wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:47 PM BST

PDB ID	:	5GAD
EMDB ID:	:	EMD-8000
Title	:	RNC-SRP-SR complex early state
Authors	:	Jomaa, A.; Boehringer, D.; Leibundgut, M.; Ban, N.
Deposited on	:	2015-11-24
Resolution	:	3.70 Å(reported)
Based on PDB ID	:	?

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

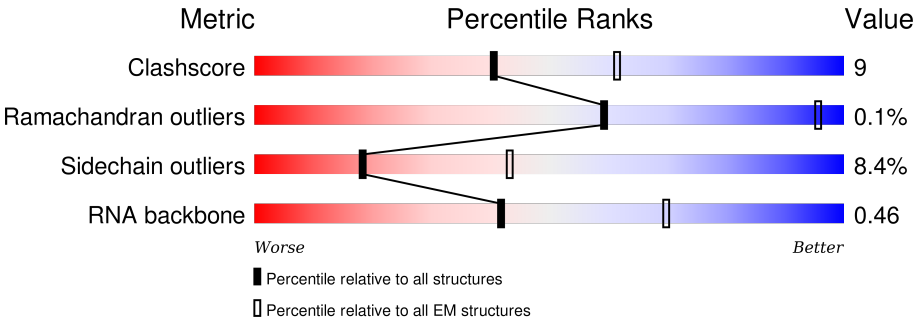
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	113	12% 15% 11% • 62%
2	2	3	33% 33% 33%
3	A	2903	54% 37% 8% ••
4	B	120	73% 24% •
5	C	273	70% 26% ••
6	D	209	78% 21% •
7	E	201	78% 21% •
8	F	179	59% 35% ••

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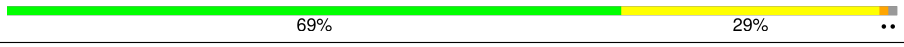
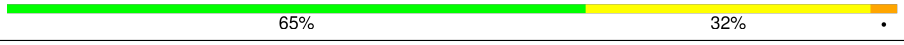
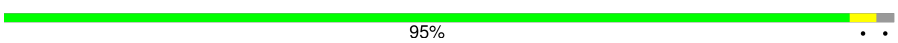
Mol	Chain	Length	Quality of chain
9	G	177	
10	H	149	
11	I	165	
12	J	142	
13	K	142	
14	L	123	
15	M	144	
16	N	136	
17	O	127	
18	P	117	
19	Q	115	
20	R	118	
21	S	103	
22	T	110	
23	U	100	
24	V	104	
25	W	94	
26	X	85	
27	Y	78	
28	Z	63	
29	a	59	
30	b	57	
31	c	55	
32	d	46	
33	e	65	

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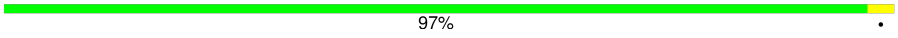
Mol	Chain	Length	Quality of chain
34	f	38	
35	i	450	
36	k	18	
37	l	497	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 98006 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 ESRP 4.5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	43	926	413	174	296	43	0	0

- Molecule 2 is a RNA chain called tRNA CCAend.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	3	62	28	11	20	3	0	0

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	A	2883	61902	27613	11397	20009	2883	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

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

- Molecule 5 is a protein called 50S ribosomal protein L2.

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

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

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

- Molecule 8 is a protein called 50S ribosomal protein L5.

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

- Molecule 9 is a protein called 50S ribosomal protein L6.

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

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	125	Total	C	N	O	S	0	0
			946	599	169	175	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	85	VAL	SER	conflict	UNP P0A7J3
I	86	THR	MET	conflict	UNP P0A7J3

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

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

- Molecule 15 is a protein called 50S ribosomal protein L15.

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

- Molecule 16 is a protein called 50S ribosomal protein L16.

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

- Molecule 17 is a protein called 50S ribosomal protein L17.

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

- Molecule 18 is a protein called 50S ribosomal protein L18.

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

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called 50S ribosomal protein L21.

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

- Molecule 22 is a protein called 50S ribosomal protein L22.

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

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	95	Total 756	C 479	N 141	O 135	S 1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L24.

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

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	76	Total 580	C 359	N 117	O 103	S 1	0	0

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

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

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	c	51	Total	C	N	O	0	0
			414	266	76	72		

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a protein called Signal recognition particle protein Ffh.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	450	Total	C	N	O	S	0	0
			3337	2109	600	610	18		

- Molecule 36 is a protein called 1A9L SS.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	18	Total	C	N	O	S	0	0
			137	94	20	22	1		

- Molecule 37 is a protein called Signal recognition particle receptor FtsY.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	198	Total	C	N	O	S	0	0
			1492	944	266	277	5		

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	P	1	Total	Mg	0
			1	1	
38	i	1	Total	Mg	0
			1	1	
38	D	1	Total	Mg	0
			1	1	
38	E	1	Total	Mg	0
			1	1	
38	B	11	Total	Mg	0
			11	11	
38	b	1	Total	Mg	0
			1	1	
38	C	2	Total	Mg	0
			2	2	
38	A	412	Total	Mg	0
			412	412	
38	2	1	Total	Mg	0
			1	1	

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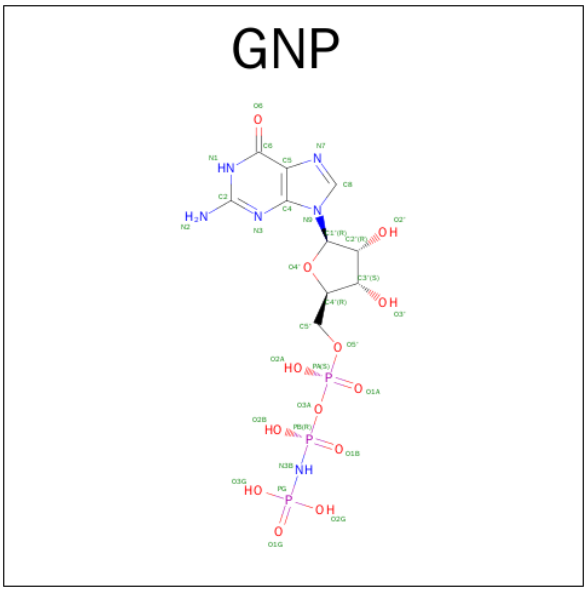
Mol	Chain	Residues	Atoms	AltConf
38	l	1	Total Mg 1 1	0
38	R	1	Total Mg 1 1	0

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
39	f	1	Total Zn 1 1	0

- Molecule 40 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



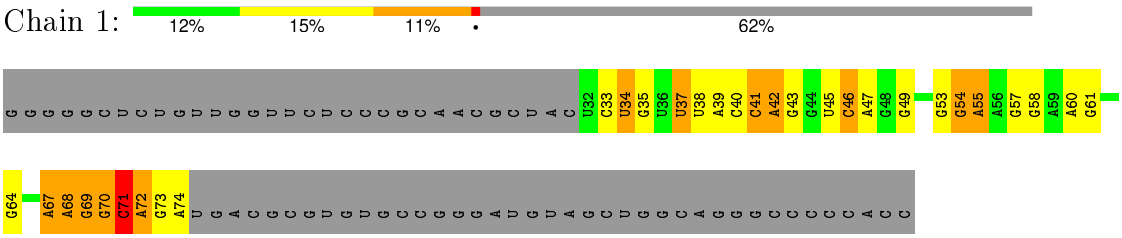
Mol	Chain	Residues	Atoms	AltConf
40	i	1	Total C N O P 32 10 6 13 3	0
40	l	1	Total C N O P 32 10 6 13 3	0

3 Residue-property plots (i)

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

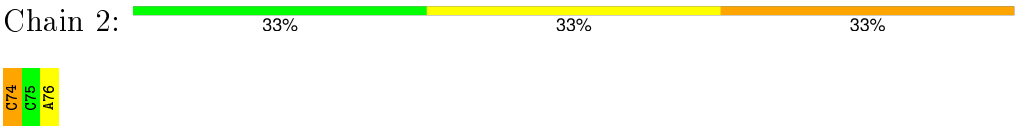
- Molecule 1: ESRP 4.5S RNA

Chain 1:



