C8	2.54	0.43
1:A:518:C:O2'	1:A:519:C:OP2	2.29	0.43
1:A:820:U:N3	1:A:873:A:N7	2.67	0.43
10:J:24:VAL:HG21	10:J:37:PRO:HD3	2.00	0.43
20:T:74:LYS:HB2	20:T:75:ASN:H	1.49	0.43
22:W:13:VAL:HG22	22:W:24:VAL:HG22	2.01	0.43
23:X:167:PRO:HG2	23:X:170:VAL:HG22	2.01	0.43
1:A:1171:G:C6	1:A:1172:C:N4	2.87	0.43
1:A:1520:G:H2'	1:A:1521:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:G:H2'	1:A:23:C:C6	2.54	0.43
1:A:41:G:C6	1:A:402:G:C6	3.07	0.43
1:A:603:U:H2'	1:A:604:G:C8	2.54	0.43
1:A:620:C:N4	1:A:621:A:C6	2.87	0.43
1:A:628:G:H2'	1:A:629:G:H8	1.84	0.43
4:D:185:PHE:CZ	4:D:189:PRO:HD3	2.54	0.43
1:A:1343:G:OP1	9:I:125:TYR:HE2	2.02	0.43
9:I:13:ALA:HB2	9:I:68:GLY:HA3	2.01	0.43
17:Q:32:TYR:C	17:Q:34:LYS:H	2.22	0.43
1:A:1187:G:H3'	1:A:1188:A:C8	2.54	0.42
1:A:579:G:H2'	1:A:580:U:C6	2.54	0.42
1:A:679:C:N4	1:A:680:C:N4	2.67	0.42
5:E:79:GLU:HA	5:E:91:LEU:O	2.18	0.42
19:S:40:ILE:CD1	19:S:62:ILE:HD11	2.45	0.42
1:A:542:G:C2	1:A:543:C:C2	3.07	0.42
1:A:660:G:H1	1:A:745:C:N4	2.17	0.42
13:M:91:ARG:HD2	13:M:96:LEU:HD12	2.00	0.42
25:Z:51:C:N3	25:Z:63:G:N2	2.54	0.42
1:A:102:G:C2	1:A:103:C:C2	3.07	0.42
1:A:1076:C:C2	1:A:1082:G:C2	3.08	0.42
1:A:1279:A:H1'	1:A:1282:C:N4	2.34	0.42
1:A:1290:G:H5'	7:G:35:LYS:NZ	2.34	0.42
1:A:1468:A:H3'	1:A:1469:G:H8	1.82	0.42
1:A:515:G:C6	1:A:516:U:N3	2.87	0.42
1:A:585:G:C6	1:A:586:C:C4	3.07	0.42
1:A:774:G:C2	1:A:806:C:N3	2.88	0.42
1:A:874:G:C6	1:A:875:C:C4	3.07	0.42
1:A:877:C:H2'	1:A:878:G:C8	2.52	0.42
14:N:32:SER:HB3	14:N:41:ARG:HG2	2.02	0.42
1:A:1300:G:O2'	1:A:1303:C:N4	2.52	0.42
1:A:1526:G:C2	1:A:1527:C:C2	3.08	0.42
1:A:502:G:H2'	1:A:503:C:C6	2.55	0.42
1:A:545:C:N4	1:A:546:G:C6	2.87	0.42
1:A:866:C:C4	1:A:867:G:H1'	2.55	0.42
1:A:887:G:H2'	1:A:888:G:O4'	2.19	0.42
1:A:924:C:H2'	1:A:925:G:H8	1.80	0.42
1:A:96:U:H2'	1:A:97:G:H8	1.84	0.42
3:C:23:TYR:CD1	10:J:11:PHE:HZ	2.38	0.42
3:C:26:LYS:H	3:C:26:LYS:HG2	1.59	0.42
3:C:64:VAL:HG21	3:C:97:LYS:HD2	2.01	0.42
4:D:132:ARG:HD3	4:D:151:LYS:HZ2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:CYS:C	4:D:33:MET:N	2.71	0.42
8:H:95:VAL:HB	8:H:99:GLU:HB3	2.01	0.42
25:Z:21:A:C5	25:Z:48:C:C2	3.06	0.42
1:A:858:G:H3'	1:A:869:G:H1	1.85	0.42
1:A:966:G:C4	25:Z:34:C:H5'	2.54	0.42
10:J:4:ILE:HD11	10:J:77:PRO:HB3	2.02	0.42
19:S:80:TYR:CZ	19:S:81:ARG:HD3	2.54	0.42
23:X:17:ARG:HG3	23:X:28:ILE:HG13	2.02	0.42
1:A:1110:A:N6	1:A:1111:A:N1	2.67	0.42
1:A:1370:G:C5'	9:I:12:GLU:HG3	2.50	0.42
1:A:1387:G:C2	1:A:1388:C:C2	3.08	0.42
1:A:1494:G:C6	1:A:1495:U:C4	3.07	0.42
1:A:340:U:H2'	1:A:341:C:H6	1.84	0.42
1:A:370:C:H2'	1:A:371:G:C8	2.55	0.42
1:A:429:U:H1'	1:A:430:A:H5''	2.01	0.42
1:A:918:A:C6	1:A:919:A:C6	3.08	0.42
3:C:139:GLN:HE22	3:C:170:GLN:HE22	1.67	0.42
7:G:65:ALA:CA	7:G:127:ALA:HB1	2.48	0.42
18:R:31:LEU:O	18:R:69:THR:HG21	2.20	0.42
23:X:16:VAL:HG22	23:X:31:THR:HA	2.00	0.42
24:Y:32:A:H3'	24:Y:33:A:C5'	2.47	0.42
1:A:104:G:H4'	1:A:174:C:H5'	2.00	0.42
1:A:9:G:H2'	1:A:10:A:O4'	2.20	0.42
1:A:120:A:C5	1:A:122:G:C6	3.07	0.42
1:A:236:G:C6	1:A:237:C:C4	3.08	0.42
1:A:319:G:C2	1:A:320:C:C2	3.08	0.42
1:A:402:G:C2	1:A:403:C:C2	3.08	0.42
1:A:451:A:C6	1:A:480:U:H2'	2.54	0.42
1:A:721:G:H1'	1:A:722:A:C2	2.53	0.42
1:A:761:G:C5	1:A:762:C:C4	3.07	0.42
16:P:7:ALA:O	16:P:17:TYR:HA	2.20	0.42
23:X:95:ASP:HB3	23:X:96:GLU:H	1.74	0.42
25:Z:41:C:C2'	25:Z:42:G:O4'	2.67	0.42
25:Z:64:G:C5	25:Z:65:C:C4	3.07	0.42
1:A:1001:A:C2	1:A:1041:A:C6	3.08	0.42
1:A:19:C:H2'	1:A:20:U:H6	1.82	0.42
1:A:132:C:C4	1:A:231:G:N1	2.87	0.42
1:A:42:G:C2	1:A:43:C:C2	3.08	0.42
1:A:577:G:C6	1:A:578:C:C4	3.07	0.42
1:A:755:G:N1	1:A:756:C:C4	2.87	0.42
1:A:975:A:N6	1:A:1367:C:O4'	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3:ARG:HD2	4:D:118:ARG:CZ	2.50	0.42
5:E:78:HIS:NE2	5:E:142:LEU:HD23	2.35	0.42
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.95	0.42
25:Z:13:C:H2'	25:Z:14:A:H8	1.85	0.42
1:A:1103:C:C5'	2:B:98:LEU:HD13	2.50	0.42
1:A:1114:C:C2	1:A:1187:G:N2	2.88	0.42
1:A:1154:G:H2'	1:A:1155:G:C8	2.54	0.42
1:A:116:A:H2'	1:A:117:G:C8	2.54	0.42
1:A:262:A:H5'	20:T:74:LYS:HZ3	1.85	0.42
1:A:354:G:N1	1:A:355:C:C4	2.88	0.42
1:A:590:C:C2	1:A:650:G:C2	3.08	0.42
3:C:28:GLN:OE1	3:C:32:LEU:CG	2.68	0.42
1:A:429:U:P	4:D:36:ARG:HH12	2.42	0.42
8:H:85:ARG:HG3	8:H:85:ARG:HH11	1.85	0.42
12:L:7:ILE:H	12:L:7:ILE:HG12	1.40	0.42
19:S:12:ASP:HB3	19:S:14:HIS:HD2	1.81	0.42
1:A:1251:A:H2'	1:A:1252:A:O4'	2.19	0.42
1:A:1278:U:H5''	1:A:1279:A:O4'	2.19	0.42
1:A:1292:U:H2'	1:A:1293:G:C8	2.54	0.42
1:A:1368:G:N2	1:A:1369:C:C2	2.88	0.42
1:A:1347:G:HO2'	1:A:1373:G:H1	1.66	0.42
1:A:1513:A:C6	1:A:1523:G:C6	3.08	0.42
1:A:289:G:C2	1:A:290:C:C2	3.07	0.42
1:A:348:G:H2'	1:A:349:A:H8	1.85	0.42
1:A:433:C:H2'	1:A:434:U:C6	2.55	0.42
1:A:657:G:H4'	15:O:28:GLN:HG3	2.02	0.42
1:A:863:U:H2'	1:A:865:A:OP2	2.19	0.42
1:A:77:G:H1	1:A:92:C:N4	2.18	0.42
3:C:29:TYR:CE1	3:C:33:LEU:HB2	2.54	0.42
3:C:29:TYR:HA	3:C:32:LEU:HD12	2.02	0.42
4:D:53:ASP:O	4:D:57:ARG:HD2	2.20	0.42
7:G:140:ASP:O	7:G:144:MET:HG2	2.20	0.42
11:K:62:GLN:CG	11:K:97:ALA:HB2	2.50	0.42
13:M:91:ARG:HE	13:M:96:LEU:HB2	1.83	0.42
17:Q:17:LYS:HA	17:Q:49:GLU:HG3	2.01	0.42
19:S:6:LYS:HB2	19:S:7:LYS:H	1.72	0.42
25:Z:54:5MU:C2	25:Z:58:A:N7	2.86	0.42
1:A:1110:A:N6	1:A:1111:A:C6	2.88	0.41
1:A:1283:G:C2	1:A:1284:C:C4	3.07	0.41
1:A:1409:C:H2'	1:A:1410:G:H8	1.83	0.41
1:A:400:C:H2'	1:A:401:C:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:C:N3	18:R:74:ARG:NH1	2.62	0.41
1:A:951:G:C2	1:A:952:U:C2	3.08	0.41
8:H:73:ASP:HA	8:H:74:PRO:HD2	1.87	0.41
9:I:26:VAL:HA	9:I:61:ALA:O	2.20	0.41
11:K:84:VAL:HG23	11:K:110:ASP:HA	2.02	0.41
25:Z:36:U:H2'	25:Z:37:A:O4'	2.20	0.41
1:A:1017:G:C6	1:A:1018:C:C4	3.08	0.41
1:A:1141:C:H2'	1:A:1142:G:C8	2.55	0.41
1:A:13:U:H3	1:A:915:A:N6	2.17	0.41
1:A:1425:U:H2'	1:A:1426:C:C6	2.55	0.41
1:A:1443:G:N1	1:A:1444:C:C4	2.88	0.41
1:A:181:G:H4'	1:A:182:U:H5'	2.02	0.41
1:A:333:G:N1	1:A:334:C:C4	2.88	0.41
1:A:681:C:C2	1:A:710:G:N2	2.87	0.41
1:A:926:G:C2	24:Y:35:A:C8	3.08	0.41
3:C:6:HIS:CB	14:N:49:HIS:HB3	2.50	0.41
4:D:132:ARG:HG3	4:D:132:ARG:O	2.20	0.41
8:H:16:ALA:O	8:H:20:TYR:N	2.51	0.41
23:X:11:ILE:HG21	23:X:16:VAL:HG11	2.01	0.41
23:X:9:GLU:HG2	23:X:35:LEU:HD22	2.01	0.41
25:Z:31:G:C2	25:Z:40:C:C2	3.08	0.41
25:Z:7:G:N1	25:Z:49:G:C5	2.88	0.41
1:A:1015:A:H2'	1:A:1016:A:C8	2.55	0.41
1:A:1255:G:H2'	1:A:1279:A:N6	2.35	0.41
1:A:1374:A:C6	1:A:1375:A:C8	3.08	0.41
1:A:189(J):G:C6	1:A:189(K):U:C4	3.09	0.41
1:A:251:G:N1	1:A:266:G:C6	2.89	0.41
1:A:276:G:C6	1:A:277:C:C4	3.09	0.41
1:A:406:G:H1	1:A:436:C:H42	1.67	0.41
1:A:43:C:H2'	1:A:44:G:C8	2.55	0.41
9:I:18:PHE:HD2	9:I:62:TYR:CD2	2.37	0.41
17:Q:59:ILE:CG2	17:Q:71:PHE:HB3	2.50	0.41
25:Z:65:C:H2'	25:Z:66:C:O4'	2.20	0.41
1:A:1116:C:H2'	1:A:1117:G:O4'	2.21	0.41
1:A:1177:G:H3'	1:A:1178:G:H8	1.86	0.41
1:A:1206:G:C6	1:A:1207:G:C5	3.08	0.41
1:A:761:G:C6	1:A:762:C:N3	2.88	0.41
1:A:891:U:H2'	1:A:892:A:H8	1.84	0.41
1:A:903:G:C6	1:A:904:C:C4	3.08	0.41
1:A:91:C:N4	1:A:92:C:N4	2.68	0.41
1:A:925:G:C2	1:A:927:G:C8	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:ARG:HG2	2:B:53:ARG:NH1	2.36	0.41
14:N:9:LYS:HE3	14:N:20:ALA:HA	2.02	0.41
24:Y:31:U:H3'	24:Y:32:A:C5'	2.50	0.41
1:A:1019:C:H2'	1:A:1020:U:O4'	2.20	0.41
1:A:1058:G:C6	1:A:1059:C:C4	3.09	0.41
1:A:1105:A:N3	1:A:1106:G:C8	2.88	0.41
1:A:112:G:H21	1:A:354:G:H5'	1.85	0.41
1:A:1353:G:N1	1:A:1354:C:C4	2.88	0.41
1:A:52:G:C6	1:A:53:A:C5	3.09	0.41
1:A:29:G:C2	1:A:555:C:N3	2.88	0.41
1:A:583:A:H2'	1:A:584:G:O4'	2.20	0.41
1:A:731:G:H8	1:A:731:G:O5'	2.03	0.41
1:A:825:G:C2	1:A:826:C:C2	3.08	0.41
1:A:886:G:O6	1:A:887:G:C6	2.73	0.41
1:A:938:A:H5'	7:G:76:ARG:HH21	1.86	0.41
1:A:947:G:C5	1:A:948:C:C4	3.08	0.41