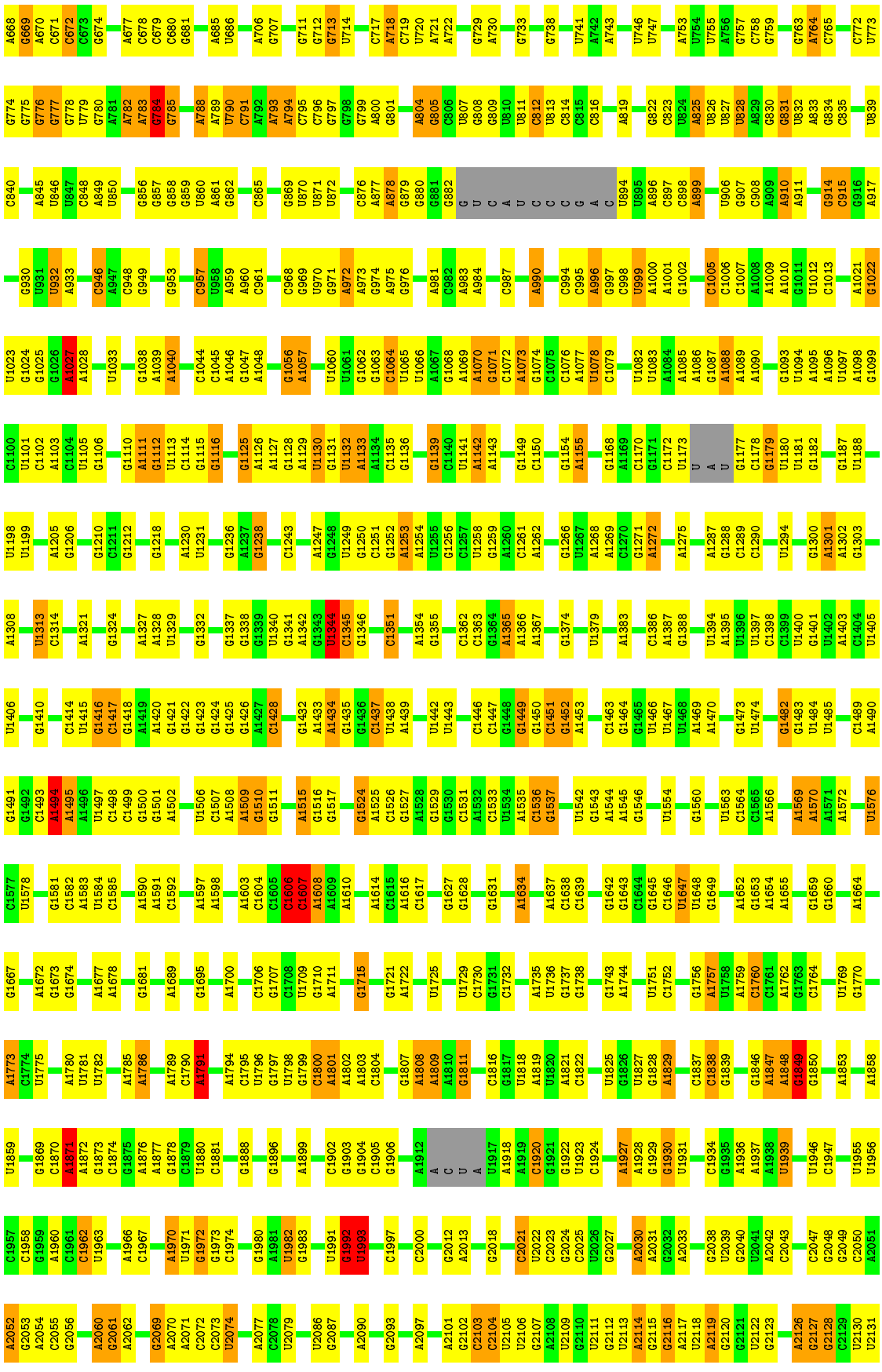
- Molecule 2: tRNA CCAend

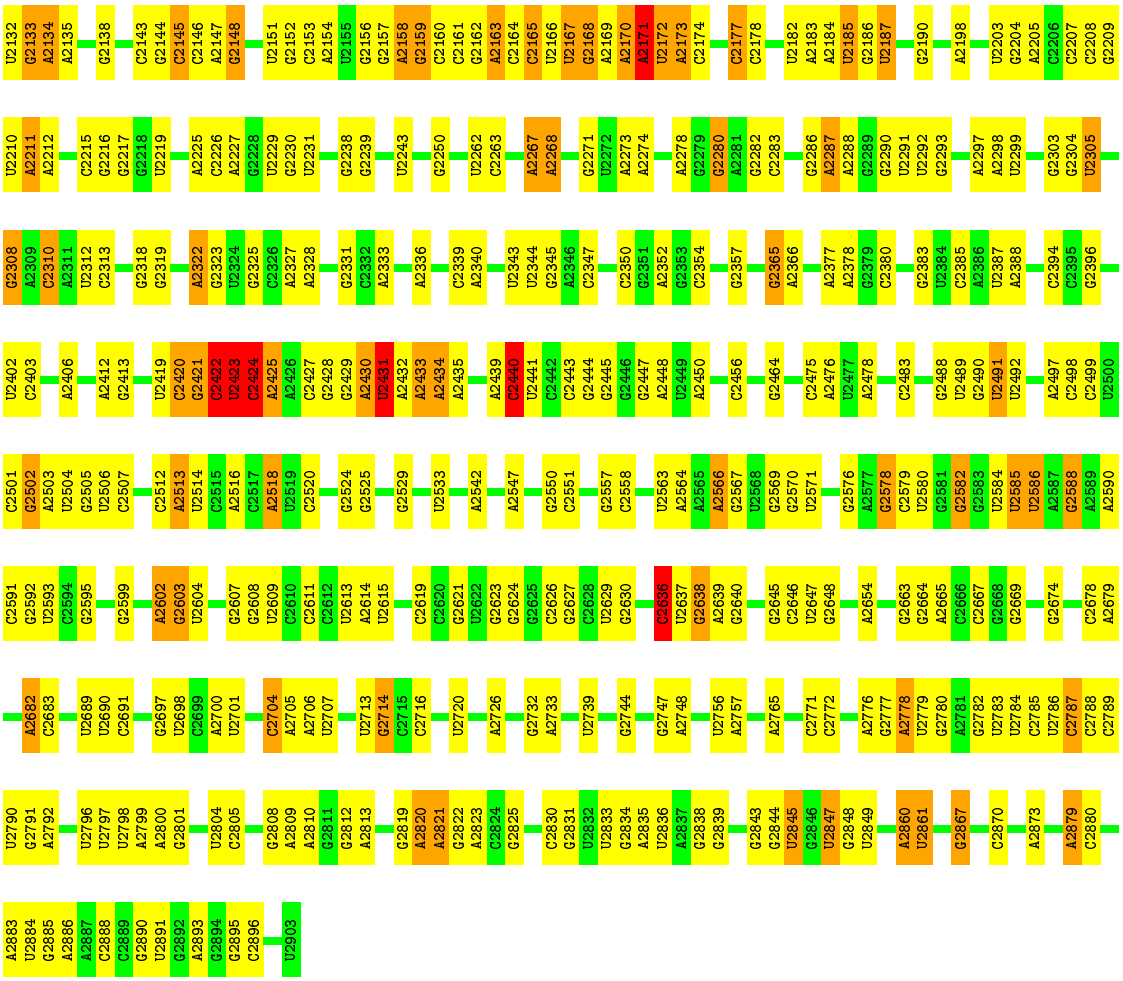
Chain 2:



- Molecule 3: 23S rRNA

Chain A:



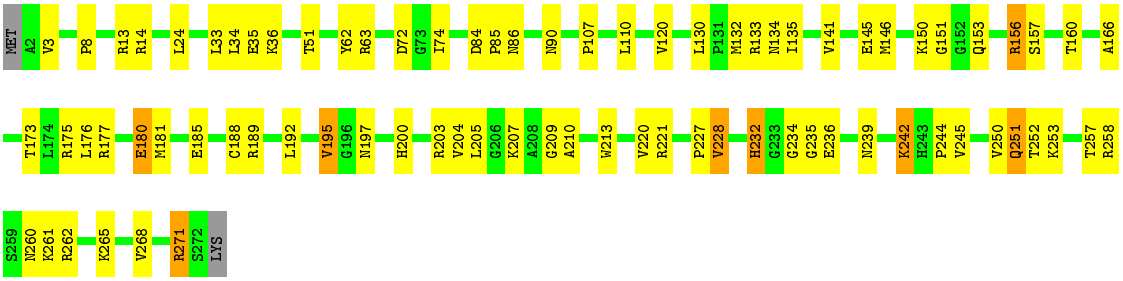


- Molecule 4: 5S rRNA

Chain B:

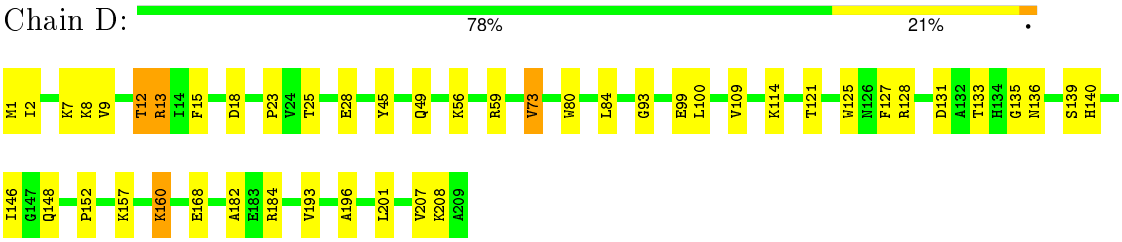
- Molecule 5: 50S ribosomal protein L2

Chain C:



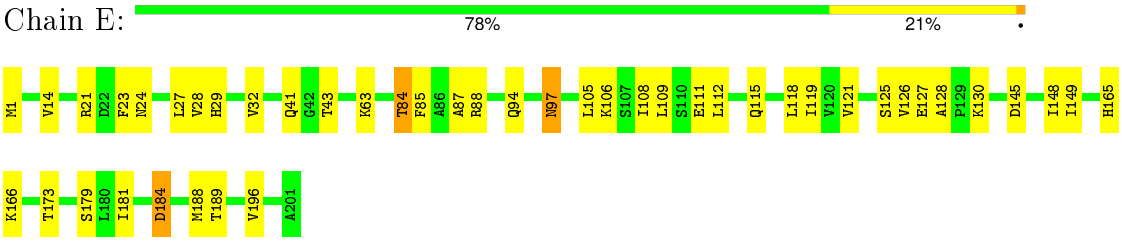
- Molecule 6: 50S ribosomal protein L3

Chain D:



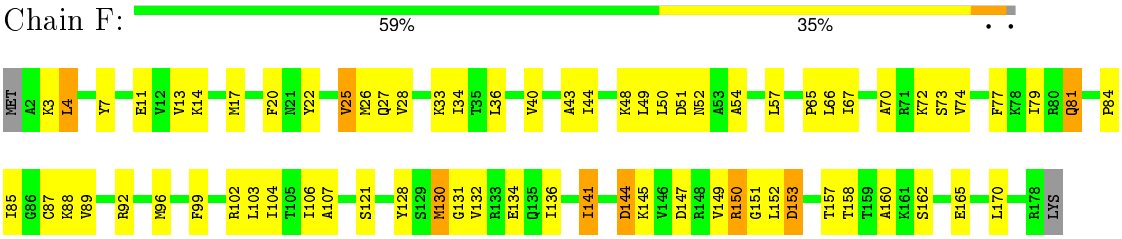
• Molecule 7: 50S ribosomal protein L4

Chain E:



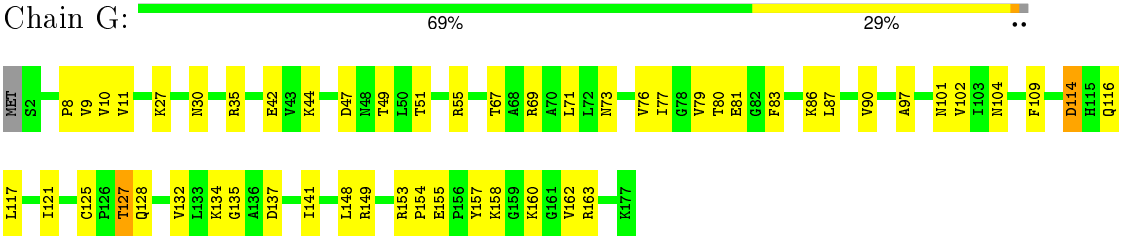
• Molecule 8: 50S ribosomal protein L5

Chain F:



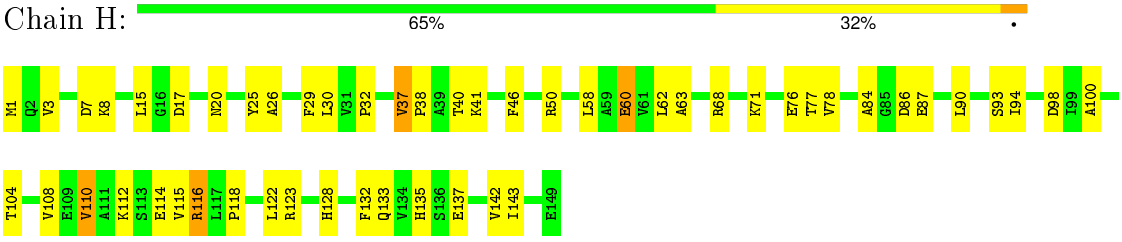
• Molecule 9: 50S ribosomal protein L6

Chain G:



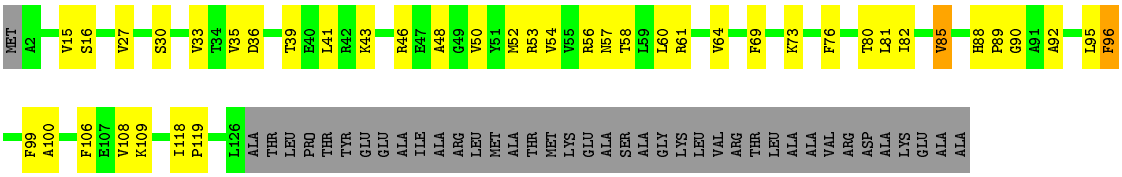
• Molecule 10: 50S ribosomal protein L9

Chain H:



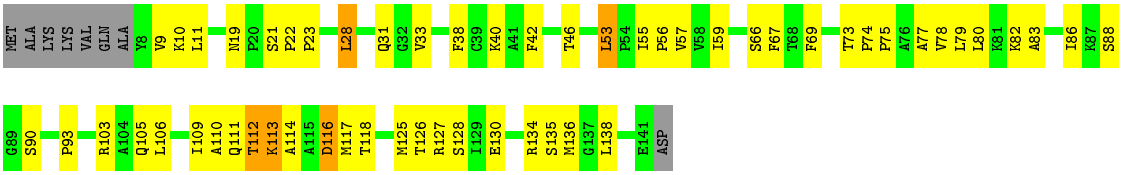
• Molecule 11: 50S ribosomal protein L10

Chain I:



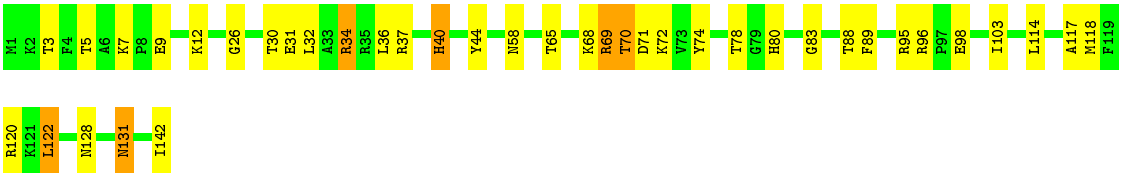
- Molecule 12: 50S ribosomal protein L11

Chain J:



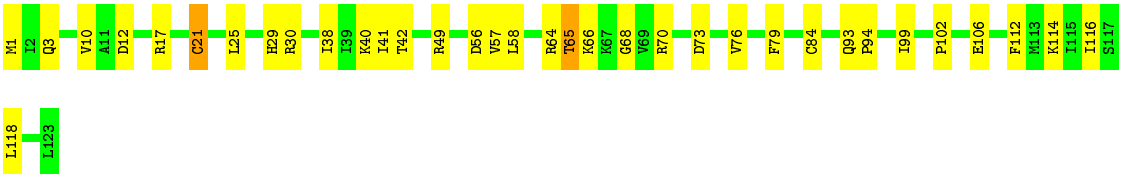
- Molecule 13: 50S ribosomal protein L13

Chain K:



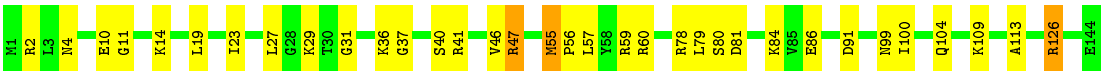
- Molecule 14: 50S ribosomal protein L14

Chain L:



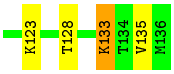
- Molecule 15: 50S ribosomal protein L15

Chain M:



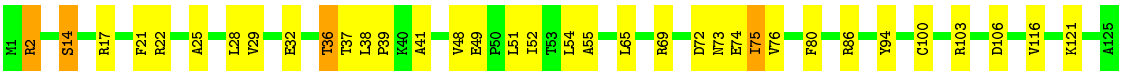
- Molecule 16: 50S ribosomal protein L16

Chain N:



• Molecule 17: 50S ribosomal protein L17

Chain O:



• Molecule 18: 50S ribosomal protein L18

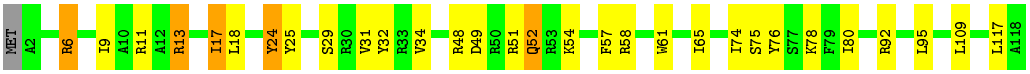
Chain P:

• Molecule 19: 50S ribosomal protein L19

Chain Q:

• Molecule 20: 50S ribosomal protein L20

Chain R:

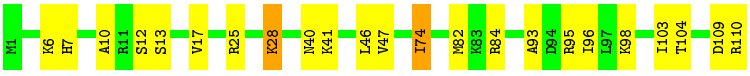


• Molecule 21: 50S ribosomal protein L21

Chain S:

• Molecule 22: 50S ribosomal protein L22

Chain T:

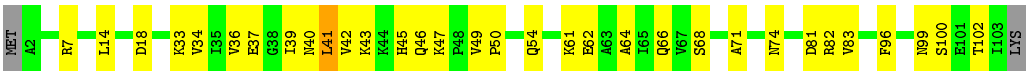


• Molecule 23: 50S ribosomal protein L23

Chain U:

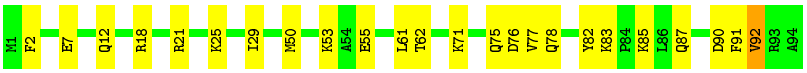
• Molecule 24: 50S ribosomal protein L24

Chain V:



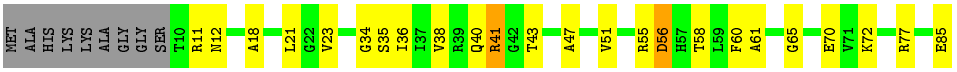
• Molecule 25: 50S ribosomal protein L25

Chain W:



• Molecule 26: 50S ribosomal protein L27

Chain X:

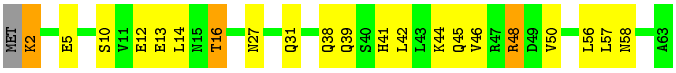


• Molecule 27: 50S ribosomal protein L28

Chain Y:

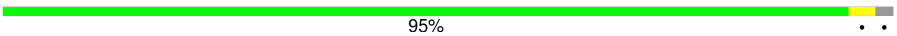
• Molecule 28: 50S ribosomal protein L29

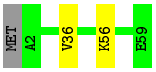
Chain Z:



• Molecule 29: 50S ribosomal protein L30

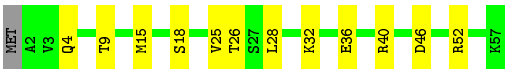
Chain a:





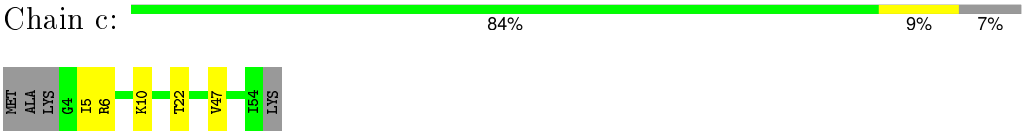
• Molecule 30: 50S ribosomal protein L32

Chain b:



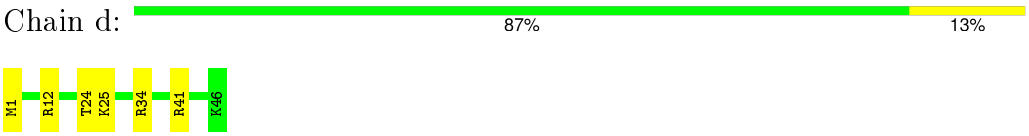
- Molecule 31: 50S ribosomal protein L33

Chain c:



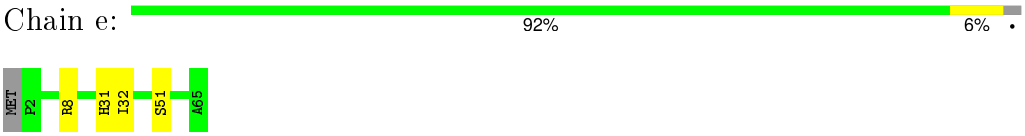
- Molecule 32: 50S ribosomal protein L34

Chain d:



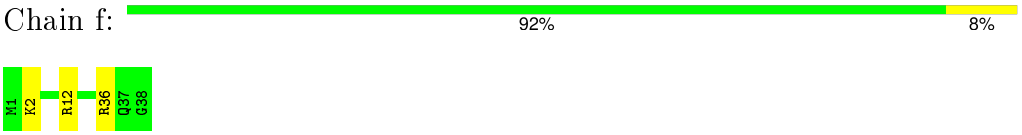
- Molecule 33: 50S ribosomal protein L35

Chain e:



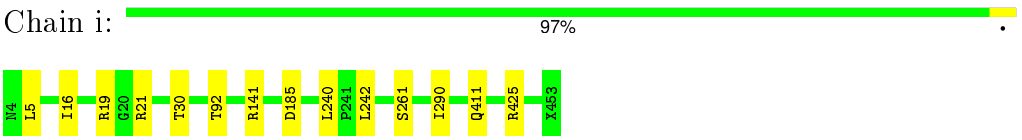
- Molecule 34: 50S ribosomal protein L36

Chain f:



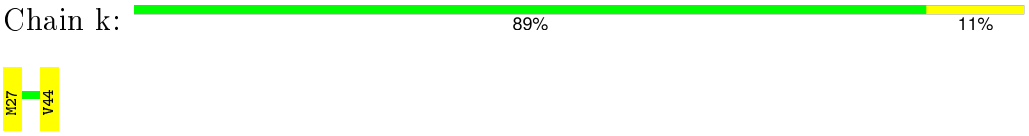
- Molecule 35: Signal recognition particle protein Ffh

Chain i:



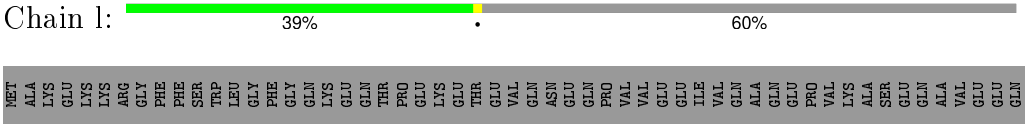
- Molecule 36: 1A9L SS

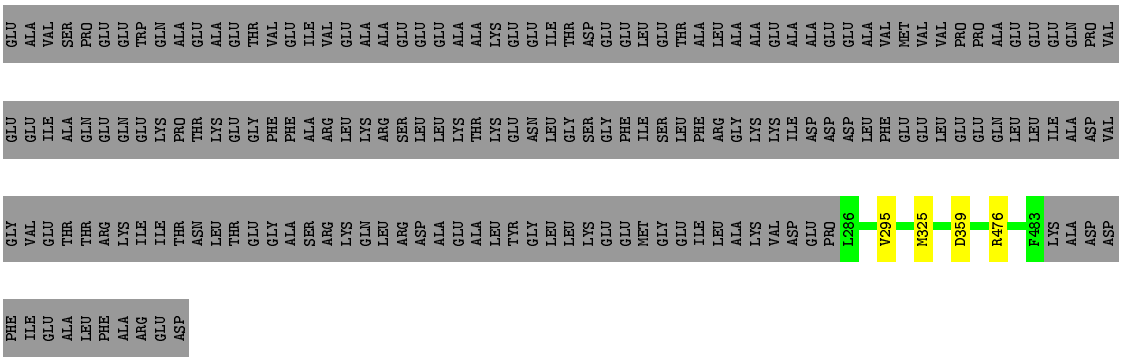
Chain k:



- Molecule 37: Signal recognition particle receptor FtsY

Chain l:




GLU ALA VAL SER PRO GLU GLU TRP GLN ALA GLU ALA GLU THR VAL GLU ILE VAL GLU ALA ALA GLU GLU GLU ALA ALA LYS GLU GLU ILE THR ASP GLU GLU LEU GLU THR ALA LEU ALA ALA GLU ALA ALA GLU GLU ALA VAL MET VAL VAL PRO PRO ALA GLU GLU GLN PRO VAL
GLU GLU ILE ALA GLN GLU GLN GLU LYS PRO THR LYS GLU GLY PHE PHE ALA ARG LEU LYS ARG SER LEU LEU LYS THR LYS GLU ASN LEU GLY SER GLY PHE ILE SER LEU PHE ARG GLY LYS LYS ILE ASP ASP LEU PHE GLU GLU LEU GLU GLU GLN LEU LEU ILE ALA ASP VAL
GLY VAL GLU THR THR ARG LYS ILE ILE THR ASN LEU THR GLU GLY ALA SER ARG LYS GLN LEU ARG ASP ALA GLU ALA LEU TYR GLY LEU LEU LYS GLU GLU MET GLY GLU ILE LEU ALA LYS VAL ASP GLU PRO L286 V295 M325 D359 R476 F483 LYS ALA ASP ASP
PHE ILE GLU ALA LEU PHE ALA ARG GLU ASP

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	81197	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, GNP

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	1	0.30	0/1037	0.99	2/1616 (0.1%)
10	H	0.42	0/1121	0.57	0/1515
11	I	0.48	0/958	0.62	1/1292 (0.1%)
12	J	0.58	0/993	0.69	1/1341 (0.1%)
13	K	0.46	0/1152	0.57	0/1551
14	L	0.45	0/955	0.63	0/1279
15	M	0.47	0/1062	0.64	0/1413
16	N	0.48	0/1093	0.59	0/1460
17	O	0.47	0/1006	0.67	0/1345
18	P	0.41	0/910	0.56	0/1219
19	Q	0.48	0/929	0.60	0/1242
2	2	0.56	0/68	1.26	1/103 (1.0%)
20	R	0.56	0/960	0.59	0/1278
21	S	0.46	0/829	0.62	0/1107
22	T	0.52	0/864	0.71	0/1156
23	U	0.64	3/763 (0.4%)	0.73	1/1021 (0.1%)
24	V	0.38	0/787	0.54	0/1051
25	W	0.40	0/766	0.57	0/1025
26	X	0.50	0/587	0.60	0/776
27	Y	0.48	0/635	0.61	0/848
28	Z	0.33	0/500	0.47	0/661
29	a	0.38	0/453	0.56	0/605
3	A	0.68	13/69329 (0.0%)	1.17	188/108152 (0.2%)
30	b	0.43	0/450	0.62	0/599
31	c	0.44	0/421	0.61	0/561
32	d	0.51	0/380	0.66	0/498
33	e	0.47	0/513	0.62	0/676
34	f	0.49	0/303	0.58	0/397
35	i	0.31	0/2942	0.51	0/3950
36	k	0.32	0/137	0.58	0/186
37	l	0.37	0/1511	1.08	3/2040 (0.1%)
4	B	0.51	0/2872	1.04	1/4478 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
5	C	0.48	0/2121	0.65	0/2852
6	D	0.47	0/1586	0.63	0/2134
7	E	0.44	0/1571	0.61	1/2113 (0.0%)
8	F	0.39	0/1434	0.56	0/1926
9	G	0.39	0/1343	0.58	0/1816
All	All	0.61	16/105341 (0.0%)	1.04	199/157282 (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
12	J	0	1
35	i	0	1
5	C	0	1
9	G	0	1
All	All	0	4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2542	A	N9-C4	-6.88	1.33	1.37
23	U	89	GLU	N-CA	6.84	1.60	1.46
3	A	1254	A	N9-C4	-6.35	1.34	1.37
3	A	2114	A	N9-C4	6.24	1.41	1.37
3	A	1321	A	N9-C4	6.01	1.41	1.37
3	A	563	A	N9-C4	-5.91	1.34	1.37
3	A	776	G	N9-C4	5.90	1.42	1.38
23	U	88	LYS	C-N	5.87	1.47	1.34
3	A	1490	A	N9-C4	5.76	1.41	1.37
3	A	1010	A	N9-C4	-5.62	1.34	1.37
3	A	586	A	N3-C4	-5.47	1.31	1.34
3	A	1254	A	N3-C4	-5.36	1.31	1.34
3	A	960	A	N9-C4	-5.16	1.34	1.37
3	A	1678	A	N9-C4	-5.14	1.34	1.37
3	A	514	A	N9-C4	-5.11	1.34	1.37
23	U	88	LYS	CA-C	5.09	1.66	1.52