4:D:10:ARG:HG3	4:D:11:LEU:N	2.36	0.41
8:H:97:VAL:HA	8:H:100:ILE:HD11	2.01	0.41
1:A:1291:G:H4'	9:I:39:GLY:HA3	2.01	0.41
11:K:58:PRO:HB2	11:K:93:GLN:HG3	2.01	0.41
15:O:75:PRO:O	15:O:78:TYR:HB3	2.21	0.41
25:Z:14:A:N3	25:Z:14:A:H2'	2.34	0.41
25:Z:41:C:H2'	25:Z:42:G:C8	2.55	0.41
1:A:1001(A):G:C6	1:A:1002:G:C6	3.09	0.41
1:A:1127:G:H21	1:A:1147:C:N4	2.17	0.41
1:A:1233:G:C2	1:A:1234:C:C2	3.09	0.41
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.53	0.41
1:A:241:C:C2	1:A:286:G:C2	3.09	0.41
1:A:399:G:H2'	1:A:400:C:C6	2.55	0.41
1:A:456:C:C2	1:A:476:G:C2	3.09	0.41
1:A:505:G:OP2	1:A:535:A:H5'	2.19	0.41
1:A:864:A:H2'	1:A:865:A:N9	2.34	0.41
1:A:988:G:C6	1:A:989:C:C4	3.08	0.41
2:B:158:LEU:HA	2:B:159:PRO:HD2	1.98	0.41
5:E:82:VAL:HG21	5:E:138:ALA:HA	2.03	0.41
1:A:1235:U:O2'	1:A:1305:G:O5'	2.39	0.41
1:A:1443:G:C2	1:A:1444:C:N3	2.88	0.41
1:A:127:G:N2	1:A:235:C:C2	2.89	0.41
1:A:563:A:C2	1:A:567:G:C5	3.08	0.41
1:A:636:U:H2'	1:A:637:G:H8	1.86	0.41
1:A:66:G:N1	1:A:67:C:C4	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:G:C2	1:A:708:C:C2	3.09	0.41
1:A:748:C:H4'	1:A:749:C:H5'	2.02	0.41
1:A:865:A:O5'	1:A:865:A:H8	2.04	0.41
1:A:942:G:N3	1:A:942:G:H2'	2.35	0.41
2:B:55:PHE:HB3	2:B:221:LEU:HD23	2.03	0.41
1:A:1205:U:H4'	3:C:195:VAL:CG2	2.51	0.41
3:C:34:LEU:HD12	14:N:25:VAL:HG21	2.03	0.41
5:E:125:SER:O	5:E:126:ARG:HD3	2.20	0.41
12:L:40:VAL:HG23	12:L:56:ALA:HB2	2.03	0.41
23:X:123:ARG:HD2	24:Y:39:U:O2	2.21	0.41
25:Z:17:C:O2	25:Z:17:C:C2'	2.68	0.41
1:A:1060:C:H5''	10:J:51:ARG:HH11	1.86	0.41
1:A:1205:U:H4'	3:C:195:VAL:HG21	2.02	0.41
1:A:1207:G:C6	1:A:1208:C:C4	3.08	0.41
1:A:1243:C:C2	1:A:1295:G:C2	3.09	0.41
1:A:1309:G:N7	13:M:99:ARG:NH2	2.68	0.41
1:A:1387:G:N2	1:A:1388:C:C2	2.88	0.41
1:A:1445:C:O2	1:A:1458:G:C2	2.73	0.41
1:A:333:G:C2	1:A:334:C:C2	3.08	0.41
1:A:384:G:C6	1:A:385:C:N4	2.89	0.41
1:A:471:G:C2'	1:A:472:A:H5'	2.50	0.41
1:A:83:U:H2'	1:A:84:U:O4'	2.21	0.41
1:A:980:C:H1'	14:N:19:ARG:HG2	2.02	0.41
2:B:96:ARG:HG2	2:B:98:LEU:HG	2.03	0.41
3:C:34:LEU:HD23	3:C:35:GLU:HG3	2.03	0.41
4:D:201:GLN:HA	4:D:204:ILE:HD12	2.03	0.41
8:H:6:ILE:HD12	8:H:31:PHE:HD2	1.85	0.41
6:F:43:LEU:HD21	18:R:35:ARG:HB3	2.01	0.41
1:A:1177:G:H3'	1:A:1178:G:C8	2.55	0.41
1:A:1050:G:C2	1:A:1209:C:O2	2.74	0.41
1:A:1271:G:H8	1:A:1271:G:O5'	2.03	0.41
1:A:1423:G:C2	1:A:1424:C:C2	3.09	0.41
1:A:399:G:N2	1:A:400:C:C2	2.88	0.41
1:A:455:C:N4	1:A:456:C:H41	2.19	0.41
1:A:555:C:N3	1:A:556:C:C4	2.88	0.41
1:A:769:G:N1	1:A:770:C:C4	2.89	0.41
2:B:9:GLU:HB2	2:B:217:ARG:HH21	1.86	0.41
8:H:4:ASP:HA	8:H:5:PRO:HD3	1.91	0.41
18:R:51:LEU:HA	18:R:52:PRO:HD3	1.94	0.41
20:T:60:GLU:HG3	20:T:81:LYS:HE3	2.02	0.41
24:Y:30:G:C3'	24:Y:31:U:H5''	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1067:A:O5'	1:A:1067:A:C8	2.67	0.41
1:A:1164:G:N1	1:A:1165:C:C4	2.89	0.41
1:A:1472:U:H2'	1:A:1473:A:C8	2.56	0.41
1:A:402:G:C6	1:A:403:C:C4	3.09	0.41
1:A:443:C:C2	1:A:492:G:N2	2.89	0.41
1:A:576:G:H3'	1:A:577:G:C5'	2.51	0.41
1:A:944:G:O6	1:A:1337:G:C8	2.60	0.41
2:B:156:LYS:HD3	2:B:157:ARG:HG2	2.03	0.41
3:C:95:THR:HB	3:C:97:LYS:HE3	2.03	0.41
7:G:99:LEU:HA	7:G:102:ARG:NH1	2.35	0.41
13:M:84:ILE:HD12	19:S:74:PHE:CE1	2.56	0.41
18:R:38:GLU:HA	18:R:41:LYS:HB2	2.03	0.41
1:A:1134:G:N2	1:A:1141:C:C2	2.89	0.41
1:A:1236:A:H2'	1:A:1237:C:C6	2.56	0.41
1:A:1241:G:C2	1:A:1242:C:C2	3.09	0.41
1:A:1347:G:H22	1:A:1374:A:P	2.44	0.41
1:A:802:A:C8	1:A:803:G:C8	3.09	0.41
2:B:68:ILE:H	2:B:90:MET:HG2	1.85	0.41
4:D:128:VAL:HG12	4:D:129:ASN:HD22	1.85	0.41
1:A:1316:G:H4'	14:N:18:VAL:HG11	2.02	0.41
17:Q:56:VAL:HG12	17:Q:78:GLU:HB3	2.03	0.41
24:Y:30:G:C2'	24:Y:31:U:H5"	2.48	0.41
1:A:1110:A:C5	1:A:1111:A:C5	3.09	0.40
1:A:1207:G:C2	1:A:1208:C:C2	3.09	0.40
1:A:1263:C:H2'	1:A:1264:C:C6	2.56	0.40
1:A:384:G:C2	1:A:385:C:C2	3.09	0.40
1:A:557:G:N1	1:A:558:G:C2	2.89	0.40
1:A:731:G:N1	1:A:732:C:C4	2.89	0.40
1:A:807:A:H2'	1:A:808:C:C6	2.57	0.40
1:A:19:C:O2	1:A:917:G:C2	2.74	0.40
3:C:177:THR:HG23	3:C:180:ALA:HB2	2.02	0.40
7:G:74:GLU:HG2	7:G:91:VAL:HG22	2.01	0.40
20:T:79:ARG:NH2	20:T:80:ARG:HG2	2.36	0.40
25:Z:63:G:C2	25:Z:64:G:C5	3.09	0.40
1:A:1508:G:C6	1:A:1509:C:C4	3.09	0.40
1:A:145:G:N2	1:A:178:C:C2	2.90	0.40
1:A:289:G:H2'	1:A:290:C:C6	2.55	0.40
1:A:499:A:O3'	1:A:500:G:H8	2.05	0.40
1:A:590:C:H42	1:A:649:G:H1	1.69	0.40
1:A:838:G:C2	1:A:849:C:N3	2.89	0.40
1:A:832:C:O2	1:A:855:G:C2	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:87:SER:HA	5:E:125:SER:HB3	2.03	0.40
7:G:85:TYR:HB3	7:G:151:TYR:CD2	2.56	0.40
10:J:10:GLY:O	10:J:67:THR:HA	2.21	0.40
1:A:1491:G:H5''	12:L:47:LYS:HB2	2.03	0.40
19:S:80:TYR:CE2	19:S:81:ARG:NH1	2.89	0.40
25:Z:2:G:N2	25:Z:3:C:C2	2.89	0.40
1:A:1081:G:H2'	1:A:1082:G:O4'	2.22	0.40
1:A:1387:G:N1	1:A:1388:C:C4	2.90	0.40
1:A:1429:C:H2'	1:A:1430:C:C6	2.57	0.40
1:A:189:G:C6	1:A:189(L):G:C6	3.09	0.40
1:A:311:C:H2'	1:A:312:C:C6	2.56	0.40
1:A:491:G:O2'	1:A:492:G:H5'	2.21	0.40
1:A:543:C:OP2	4:D:10:ARG:NH2	2.53	0.40
1:A:577:G:C8	1:A:816:A:C6	3.09	0.40
1:A:947:G:C6	1:A:948:C:C4	3.09	0.40
2:B:208:ILE:H	2:B:208:ILE:HG13	1.44	0.40
6:F:14:LEU:HD11	6:F:84:ASN:HB3	2.04	0.40
8:H:37:ARG:HG2	8:H:41:ARG:HH12	1.87	0.40
19:S:32:LYS:HG2	19:S:32:LYS:H	1.69	0.40
25:Z:68:C:H2'	25:Z:69:C:O4'	2.22	0.40
1:A:309:G:H2'	1:A:310:G:C8	2.55	0.40
1:A:658:G:H2'	1:A:659:U:C6	2.56	0.40
1:A:725:G:C2	1:A:726:C:C2	3.09	0.40
1:A:823:G:C6	1:A:824:C:N4	2.90	0.40
1:A:988:G:C2	1:A:989:C:C2	3.09	0.40
1:A:98:G:C2	1:A:99:U:C2	3.09	0.40
2:B:25:ASN:HA	2:B:26:PRO:HD3	1.87	0.40
4:D:101:LEU:O	4:D:105:VAL:HG23	2.20	0.40
4:D:173:TRP:CD1	4:D:174:LEU:HG	2.56	0.40
4:D:83:SER:HA	4:D:89:THR:HG23	2.03	0.40
1:A:694:A:H5'	11:K:53:SER:HB2	2.03	0.40
16:P:39:TYR:CD1	16:P:73:LEU:HD21	2.56	0.40
1:A:254:G:OP1	17:Q:69:LYS:HB2	2.22	0.40
24:Y:22:G:C2	24:Y:23:C:O2	2.75	0.40
1:A:1084:G:H2'	1:A:1085:U:C5	2.57	0.40
1:A:1283:G:C6	1:A:1284:C:N4	2.90	0.40
1:A:1343:G:C6	1:A:1344:C:N4	2.90	0.40
1:A:143:A:H8	1:A:143:A:O5'	2.04	0.40
1:A:1491:G:H4'	12:L:47:LYS:HB2	2.04	0.40
1:A:168:G:C6	1:A:169:C:N4	2.90	0.40
1:A:568:G:C2	1:A:569:C:C4	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:912:C:H2'	1:A:913:A:C8	2.57	0.40
1:A:946:A:H2'	1:A:947:G:C8	2.56	0.40
3:C:156:ARG:HB3	3:C:159:GLY:HA2	2.03	0.40
5:E:42:GLY:HA2	5:E:65:ASN:O	2.22	0.40
7:G:29:LYS:HB3	7:G:105:VAL:HG21	2.04	0.40
10:J:39:PRO:HB2	10:J:40:LEU:H	1.78	0.40
14:N:13:THR:HG22	14:N:15:LYS:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	178 (77%)	41 (18%)	13 (6%)	2	27
3	C	204/239 (85%)	173 (85%)	25 (12%)	6 (3%)	6	43
4	D	206/209 (99%)	174 (84%)	25 (12%)	7 (3%)	5	40
5	E	148/162 (91%)	130 (88%)	16 (11%)	2 (1%)	14	57
6	F	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	9	51
7	G	153/156 (98%)	133 (87%)	17 (11%)	3 (2%)	9	51
8	H	136/138 (99%)	117 (86%)	17 (12%)	2 (2%)	13	57
9	I	125/128 (98%)	101 (81%)	18 (14%)	6 (5%)	3	31
10	J	96/105 (91%)	77 (80%)	11 (12%)	8 (8%)	1	18
11	K	117/129 (91%)	97 (83%)	16 (14%)	4 (3%)	5	40
12	L	122/132 (92%)	95 (78%)	24 (20%)	3 (2%)	7	46
13	M	116/126 (92%)	94 (81%)	19 (16%)	3 (3%)	7	45
14	N	58/61 (95%)	44 (76%)	14 (24%)	0	100	100
15	O	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	16	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	81/88 (92%)	76 (94%)	5 (6%)	0	100	100
17	Q	97/105 (92%)	85 (88%)	11 (11%)	1 (1%)	19	64
18	R	71/88 (81%)	59 (83%)	9 (13%)	3 (4%)	3	34
19	S	78/93 (84%)	62 (80%)	15 (19%)	1 (1%)	15	59
20	T	97/106 (92%)	81 (84%)	10 (10%)	6 (6%)	2	25
21	V	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
22	W	69/72 (96%)	58 (84%)	9 (13%)	2 (3%)	6	43
23	X	160/171 (94%)	135 (84%)	21 (13%)	4 (2%)	7	46
All	All	2573/2781 (92%)	2158 (84%)	338 (13%)	77 (3%)	9	42