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	l	476	ARG	NE-CZ-NH2	-25.15	107.72	120.30
37	l	476	ARG	NE-CZ-NH1	-25.05	107.78	120.30
37	l	476	ARG	NH1-CZ-NH2	22.82	144.50	119.40
3	A	2423	U	C6-N1-C2	-12.22	113.67	121.00
3	A	1838	C	C6-N1-C2	9.47	124.09	120.30
3	A	2422	C	O4'-C1'-N1	9.25	115.60	108.20
3	A	2423	U	C5-C6-N1	8.77	127.08	122.70
3	A	1584	U	C2-N1-C1'	8.48	127.88	117.70
3	A	776	G	C8-N9-C4	-8.25	103.10	106.40
3	A	2431	U	N3-C2-O2	-8.03	116.58	122.20
3	A	275	C	C6-N1-C2	-7.84	117.17	120.30
3	A	1760	C	C6-N1-C2	7.60	123.34	120.30
3	A	1584	U	N1-C2-O2	7.30	127.91	122.80
3	A	2422	C	N3-C2-O2	-7.27	116.81	121.90
1	1	71	C	C6-N1-C2	-7.20	117.42	120.30
3	A	2431	U	C5-C4-O4	7.01	130.10	125.90
3	A	1992	G	C4-C5-N7	7.00	113.60	110.80
3	A	2424	C	O4'-C1'-N1	6.97	113.78	108.20
3	A	2177	C	C6-N1-C2	-6.92	117.53	120.30
3	A	214	G	N3-C4-C5	-6.90	125.15	128.60
3	A	2636	C	C2-N1-C1'	6.87	126.36	118.80
3	A	1027	A	C8-N9-C4	6.80	108.52	105.80
3	A	2207	C	C6-N1-C2	-6.80	117.58	120.30
3	A	2614	A	C6-N1-C2	-6.80	114.52	118.60
3	A	137	U	C5-C4-O4	-6.78	121.83	125.90
3	A	2422	C	C6-N1-C2	-6.74	117.61	120.30
3	A	1849	G	C8-N9-C4	-6.70	103.72	106.40
3	A	1607	C	C6-N1-C2	-6.65	117.64	120.30
3	A	1064	C	C6-N1-C2	-6.61	117.65	120.30
3	A	102	U	C2-N1-C1'	6.61	125.63	117.70
3	A	776	G	C4-N9-C1'	6.58	135.06	126.50
3	A	2456	C	C6-N1-C2	-6.56	117.67	120.30
3	A	2000	C	C6-N1-C2	6.56	122.92	120.30
3	A	2542	A	C2-N3-C4	-6.53	107.33	110.60
3	A	1652	A	C8-N9-C4	6.51	108.40	105.80
3	A	784	G	P-O3'-C3'	6.49	127.48	119.70
3	A	1849	G	N7-C8-N9	6.48	116.34	113.10
3	A	1531	C	C5-C6-N1	6.44	124.22	121.00
3	A	805	G	C8-N9-C4	6.39	108.96	106.40
3	A	12	U	N3-C2-O2	-6.38	117.74	122.20
3	A	1313	U	N3-C2-O2	-6.37	117.74	122.20
3	A	906	U	C5-C4-O4	6.37	129.72	125.90
3	A	776	G	N3-C4-C5	-6.28	125.46	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1272	A	C8-N9-C4	6.25	108.30	105.80
3	A	832	U	C5-C6-N1	-6.25	119.58	122.70
3	A	1606	C	N3-C2-O2	-6.24	117.53	121.90
3	A	2104	C	C6-N1-C2	-6.23	117.81	120.30
3	A	758	C	C6-N1-C2	-6.22	117.81	120.30
3	A	130	C	N3-C4-C5	6.18	124.37	121.90
3	A	2499	C	N1-C2-O2	6.18	122.61	118.90
3	A	1695	G	N9-C4-C5	-6.18	102.93	105.40
3	A	1128	G	C8-N9-C4	6.15	108.86	106.40
3	A	2542	A	N3-C4-C5	6.14	131.10	126.80
3	A	2704	C	C6-N1-C2	-6.14	117.84	120.30
3	A	611	C	C6-N1-C2	-6.12	117.85	120.30
3	A	483	A	C8-N9-C4	6.11	108.24	105.80
3	A	1362	C	C6-N1-C2	-6.09	117.86	120.30
3	A	2077	A	C6-N1-C2	-6.07	114.96	118.60
3	A	1848	A	C8-N9-C4	-6.07	103.37	105.80
3	A	733	G	C4-C5-N7	6.06	113.22	110.80
3	A	2109	U	C6-N1-C2	-6.02	117.39	121.00
3	A	804	A	C8-N9-C4	6.02	108.21	105.80
3	A	1584	U	C5-C6-N1	5.99	125.70	122.70
23	U	88	LYS	CB-CA-C	5.99	122.38	110.40
3	A	1072	C	C6-N1-C2	-5.99	117.91	120.30
3	A	2171	A	O4'-C1'-N9	5.99	112.99	108.20
3	A	102	U	N1-C2-O2	5.97	126.98	122.80
3	A	2433	A	N1-C2-N3	5.95	132.28	129.30
3	A	1992	G	N9-C4-C5	-5.95	103.02	105.40
3	A	774	G	C8-N9-C4	5.94	108.78	106.40
3	A	832	U	C2-N3-C4	-5.93	123.44	127.00
3	A	1531	C	C6-N1-C2	-5.93	117.93	120.30
3	A	2691	C	C6-N1-C2	5.92	122.67	120.30
3	A	2052	A	N1-C6-N6	5.89	122.14	118.60
3	A	2153	C	C5-C6-N1	5.89	123.95	121.00
3	A	2423	U	N3-C4-C5	-5.87	111.08	114.60
3	A	1584	U	N3-C2-O2	-5.87	118.09	122.20
12	J	53	LEU	CA-CB-CG	5.85	128.76	115.30
3	A	790	U	N1-C2-O2	5.85	126.89	122.80
3	A	1261	C	C6-N1-C2	5.83	122.63	120.30
3	A	1470	A	C8-N9-C4	-5.83	103.47	105.80
3	A	987	C	N3-C4-C5	5.82	124.23	121.90
3	A	776	G	O4'-C1'-N9	5.82	112.86	108.20
3	A	2820	A	C8-N9-C4	5.81	108.12	105.80
3	A	2845	U	C2-N3-C4	-5.78	123.53	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2440	C	C6-N1-C2	5.77	122.61	120.30
3	A	2580	U	C6-N1-C2	-5.74	117.56	121.00
3	A	741	U	C5-C6-N1	-5.71	119.84	122.70
3	A	1643	G	C8-N9-C4	-5.71	104.11	106.40
3	A	793	A	C5-C6-N6	-5.71	119.14	123.70
3	A	205	G	O4'-C1'-N9	5.70	112.76	108.20
7	E	109	LEU	CA-CB-CG	-5.69	102.22	115.30
3	A	141	G	N7-C8-N9	5.67	115.93	113.10
3	A	1526	C	C6-N1-C2	-5.65	118.04	120.30
3	A	1045	C	C6-N1-C2	5.65	122.56	120.30
11	I	95	LEU	CA-CB-CG	5.63	128.25	115.30
3	A	1604	C	C5-C6-N1	-5.62	118.19	121.00
1	1	71	C	C5-C6-N1	5.62	123.81	121.00
3	A	2636	C	C6-N1-C1'	-5.62	114.06	120.80
3	A	1993	U	C5-C6-N1	-5.62	119.89	122.70
3	A	1871	A	C8-N9-C4	-5.61	103.56	105.80
3	A	1303	G	C8-N9-C4	5.57	108.63	106.40
3	A	2145	C	C6-N1-C2	-5.56	118.08	120.30
3	A	776	G	N7-C8-N9	5.55	115.88	113.10
3	A	76	C	C5-C6-N1	5.55	123.78	121.00
3	A	783	A	C8-N9-C4	-5.55	103.58	105.80
3	A	2582	G	N3-C4-C5	-5.54	125.83	128.60
3	A	130	C	C6-N1-C2	5.54	122.52	120.30
3	A	1659	G	N3-C4-C5	5.52	131.36	128.60
3	A	2243	U	C5-C6-N1	-5.50	119.95	122.70
3	A	1848	A	N7-C8-N9	5.50	116.55	113.80
3	A	793	A	C2-N3-C4	5.50	113.35	110.60
3	A	2588	G	N3-C4-C5	5.49	131.34	128.60
3	A	972	A	N1-C6-N6	-5.48	115.31	118.60
3	A	2380	C	C6-N1-C2	-5.48	118.11	120.30