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
2	B	24	TRP
8	H	105	ARG
10	J	39	PRO
10	J	40	LEU
10	J	60	ARG
11	K	101	SER
18	R	87	ARG
23	X	54	PRO
2	B	16	HIS
2	B	17	PHE
2	B	132	LYS
2	B	207	ALA
4	D	5	ILE
4	D	32	ALA
7	G	7	ALA
7	G	55	GLY
9	I	56	LEU
13	M	99	ARG
17	Q	99	SER
20	T	70	SER
22	W	2	LYS
3	C	12	LEU
3	C	168	ALA
5	E	142	LEU
9	I	33	PHE

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Mol	Chain	Res	Type
10	J	55	LYS
10	J	72	VAL
12	L	27	LEU
20	T	49	ALA
23	X	8	ASN
2	B	183	PRO
2	B	228	GLY
3	C	108	ASN
4	D	129	ASN
9	I	44	VAL
10	J	34	VAL
11	K	14	VAL
11	K	37	GLY
11	K	117	ASN
13	M	14	ARG
18	R	17	SER
20	T	95	ALA
20	T	97	ALA
23	X	154	PRO
2	B	9	GLU
2	B	130	ARG
2	B	194	PRO
2	B	229	VAL
3	C	127	ARG
3	C	181	ASN
4	D	18	LYS
4	D	30	LYS
6	F	51	PRO
6	F	70	ASP
8	H	54	ASP
9	I	54	ASP
9	I	121	ARG
10	J	54	PHE
12	L	25	PRO
12	L	26	ALA
13	M	5	ALA
18	R	45	SER
23	X	125	ARG
2	B	131	PRO
5	E	124	GLY
19	S	8	GLY
9	I	90	PRO

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Mol	Chain	Res	Type
10	J	31	GLY
4	D	167	GLY
20	T	96	GLY
3	C	14	ILE
22	W	49	PRO
7	G	112	PRO
15	O	75	PRO
20	T	69	GLY
4	D	172	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	150 (74%)	52 (26%)	0	6
3	C	160/188 (85%)	138 (86%)	22 (14%)	4	28
4	D	180/181 (99%)	136 (76%)	44 (24%)	1	7
5	E	115/123 (94%)	90 (78%)	25 (22%)	1	10
6	F	90/90 (100%)	76 (84%)	14 (16%)	3	23
7	G	126/127 (99%)	107 (85%)	19 (15%)	3	24
8	H	119/119 (100%)	94 (79%)	25 (21%)	1	11
9	I	98/99 (99%)	83 (85%)	15 (15%)	3	23
10	J	87/92 (95%)	75 (86%)	12 (14%)	4	28
11	K	90/99 (91%)	76 (84%)	14 (16%)	3	23
12	L	104/109 (95%)	83 (80%)	21 (20%)	1	12
13	M	94/101 (93%)	81 (86%)	13 (14%)	4	28
14	N	49/50 (98%)	38 (78%)	11 (22%)	1	9
15	O	79/80 (99%)	62 (78%)	17 (22%)	1	10
16	P	72/74 (97%)	59 (82%)	13 (18%)	2	16
17	Q	94/97 (97%)	81 (86%)	13 (14%)	4	28
18	R	64/77 (83%)	47 (73%)	17 (27%)	0	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	S	71/80 (89%)	58 (82%)	13 (18%)	2	15
20	T	76/82 (93%)	59 (78%)	17 (22%)	1	9
21	V	19/22 (86%)	15 (79%)	4 (21%)	1	10
22	W	61/63 (97%)	56 (92%)	5 (8%)	14	51
23	X	145/150 (97%)	118 (81%)	27 (19%)	2	14
All	All	2195/2323 (94%)	1782 (81%)	413 (19%)	5	14