3	A	825	A	C6-N1-C2	-5.47	115.32	118.60
3	A	946	C	N3-C2-O2	-5.45	118.08	121.90
3	A	1314	C	C6-N1-C2	-5.45	118.12	120.30
3	A	2022	U	C6-N1-C2	5.45	124.27	121.00
3	A	2595	G	C4-N9-C1'	-5.45	119.42	126.50
3	A	2498	C	C6-N1-C2	-5.44	118.12	120.30
3	A	816	C	C6-N1-C2	-5.44	118.12	120.30
3	A	2153	C	C6-N1-C2	-5.43	118.13	120.30
3	A	410	G	N3-C4-C5	-5.42	125.89	128.60
3	A	613	A	P-O3'-C3'	5.42	126.20	119.70
3	A	642	U	O4'-C1'-N1	5.42	112.53	108.20
3	A	1172	C	C6-N1-C2	-5.42	118.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1584	U	C6-N1-C1'	-5.41	113.63	121.20
3	A	1072	C	C5-C6-N1	5.40	123.70	121.00
4	B	42	C	C6-N1-C2	-5.39	118.14	120.30
3	A	790	U	C2-N1-C1'	5.38	124.16	117.70
3	A	135	U	C5-C6-N1	5.37	125.38	122.70
3	A	755	U	C5-C6-N1	-5.36	120.02	122.70
3	A	972	A	N9-C4-C5	5.35	107.94	105.80
3	A	906	U	O4'-C1'-N1	5.33	112.46	108.20
3	A	809	G	N3-C4-C5	-5.33	125.94	128.60
3	A	2614	A	C5-C6-N1	5.32	120.36	117.70
3	A	569	U	C5-C6-N1	-5.32	120.04	122.70
3	A	206	U	C2-N1-C1'	5.31	124.08	117.70
3	A	1970	A	N1-C2-N3	5.31	131.95	129.30
3	A	793	A	C5-C6-N1	5.30	120.35	117.70
3	A	2645	G	C4-N9-C1'	5.30	133.39	126.50
3	A	12	U	N1-C2-O2	5.30	126.51	122.80
3	A	2423	U	N1-C2-N3	5.30	118.08	114.90
3	A	1351	C	C6-N1-C2	5.29	122.42	120.30
3	A	2542	A	C8-N9-C4	5.28	107.91	105.80
3	A	280	U	P-O3'-C3'	5.28	126.03	119.70
3	A	828	U	C5-C6-N1	-5.28	120.06	122.70
3	A	1078	U	C5-C6-N1	5.27	125.33	122.70
3	A	1606	C	N1-C2-O2	5.26	122.06	118.90
3	A	2645	G	N3-C4-C5	-5.26	125.97	128.60
3	A	375	G	N3-C4-C5	-5.25	125.97	128.60
3	A	2114	A	C8-N9-C4	-5.24	103.70	105.80
3	A	264	C	N3-C2-O2	-5.23	118.24	121.90
3	A	1642	G	N3-C4-C5	5.23	131.21	128.60
3	A	271	G	C8-N9-C4	5.22	108.49	106.40
3	A	1494	A	P-O3'-C3'	5.22	125.97	119.70
3	A	1664	A	C8-N9-C4	-5.22	103.71	105.80
3	A	1848	A	O4'-C1'-N9	5.21	112.37	108.20
3	A	2516	A	C8-N9-C4	5.19	107.88	105.80
3	A	128	C	C6-N1-C2	5.19	122.38	120.30
3	A	672	C	N3-C2-O2	-5.19	118.27	121.90
2	2	74	C	C5-C6-N1	5.18	123.59	121.00
3	A	2000	C	C5-C6-N1	-5.18	118.41	121.00
3	A	375	G	N3-C4-N9	5.18	129.11	126.00
3	A	1958	C	C6-N1-C2	-5.17	118.23	120.30
3	A	1617	C	C2-N3-C4	-5.17	117.31	119.90
3	A	906	U	C2-N1-C1'	-5.14	111.53	117.70
3	A	76	C	C6-N1-C2	-5.14	118.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1102	C	C6-N1-C2	-5.14	118.24	120.30
3	A	2022	U	C5-C6-N1	-5.14	120.13	122.70
3	A	1125	G	C8-N9-C4	-5.12	104.35	106.40
3	A	1617	C	C5-C6-N1	-5.12	118.44	121.00
3	A	30	G	C8-N9-C4	5.12	108.45	106.40
3	A	2090	A	C8-N9-C4	5.11	107.84	105.80
3	A	2580	U	N3-C2-O2	-5.11	118.63	122.20
3	A	804	A	C2-N3-C4	-5.10	108.05	110.60
3	A	1791	A	N1-C6-N6	-5.10	115.54	118.60
3	A	2847	U	C5-C6-N1	-5.09	120.15	122.70
3	A	2267	A	C8-N9-C4	-5.09	103.77	105.80
3	A	2074	U	C2-N1-C1'	5.08	123.80	117.70
3	A	2310	C	C6-N1-C2	-5.07	118.27	120.30
3	A	418	C	C6-N1-C2	-5.06	118.27	120.30
3	A	2013	A	C6-N1-C2	-5.06	115.56	118.60
3	A	2424	C	C5'-C4'-O4'	5.05	115.16	109.10
3	A	2365	G	C8-N9-C4	5.04	108.42	106.40
3	A	809	G	C8-N9-C4	-5.03	104.39	106.40
3	A	2431	U	C4-C5-C6	5.03	122.72	119.70
3	A	1344	U	C5-C6-N1	-5.03	120.19	122.70
3	A	2115	G	N3-C4-C5	-5.03	126.09	128.60
3	A	66	C	N3-C2-O2	-5.03	118.38	121.90
3	A	1652	A	N7-C8-N9	-5.03	111.29	113.80
3	A	2074	U	N3-C2-O2	-5.03	118.68	122.20
3	A	516	C	C6-N1-C2	5.02	122.31	120.30
3	A	1570	A	C8-N9-C4	5.02	107.81	105.80
3	A	102	U	C6-N1-C1'	-5.02	114.17	121.20
3	A	1769	U	C5-C6-N1	-5.02	120.19	122.70
3	A	906	U	C6-N1-C1'	5.02	128.22	121.20
3	A	277	G	C4-N9-C1'	5.00	133.00	126.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	232	HIS	Peptide
9	G	47	ASP	Peptide
12	J	19	ASN	Peptide
35	i	240	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	926	0	467	26	0
2	2	62	0	34	1	0
3	A	61902	0	31133	685	0
4	B	2569	0	1301	20	0
5	C	2082	0	2154	51	0
6	D	1565	0	1616	35	0
7	E	1552	0	1619	24	0
8	F	1410	0	1444	43	0
9	G	1323	0	1371	32	0
10	H	1110	0	1148	25	0
11	I	946	0	978	31	0
12	J	979	0	1028	38	0
13	K	1129	0	1162	24	0
14	L	946	0	1023	19	0
15	M	1053	0	1129	26	0
16	N	1074	0	1157	23	0
17	O	993	0	1034	25	0
18	P	900	0	935	20	0
19	Q	917	0	962	18	0
20	R	947	0	1019	23	0
21	S	816	0	839	20	0
22	T	857	0	922	13	0
23	U	756	0	817	21	0
24	V	779	0	831	18	0
25	W	753	0	780	14	0
26	X	580	0	594	16	0
27	Y	625	0	652	17	0
28	Z	501	0	529	16	0
29	a	449	0	488	0	0
30	b	444	0	458	0	0
31	c	414	0	442	0	0
32	d	377	0	418	0	0
33	e	504	0	572	0	0
34	f	302	0	340	0	0
35	i	3337	0	3457	0	0
36	k	137	0	168	0	0
37	l	1492	0	1544	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	2	1	0	0	0	0
38	A	412	0	0	0	0
38	B	11	0	0	0	0
38	C	2	0	0	0	0
38	D	1	0	0	0	0
38	E	1	0	0	0	0
38	P	1	0	0	0	0
38	R	1	0	0	0	0
38	b	1	0	0	0	0
38	i	1	0	0	0	0
38	l	1	0	0	0	0
39	f	1	0	0	0	0
40	i	32	0	13	0	0
40	l	32	0	13	0	0
All	All	98006	0	66591	1182	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 9.