All (413) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	10	LEU
2	B	16	HIS
2	B	21	ARG
2	B	23	ARG
2	B	24	TRP
2	B	25	ASN
2	B	28	PHE
2	B	44	LEU
2	B	53	ARG
2	B	61	LEU
2	B	64	ARG
2	B	67	THR
2	B	75	LYS
2	B	76	GLN
2	B	78	GLN
2	B	87	ARG
2	B	93	VAL
2	B	96	ARG
2	B	97	TRP
2	B	102	LEU
2	B	108	ILE
2	B	114	ARG
2	B	122	PHE
2	B	126	GLU
2	B	127	ILE
2	B	140	HIS
2	B	141	GLU
2	B	142	LEU
2	B	144	ARG

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Mol	Chain	Res	Type
2	B	153	ARG
2	B	155	LEU
2	B	160	ASP
2	B	178	ARG
2	B	179	LYS
2	B	180	LEU
2	B	187	LEU
2	B	190	THR
2	B	191	ASP
2	B	193	ASP
2	B	196	LEU
2	B	198	ASP
2	B	200	ILE
2	B	204	ASN
2	B	205	ASP
2	B	208	ILE
2	B	211	ILE
2	B	213	LEU
2	B	215	LEU
2	B	220	ASP
2	B	226	ARG
2	B	233	SER
3	C	3	ASN
3	C	11	ARG
3	C	33	LEU
3	C	34	LEU
3	C	38	ARG
3	C	43	LEU
3	C	52	LEU
3	C	64	VAL
3	C	82	GLU
3	C	87	LEU
3	C	90	GLU
3	C	94	LEU
3	C	97	LYS
3	C	98	ASN
3	C	108	ASN
3	C	111	LEU
3	C	126	ARG
3	C	144	SER
3	C	166	GLU
3	C	167	TRP

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Mol	Chain	Res	Type
3	C	188	LEU
3	C	191	THR
4	D	13	ARG
4	D	14	ARG
4	D	15	GLU
4	D	19	LEU
4	D	25	ARG
4	D	28	SER
4	D	33	MET
4	D	35	ARG
4	D	36	ARG
4	D	38	TYR
4	D	45	GLN
4	D	47	ARG
4	D	50	ARG
4	D	57	ARG
4	D	59	ARG
4	D	64	LEU
4	D	66	ARG
4	D	70	ILE
4	D	73	ARG
4	D	75	PHE
4	D	78	LEU
4	D	83	SER
4	D	92	VAL
4	D	114	ARG
4	D	115	ARG
4	D	118	ARG
4	D	122	ARG
4	D	125	HIS
4	D	131	ARG
4	D	132	ARG
4	D	134	ASP
4	D	141	ARG
4	D	144	ASP
4	D	146	ILE
4	D	151	LYS
4	D	152	SER
4	D	153	ARG
4	D	162	LEU
4	D	165	MET
4	D	174	LEU

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Mol	Chain	Res	Type
4	D	181	MET
4	D	187	ARG
4	D	190	ASP
4	D	193	ASP
5	E	5	ASP
5	E	12	LEU
5	E	13	ILE
5	E	15	ARG
5	E	19	MET
5	E	24	ARG
5	E	25	ARG
5	E	27	ARG
5	E	32	VAL
5	E	36	ASP
5	E	47	LYS
5	E	80	ILE
5	E	87	SER
5	E	107	ARG
5	E	118	ILE
5	E	120	THR
5	E	123	LEU
5	E	126	ARG
5	E	129	ILE
5	E	130	ASN
5	E	133	TYR
5	E	137	GLU
5	E	142	LEU
5	E	148	VAL
5	E	149	GLU
6	F	3	ARG
6	F	7	ASN
6	F	19	LEU
6	F	28	ARG
6	F	31	GLU
6	F	36	ARG
6	F	47	ARG
6	F	55	ASP
6	F	61	LEU
6	F	70	ASP
6	F	74	ASP
6	F	77	ARG
6	F	82	ARG

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Mol	Chain	Res	Type
6	F	98	LEU
7	G	6	ARG
7	G	8	GLU
7	G	12	LEU
7	G	14	PRO
7	G	45	ASP
7	G	61	VAL
7	G	62	PHE
7	G	72	ARG
7	G	74	GLU
7	G	76	ARG
7	G	79	ARG
7	G	80	VAL
7	G	91	VAL
7	G	96	GLN
7	G	104	LEU
7	G	111	ARG
7	G	136	LYS
7	G	149	ARG
7	G	156	TRP
8	H	2	LEU
8	H	6	ILE
8	H	11	THR
8	H	14	ARG
8	H	18	ARG
8	H	21	LYS
8	H	25	ASP
8	H	39	LEU
8	H	41	ARG
8	H	50	ARG
8	H	59	LEU
8	H	60	ARG
8	H	68	ARG
8	H	84	ARG
8	H	85	ARG
8	H	92	ARG
8	H	93	VAL
8	H	104	ARG
8	H	119	LEU
8	H	122	ARG
8	H	125	ARG
8	H	127	LEU

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Mol	Chain	Res	Type
8	H	129	VAL
8	H	133	LEU
8	H	134	ILE
9	I	32	ASP
9	I	38	GLN
9	I	44	VAL
9	I	56	LEU
9	I	60	ASP
9	I	64	THR
9	I	65	VAL
9	I	78	LYS
9	I	85	LEU
9	I	87	GLN
9	I	91	ASP
9	I	97	LYS
9	I	102	LEU
9	I	121	ARG
9	I	127	LYS
10	J	8	LEU
10	J	16	LEU
10	J	38	ILE
10	J	42	THR
10	J	48	THR
10	J	57	LYS
10	J	60	ARG
10	J	61	GLU
10	J	71	LEU
10	J	74	ILE
10	J	79	ARG
10	J	99	LYS
11	K	18	ARG
11	K	29	ILE
11	K	34	ASP
11	K	40	ILE
11	K	48	ILE
11	K	63	LEU
11	K	77	MET
11	K	84	VAL
11	K	91	ARG
11	K	96	ARG
11	K	116	HIS
11	K	117	ASN

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Mol	Chain	Res	Type
11	K	120	ARG
11	K	126	ARG
12	L	6	THR
12	L	7	ILE
12	L	12	ARG
12	L	17	LYS
12	L	33	ARG
12	L	34	ARG
12	L	39	VAL
12	L	41	ARG
12	L	42	THR
12	L	46	LYS
12	L	53	ARG
12	L	58	VAL
12	L	59	ARG
12	L	66	VAL
12	L	79	GLU
12	L	91	LYS
12	L	92	ASP
12	L	97	ARG
12	L	110	VAL
12	L	113	ARG
12	L	117	ARG
13	M	12	ASN
13	M	15	VAL
13	M	32	GLU
13	M	47	ASP
13	M	56	LEU
13	M	65	LYS
13	M	66	LEU
13	M	90	LEU
13	M	98	VAL
13	M	102	ARG
13	M	109	THR
13	M	115	LYS
13	M	116	THR
14	N	3	ARG
14	N	9	LYS
14	N	13	THR
14	N	17	LYS
14	N	18	VAL
14	N	26	ARG

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Mol	Chain	Res	Type
14	N	32	SER
14	N	33	VAL
14	N	35	ARG
14	N	40	CYS
14	N	46	GLU
15	O	17	ARG
15	O	21	ASP
15	O	22	THR
15	O	32	LEU
15	O	38	ARG
15	O	39	LEU
15	O	41	GLU
15	O	43	LEU
15	O	48	LYS
15	O	54	ARG
15	O	56	LEU
15	O	58	MET
15	O	65	ARG
15	O	70	LEU
15	O	71	GLN
15	O	77	ARG
15	O	83	GLU
16	P	9	PHE
16	P	12	LYS
16	P	20	VAL
16	P	23	ASP
16	P	28	ARG
16	P	29	ASP
16	P	35	LYS
16	P	44	THR
16	P	62	VAL
16	P	67	THR
16	P	69	THR
16	P	72	ARG
16	P	73	LEU
17	Q	15	MET
17	Q	16	GLN
17	Q	38	ARG
17	Q	41	LYS
17	Q	53	LEU
17	Q	55	ASP
17	Q	63	ARG

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Mol	Chain	Res	Type
17	Q	68	ARG
17	Q	70	ARG
17	Q	82	MET
17	Q	89	LEU
17	Q	93	GLN
17	Q	100	LYS
18	R	18	ARG
18	R	19	LYS
18	R	22	VAL
18	R	28	GLU
18	R	34	TYR
18	R	36	ASN
18	R	47	THR
18	R	53	ARG
18	R	54	ARG
18	R	55	ARG
18	R	59	SER
18	R	62	GLU
18	R	63	GLN
18	R	66	LEU
18	R	75	ILE
18	R	81	PHE
18	R	87	ARG
19	S	5	LEU
19	S	7	LYS
19	S	15	LEU
19	S	18	LYS
19	S	19	VAL
19	S	27	GLU
19	S	29	ARG
19	S	36	ARG
19	S	39	THR
19	S	43	GLU
19	S	63	THR
19	S	77	THR
19	S	81	ARG
20	T	10	LEU
20	T	15	ARG
20	T	18	GLN
20	T	20	LEU
20	T	23	ARG
20	T	25	ARG

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Mol	Chain	Res	Type
20	T	45	GLN
20	T	56	MET
20	T	57	ARG
20	T	62	LEU
20	T	68	LYS
20	T	71	THR
20	T	72	LEU
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
21	V	6	ARG
21	V	7	ARG
21	V	12	LYS
21	V	21	TYR
22	W	8	ARG
22	W	19	ASN
22	W	23	ARG
22	W	27	ASP
22	W	32	ILE
23	X	3	LYS
23	X	4	GLU
23	X	19	VAL
23	X	22	ASP
23	X	26	LEU
23	X	31	THR
23	X	35	LEU
23	X	37	LEU
23	X	43	LEU
23	X	61	ASP
23	X	71	MET
23	X	74	LYS
23	X	87	SER
23	X	91	ARG
23	X	95	ASP
23	X	103	LEU
23	X	117	LYS
23	X	118	VAL
23	X	123	ARG
23	X	125	ARG
23	X	126	GLU
23	X	131	GLU

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Mol	Chain	Res	Type
23	X	135	ARG
23	X	143	ASP
23	X	156	MET
23	X	164	LEU
23	X	170	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	HIS
2	B	76	GLN
2	B	204	ASN
3	C	3	ASN
3	C	31	HIS
3	C	108	ASN
3	C	123	GLN
3	C	139	GLN
3	C	170	GLN
4	D	42	GLN
4	D	43	HIS
4	D	103	ASN
4	D	116	GLN
4	D	129	ASN
4	D	160	GLN
4	D	199	ASN
4	D	201	GLN
5	E	73	ASN
5	E	130	ASN
6	F	7	ASN
6	F	13	ASN
6	F	73	ASN
6	F	100	ASN
7	G	68	ASN
7	G	96	GLN
8	H	15	ASN
8	H	82	HIS
10	J	68	HIS
11	K	26	ASN
11	K	62	GLN
13	M	77	ASN
17	Q	94	ASN
18	R	63	GLN

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Mol	Chain	Res	Type
19	S	53	ASN
20	T	18	GLN
20	T	73	HIS
20	T	75	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	437 (29%)	113 (7%)
24	Y	18/42 (42%)	14 (77%)	3 (16%)
25	Z	74/77 (96%)	32 (43%)	9 (12%)
All	All	1598/1641 (97%)	483 (30%)	125 (7%)

All (483) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G
1	A	13	U
1	A	16	A
1	A	18	C
1	A	22	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	40	C
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	52	G
1	A	54	C
1	A	55	A
1	A	58	C
1	A	60	A
1	A	61	G
1	A	72	C
1	A	73	G

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Mol	Chain	Res	Type
1	A	81	U
1	A	90	U
1	A	91	C
1	A	97	G
1	A	100	C
1	A	116	A
1	A	120	A
1	A	121	C
1	A	122	G
1	A	127	G
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	142	G
1	A	151	A
1	A	157	G
1	A	163	C
1	A	173	U
1	A	174	C
1	A	178	C
1	A	181	G
1	A	182	U
1	A	183	G
1	A	189(E)	U
1	A	189(F)	U
1	A	189(G)	G
1	A	189(H)	G
1	A	195	A
1	A	196	A
1	A	197	A
1	A	198	G
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	220	G
1	A	222	U
1	A	240	C
1	A	244	U
1	A	247	G
1	A	250	A
1	A	251	G

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Mol	Chain	Res	Type
1	A	252	U
1	A	253	U
1	A	266	G
1	A	267	C
1	A	279	A
1	A	280	C
1	A	281	G
1	A	282	A
1	A	283	C
1	A	289	G
1	A	298	A
1	A	301	G
1	A	315	A
1	A	316	G
1	A	321	A
1	A	324	G
1	A	325	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	340	U
1	A	345	C
1	A	347	G
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	357	G
1	A	362	G
1	A	366	C
1	A	367	U
1	A	368	U
1	A	372	C
1	A	373	A
1	A	382	A
1	A	384	G
1	A	388	G
1	A	392	G
1	A	393	A
1	A	396	G
1	A	397	A

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Mol	Chain	Res	Type
1	A	398	C
1	A	406	G
1	A	409	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	441	A
1	A	448	A
1	A	450	G
1	A	452	A
1	A	470	C
1	A	481	G
1	A	482	A
1	A	484	G
1	A	485	G
1	A	486	U
1	A	495	A
1	A	496	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	514	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	521	G
1	A	524	G
1	A	527	G
1	A	529	G
1	A	530	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	534	U

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Mol	Chain	Res	Type
1	A	545	C
1	A	547	A
1	A	548	G
1	A	550	G
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	566	G
1	A	568	G
1	A	571	U
1	A	572	A
1	A	573	A
1	A	574	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	582	U
1	A	588	G
1	A	589	C
1	A	596	C
1	A	607	A
1	A	619	U
1	A	632	A
1	A	639	G
1	A	641	U
1	A	653	A
1	A	657	G
1	A	665	A
1	A	687	A
1	A	688	G
1	A	692	U
1	A	701	C
1	A	702	A
1	A	703	G
1	A	713	G
1	A	717	C
1	A	721	G
1	A	722	A
1	A	723	U
1	A	727	G
1	A	731	G

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Mol	Chain	Res	Type
1	A	733	A
1	A	748	C
1	A	749	C
1	A	755	G
1	A	760	G
1	A	777	A
1	A	785	G
1	A	787	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	798	G
1	A	799	G
1	A	800	G
1	A	810	C
1	A	813	U
1	A	815	A
1	A	817	C
1	A	820	U
1	A	821	G
1	A	828	A
1	A	839	U
1	A	841	U
1	A	853	G
1	A	855	G
1	A	859	A
1	A	865	A
1	A	870	U
1	A	872	A
1	A	873	A
1	A	876	G
1	A	884	U
1	A	885	G
1	A	889	A
1	A	900	A
1	A	901	A
1	A	902	G
1	A	911	U
1	A	913	A
1	A	922	G
1	A	926	G
1	A	927	G

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Mol	Chain	Res	Type
1	A	932	C
1	A	934	C
1	A	935	A
1	A	942	G
1	A	943	U
1	A	950	U
1	A	960	U
1	A	961	U
1	A	965	A
1	A	966	G
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1000	U
1	A	1001	A
1	A	1002	G
1	A	1003	G
1	A	1004	A
1	A	1005	A
1	A	1016	A
1	A	1022	G
1	A	1023	G
1	A	1024	G
1	A	1025	U
1	A	1030	C
1	A	1030(C)	G
1	A	1031	G
1	A	1043	C
1	A	1045	C
1	A	1049	U
1	A	1050	G
1	A	1051	C
1	A	1053	G

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Mol	Chain	Res	Type
1	A	1054	C
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1067	A
1	A	1068	G
1	A	1074	G
1	A	1085	U
1	A	1089	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1104	G
1	A	1117	G
1	A	1118	C
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1135	U
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1145	C
1	A	1146	A
1	A	1150	U
1	A	1152	A
1	A	1157	A
1	A	1159	U
1	A	1160	G
1	A	1169	A
1	A	1171	G
1	A	1176	A
1	A	1183	A
1	A	1184	G

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Mol	Chain	Res	Type
1	A	1187	G
1	A	1191	A
1	A	1193	G
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1236	A
1	A	1237	C
1	A	1238	A
1	A	1249	C
1	A	1250	A
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1261	A
1	A	1268	A
1	A	1270	C
1	A	1275	A
1	A	1277	C
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1290	G
1	A	1296	C
1	A	1297	C

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Mol	Chain	Res	Type
1	A	1298	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1312	G
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1321	C
1	A	1323	G
1	A	1332	A
1	A	1335	C
1	A	1336	C
1	A	1337	G
1	A	1340	A
1	A	1341	U
1	A	1342	C
1	A	1345	U
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1351	U
1	A	1353	G
1	A	1357	A
1	A	1361	G
1	A	1362	C
1	A	1363	C
1	A	1363(A)	A
1	A	1364	U
1	A	1370	G
1	A	1376	U
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1394	A
1	A	1396	A
1	A	1398	A
1	A	1401	G

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Mol	Chain	Res	Type
1	A	1412	C
1	A	1415	G
1	A	1440	C
1	A	1442	G
1	A	1443	G
1	A	1445	C
1	A	1446	U
1	A	1447	A
1	A	1452	C
1	A	1456	G
1	A	1457	G
1	A	1459	C
1	A	1484	C
1	A	1488	G
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1508	G
1	A	1517	G
1	A	1520	G
1	A	1524	C
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1535	C
1	A	1538	C
24	Y	21	G
24	Y	23	C
24	Y	24	A
24	Y	26	G
24	Y	28	A
24	Y	29	G
24	Y	31	U
24	Y	32	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
24	Y	34	A
24	Y	35	A
24	Y	36	A
24	Y	37	U
24	Y	38	G
24	Y	39	U
25	Z	3	C
25	Z	4	G
25	Z	6	G
25	Z	7	G
25	Z	9	G
25	Z	13	C
25	Z	14	A
25	Z	16	C
25	Z	17	C
25	Z	17(A)	U
25	Z	18	G
25	Z	19	G
25	Z	20	U
25	Z	21	A
25	Z	26	G
25	Z	34	C
25	Z	37	A
25	Z	40	C
25	Z	42	G
25	Z	46	G7M
25	Z	47	U
25	Z	48	C
25	Z	55	PSU
25	Z	57	A
25	Z	59	A
25	Z	60	U
25	Z	61	C
25	Z	67	C
25	Z	68	C
25	Z	74	C
25	Z	75	C
25	Z	76	A

All (125) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	A	7	G
1	A	30	U
1	A	48	C
1	A	49	U
1	A	51	A
1	A	60	A
1	A	115	G
1	A	119	A
1	A	125	U
1	A	129(A)	G
1	A	181	G
1	A	197	A
1	A	202	U
1	A	243	A
1	A	250	A
1	A	251	G
1	A	266	G
1	A	279	A
1	A	281	G
1	A	289	G
1	A	328	C
1	A	329	A
1	A	344	A
1	A	351	G
1	A	356	A
1	A	366	C
1	A	367	U
1	A	372	C
1	A	421	U
1	A	428	G
1	A	429	U
1	A	481	G
1	A	484	G
1	A	496	A
1	A	509	A
1	A	518	C
1	A	531	U
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U

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Mol	Chain	Res	Type
1	A	575	G
1	A	577	G
1	A	595	G
1	A	624	C
1	A	641	U
1	A	653	A
1	A	671	G
1	A	687	A
1	A	701	C
1	A	702	A
1	A	721	G
1	A	748	C
1	A	753	A
1	A	770	C
1	A	792	A
1	A	809	G
1	A	812	C
1	A	865	A
1	A	872	A
1	A	884	U
1	A	934	C
1	A	954	G
1	A	960	U
1	A	965	A
1	A	968	A
1	A	975	A
1	A	976	G
1	A	982	U
1	A	992	U
1	A	993	G
1	A	1001	A
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1101	A
1	A	1145	C
1	A	1151	A
1	A	1182	G
1	A	1190	G
1	A	1196	U
1	A	1200	C
1	A	1201	A

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Mol	Chain	Res	Type
1	A	1213	A
1	A	1214	C
1	A	1224	G
1	A	1249	C
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1297	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1303	C
1	A	1319	A
1	A	1335	C
1	A	1336	C
1	A	1345	U
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1397	C
1	A	1400	C
1	A	1442(B)	A
1	A	1447	A
1	A	1452	C
1	A	1488	G
1	A	1493	A
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1534	A
24	Y	31	U
24	Y	35	A
24	Y	38	G
25	Z	16	C
25	Z	17	C
25	Z	17(A)	U
25	Z	33	U
25	Z	36	U
25	Z	47	U
25	Z	51	C
25	Z	60	U
25	Z	62	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$
25	OMC	Z	32	25	15,22,23	0.85	1 (6%)	20,31,34	1.92	5 (25%)
25	G7M	Z	46	25	18,26,27	2.92	3 (16%)	21,39,42	2.92	6 (28%)
25	5MU	Z	54	25	13,22,23	0.83	0	16,32,35	3.85	3 (18%)
25	PSU	Z	55	25	15,21,22	0.80	0	16,30,33	2.57	6 (37%)
25	4SU	Z	8	25	12,21,22	1.07	1 (8%)	15,30,33	1.77	6 (40%)

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
25	OMC	Z	32	25	-	0/5/27/28	0/2/2/2
25	G7M	Z	46	25	-	0/3/25/26	0/3/3/3
25	5MU	Z	54	25	-	0/3/25/26	0/2/2/2
25	PSU	Z	55	25	-	0/7/25/26	0/2/2/2
25	4SU	Z	8	25	-	0/3/25/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	32	OMC	O4'-C1'	2.61	1.45	1.41
25	Z	8	4SU	O4'-C1'	3.06	1.45	1.41
25	Z	46	G7M	C6-C5	4.24	1.49	1.41
25	Z	46	G7M	C8-N7	7.84	1.47	1.33
25	Z	46	G7M	C8-N9	8.08	1.48	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	54	5MU	C5-C4-N3	-10.69	116.37	125.35
25	Z	46	G7M	N7-C8-N9	-7.72	97.28	108.67
25	Z	46	G7M	C5-C6-N1	-6.30	115.28	123.52
25	Z	55	PSU	C4'-O4'-C1'	-4.63	104.77	109.54
25	Z	8	4SU	C5-C4-N3	-3.47	119.89	123.56
25	Z	55	PSU	C5-C6-N1	-3.22	119.89	124.38
25	Z	46	G7M	N3-C2-N1	-2.86	123.67	127.56
25	Z	8	4SU	C6-N1-C2	-2.57	117.14	121.33
25	Z	32	OMC	C6-N1-C2	-2.36	117.48	121.33
25	Z	46	G7M	CN7-N7-C8	-2.29	113.34	125.31
25	Z	32	OMC	C5-C4-N3	-2.24	118.95	121.79
25	Z	55	PSU	C5-C1'-C2'	-2.21	111.68	115.44
25	Z	8	4SU	O4'-C4'-C5'	2.13	116.92	109.29
25	Z	8	4SU	O5'-C5'-C4'	2.23	117.10	109.09
25	Z	8	4SU	O3'-C3'-C2'	2.28	119.23	111.86
25	Z	32	OMC	N4-C4-N3	2.38	120.67	116.50
25	Z	32	OMC	O4'-C1'-N1	2.40	112.65	108.10
25	Z	8	4SU	C4'-O4'-C1'	2.52	112.31	109.64
25	Z	54	5MU	O4'-C1'-N1	2.66	113.16	108.10
25	Z	55	PSU	O4'-C4'-C5'	2.80	119.31	109.29
25	Z	46	G7M	O4'-C1'-N9	3.26	114.26	108.11
25	Z	55	PSU	C3'-C2'-C1'	3.31	105.64	101.71
25	Z	32	OMC	C6-C5-C4	6.23	119.88	117.44
25	Z	46	G7M	C6-N1-C2	6.39	123.37	115.88
25	Z	55	PSU	C4-N3-C2	6.78	120.81	115.16
25	Z	54	5MU	C4-N3-C2	10.09	123.58	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Z	32	OMC	2	0
25	Z	46	G7M	4	0
25	Z	54	5MU	2	0
25	Z	55	PSU	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.



## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	6
25	Z	3
24	Y	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	55:PSU	O3'	56:C	P	5.82
1	A	841:U	O3'	848:C	P	5.50
1	A	93:G	O3'	96:U	P	4.90
1	A	84:U	O3'	88:A	P	4.32
1	A	1442(A):G	O3'	1442(B):A	P	3.51
1	Y	32:A	O3'	33:A	P	3.38
1	A	927:G	O3'	928:G	P	3.26
1	A	204:U	O3'	216:G	P	3.23
1	Z	14:A	O3'	15:G	P	3.20
1	Z	42:G	O3'	43:A	P	1.77