All (1182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1818:U:OP2	5:C:156:ARG:NH1	2.00	0.95
3:A:1168:G:H1	3:A:1181:U:H3	1.20	0.90
23:U:53:VAL:HG21	23:U:93:LEU:HD11	1.53	0.89
3:A:276:U:O2	3:A:278:A:N6	2.07	0.87
10:H:3:VAL:HG12	10:H:38:PRO:HA	1.57	0.86
3:A:1827:U:OP2	5:C:221:ARG:NH1	2.08	0.86
5:C:107:PRO:HD2	5:C:110:LEU:HD22	1.59	0.84
3:A:287:G:O6	3:A:352:A:N6	2.10	0.84
3:A:2135:A:N6	3:A:2156:G:O2'	2.10	0.83
3:A:2107:G:H1	3:A:2182:U:H3	1.22	0.82
3:A:807:U:OP2	15:M:41:ARG:NH1	2.14	0.81
23:U:53:VAL:HG11	23:U:93:LEU:HD21	1.61	0.81
1:1:49:G:H1	1:1:60:A:H61	1.30	0.80
15:M:109:LYS:HG2	15:M:126:ARG:HB2	1.64	0.80
3:A:2128:G:N3	3:A:2173:A:O2'	2.14	0.79
3:A:994:C:O2	21:S:10:LYS:NZ	2.16	0.78
23:U:87:LEU:HD13	23:U:93:LEU:HD12	1.66	0.77
18:P:15:ARG:NH2	18:P:95:SER:OG	2.18	0.77
11:I:41:LEU:HD21	11:I:96:PHE:HE1	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:614:A:O2'	3:A:616:A:N7	2.18	0.76
5:C:245:VAL:HG12	5:C:251:GLN:HA	1.67	0.76
1:1:71:C:H2'	1:1:72:A:C8	2.21	0.75
5:C:181:MET:HB2	5:C:268:VAL:HB	1.69	0.74
3:A:2599:G:N7	5:C:236:GLU:HB2	2.02	0.74
3:A:2848:G:O2'	3:A:2867:G:N2	2.19	0.74
3:A:2135:A:O2'	3:A:2159:G:O2'	2.06	0.73
3:A:331:C:H41	3:A:1210:G:H22	1.37	0.72
3:A:2119:A:N6	3:A:2167:U:O2	2.22	0.72
3:A:545:U:O2	3:A:548:G:N1	2.19	0.72
7:E:1:MET:HG3	7:E:14:VAL:HG23	1.71	0.72
3:A:95:A:HO2'	28:Z:41:HIS:N	1.87	0.72
3:A:331:C:H41	3:A:1210:G:N2	1.88	0.71
3:A:1069:A:H4'	3:A:1070:A:H5"	1.71	0.71
3:A:720:U:H2'	3:A:721:A:C8	2.24	0.71
23:U:87:LEU:CD1	23:U:93:LEU:HD12	2.21	0.71
1:1:42:A:H61	1:1:67:A:H62	1.36	0.71
3:A:2423:U:H2'	3:A:2424:C:O4'	1.89	0.71
13:K:131:ASN:N	13:K:131:ASN:OD1	2.22	0.71
13:K:70:THR:OG1	13:K:71:ASP:OD1	2.08	0.71
11:I:50:VAL:HG22	11:I:85:VAL:HG13	1.73	0.70
3:A:2163:A:OP1	3:A:2170:A:O2'	2.08	0.70
3:A:258:G:H1'	15:M:104:GLN:HE22	1.56	0.70
1:1:68:A:H2'	1:1:69:G:C8	2.26	0.70
3:A:1801:A:OP2	5:C:150:LYS:NZ	2.18	0.70
3:A:2310:C:H2'	8:F:77:PHE:HE2	1.54	0.70
3:A:971:G:H2'	3:A:972:A:O4'	1.92	0.69
3:A:1340:U:OP1	23:U:19:LYS:NZ	2.26	0.69
14:L:70:ARG:HD3	14:L:76:VAL:HG22	1.72	0.69
3:A:1536:C:H4'	3:A:1537:G:H5"	1.75	0.69
1:1:68:A:H2'	1:1:69:G:H8	1.58	0.69
3:A:2830:C:H5"	6:D:56:LYS:HE3	1.75	0.68
9:G:35:ARG:HD3	9:G:71:LEU:HD13	1.74	0.68
3:A:513:A:O2'	20:R:11:ARG:NH1	2.26	0.68
14:L:21:CYS:HA	14:L:41:ILE:HG22	1.76	0.68
3:A:362:A:H3'	3:A:363:G:H8	1.59	0.68
11:I:43:LYS:HG2	11:I:46:ARG:HH22	1.56	0.68
3:A:2122:U:OP1	3:A:2168:G:N2	2.26	0.68
14:L:79:PHE:HD1	19:Q:70:VAL:HG22	1.58	0.67
3:A:878:A:H3'	3:A:879:G:H8	1.60	0.67
3:A:358:U:H2'	3:A:359:G:H8	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:31:THR:HG22	18:P:34:HIS:H	1.59	0.67
3:A:2103:C:O2	3:A:2186:G:N1	2.27	0.67
13:K:31:GLU:HG3	13:K:142:ILE:HG13	1.77	0.66
3:A:2713:U:H3'	3:A:2714:G:H5"	1.77	0.66
12:J:79:LEU:HB3	12:J:109:ILE:HG12	1.76	0.66
3:A:370:G:O2'	3:A:424:G:OP1	2.11	0.66
3:A:2303:G:O2'	8:F:121:SER:O	2.13	0.66
3:A:572:A:OP2	21:S:80:ARG:NH2	2.27	0.66
3:A:286:U:H2'	3:A:287:G:H8	1.60	0.66
3:A:196:A:OP2	15:M:47:ARG:NH1	2.29	0.66
3:A:2216:G:H2'	3:A:2217:G:H8	1.60	0.66
27:Y:32:ASN:O	27:Y:52:SER:HA	1.95	0.66
3:A:1105:U:H2'	3:A:1106:G:C8	2.29	0.66
28:Z:10:SER:N	28:Z:13:GLU:OE1	2.26	0.66
3:A:2305:U:C2	8:F:151:GLY:HA3	2.31	0.66
3:A:286:U:H2'	3:A:287:G:C8	2.31	0.66
3:A:2209:G:H1	3:A:2215:C:H42	1.44	0.66
3:A:2590:A:H2'	3:A:2591:C:H6	1.61	0.66
10:H:84:ALA:HA	10:H:90:LEU:HA	1.78	0.66
3:A:1344:U:O2'	3:A:1345:C:OP1	2.14	0.66
16:N:50:ARG:O	16:N:54:THR:OG1	2.13	0.66
3:A:1597:A:H5"	3:A:1598:A:H5'	1.78	0.65
9:G:9:VAL:HG22	9:G:69:ARG:HE	1.61	0.65
4:B:43:C:O2	8:F:92:ARG:NH2	2.28	0.65
3:A:1794:A:H2'	3:A:1795:C:H6	1.61	0.65
7:E:87:ALA:O	7:E:88:ARG:NH2	2.30	0.65
26:X:65:GLY:HA2	26:X:85:GLU:HG2	1.78	0.65
3:A:2788:C:O2'	3:A:2809:A:N3	2.28	0.65
3:A:1007:C:OP1	13:K:37:ARG:NH2	2.29	0.65
3:A:1869:G:N2	3:A:1871:A:O2'	2.30	0.65
3:A:322:A:H5'	3:A:340:A:H1'	1.78	0.65
8:F:158:THR:HG22	8:F:160:ALA:H	1.62	0.64
3:A:860:U:H1'	3:A:2268:A:H5'	1.78	0.64
3:A:284:U:H3	3:A:356:G:H1	1.44	0.64
8:F:144:ASP:OD1	8:F:144:ASP:N	2.30	0.64
3:A:2116:G:N7	3:A:2165:C:N4	2.44	0.64
3:A:1105:U:H2'	3:A:1106:G:H8	1.63	0.64
3:A:1510:G:H2'	3:A:1511:G:C8	2.32	0.64
3:A:1980:G:O2'	3:A:1982:U:OP2	2.16	0.64
3:A:2674:G:H4'	14:L:30:ARG:HG3	1.78	0.64
3:A:825:A:H2'	3:A:826:U:O4'	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:968:C:H2'	3:A:969:G:H8	1.62	0.63
19:Q:91:ALA:HB2	19:Q:113:ARG:HA	1.80	0.63
3:A:1094:U:N3	3:A:1097:U:OP2	2.30	0.63
25:W:21:ARG:NH2	25:W:87:GLN:O	2.28	0.63
3:A:1614:A:N1	22:T:93:ALA:HB2	2.13	0.63
3:A:2151:U:H2'	3:A:2152:G:C8	2.34	0.63
20:R:58:ARG:HA	20:R:61:TRP:CE3	2.34	0.63
3:A:2424:C:H5"	3:A:2425:A:H5'	1.79	0.62
13:K:117:ALA:HA	13:K:120:ARG:HH21	1.63	0.62
16:N:14:LYS:O	16:N:71:LYS:NZ	2.32	0.62
20:R:74:ILE:HD11	20:R:78:LYS:HB3	1.80	0.62
22:T:82:MET:HB3	22:T:84:ARG:HH22	1.63	0.62
3:A:1433:A:N1	3:A:1434:A:N6	2.47	0.62
3:A:2822:G:O6	17:O:2:ARG:NH1	2.32	0.62
3:A:2809:A:H2'	3:A:2810:A:C8	2.34	0.62
3:A:2636:C:HO2'	6:D:45:TYR:HH	1.46	0.62
8:F:74:VAL:HG22	8:F:79:ILE:HD11	1.79	0.62
19:Q:4:ILE:H	19:Q:4:ILE:HD12	1.65	0.62
3:A:514:A:N3	3:A:581:C:O2'	2.32	0.62
11:I:41:LEU:HD21	11:I:96:PHE:CE1	2.34	0.62
10:H:68:ARG:HA	10:H:71:LYS:HD2	1.81	0.62
21:S:41:ILE:HB	21:S:48:LYS:HD2	1.79	0.62
17:O:49:GLU:HA	17:O:52:ILE:HD12	1.80	0.62
11:I:57:ASN:ND2	11:I:76:PHE:O	2.33	0.62
3:A:784:G:C6	5:C:228:VAL:HG11	2.35	0.62
3:A:503:A:H4'	3:A:504:A:H5'	1.82	0.61
3:A:2590:A:H2'	3:A:2591:C:C6	2.35	0.61
9:G:137:ASP:O	9:G:141:ILE:HG22	2.01	0.61
3:A:2639:A:H2'	3:A:2640:G:O4'	2.01	0.61
12:J:53:LEU:HD11	12:J:82:LYS:HD2	1.83	0.61
15:M:57:LEU:HD13	15:M:60:ARG:HH11	1.65	0.61
3:A:1079:C:O2'	12:J:134:ARG:NH1	2.33	0.61
22:T:6:LYS:HG2	22:T:104:THR:HG23	1.82	0.61
3:A:1001:A:H2'	3:A:1002:G:O4'	2.01	0.60
3:A:585:G:N7	20:R:6:ARG:NH1	2.48	0.60
3:A:1076:C:H2'	3:A:1077:A:C8	2.37	0.60
5:C:235:GLY:HA3	5:C:239:ASN:HB2	1.83	0.60
6:D:12:THR:OG1	6:D:13:ARG:N	2.34	0.60
3:A:2310:C:H2'	8:F:77:PHE:CE2	2.35	0.60
11:I:27:VAL:HG22	11:I:82:ILE:HG22	1.83	0.60
3:A:1363:C:O2'	3:A:1809:A:N3	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:570:G:H2'	3:A:2030:A:N7	2.16	0.60
3:A:299:A:N1	3:A:322:A:O2'	2.27	0.60
17:O:54:LEU:HD21	17:O:65:LEU:HD23	1.82	0.60
3:A:355:U:H2'	3:A:356:G:C8	2.37	0.60
3:A:2102:G:N2	3:A:2187:U:O2	2.31	0.60
3:A:1170:C:O2	3:A:1179:G:N2	2.34	0.60
3:A:1342:A:O2'	3:A:1344:U:OP2	2.16	0.59
8:F:44:ILE:HG21	8:F:79:ILE:HG22	1.83	0.59
15:M:81:ASP:HA	15:M:84:LYS:HD2	1.82	0.59
3:A:1251:C:OP2	20:R:6:ARG:NH2	2.35	0.59
6:D:2:ILE:HG13	6:D:100:LEU:HD21	1.83	0.59
9:G:27:LYS:NZ	9:G:27:LYS:HB3	2.17	0.59
3:A:2127:G:O2'	3:A:2128:G:O5'	2.19	0.59
3:A:1794:A:H2'	3:A:1795:C:C6	2.37	0.59
11:I:64:VAL:HG22	11:I:69:PHE:HB2	1.84	0.59
1:1:69:G:H2'	1:1:70:G:H1'	1.85	0.59
24:V:81:ASP:OD1	24:V:82:ARG:N	2.35	0.59
13:K:36:LEU:HD11	13:K:122:LEU:HB2	1.83	0.59
3:A:2819:G:H2'	3:A:2821:A:N7	2.17	0.59
7:E:97:ASN:OD1	7:E:97:ASN:N	2.34	0.59
1:1:70:G:H3'	1:1:71:C:H6	1.66	0.59
3:A:1808:A:H3'	3:A:1809:A:C8	2.38	0.59
3:A:2584:U:H3'	3:A:2585:U:H5"	1.84	0.59
3:A:878:A:H3'	3:A:879:G:C8	2.38	0.59
3:A:776:G:O2'	3:A:777:G:OP1	2.19	0.59
3:A:2831:G:OP1	6:D:56:LYS:NZ	2.35	0.58
18:P:99:TYR:OH	18:P:111:ARG:NH1	2.36	0.58
3:A:396:G:OP2	27:Y:10:LYS:NZ	2.36	0.58
21:S:37:GLU:HB3	21:S:53:PHE:CE1	2.39	0.58
3:A:1796:U:H2'	3:A:1797:G:H8	1.67	0.58
12:J:106:LEU:HB3	12:J:126:THR:HG23	1.85	0.58
3:A:2127:G:O2'	3:A:2128:G:O4'	2.20	0.58
17:O:73:ASN:HA	17:O:76:VAL:HG22	1.86	0.58
25:W:76:ASP:OD1	25:W:77:VAL:N	2.37	0.58
3:A:2205:A:H61	3:A:2219:U:H3	1.50	0.58
3:A:1130:U:O2'	3:A:1131:G:H8	1.87	0.58
3:A:2060:A:H3'	7:E:63:LYS:HZ1	1.67	0.58
3:A:2291:U:H2'	3:A:2292:U:C6	2.38	0.58
3:A:2021:C:OP1	20:R:25:TYR:OH	2.21	0.58
3:A:833:A:H2'	3:A:834:G:C8	2.38	0.58
6:D:13:ARG:HD2	6:D:15:PHE:CZ	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2412:A:H2'	3:A:2413:G:O4'	2.04	0.58
5:C:227:PRO:HG3	5:C:234:GLY:H	1.69	0.57
12:J:59:ILE:HD13	12:J:69:PHE:HB3	1.86	0.57
19:Q:16:ASP:OD1	19:Q:16:ASP:N	2.32	0.57
3:A:340:A:H2'	3:A:341:C:O4'	2.05	0.57
7:E:21:ARG:HD3	7:E:106:LYS:HB3	1.85	0.57
3:A:1187:G:OP1	21:S:85:LYS:NZ	2.31	0.57
18:P:41:ALA:HB2	18:P:48:LEU:HD21	1.86	0.57
3:A:2447:G:N2	3:A:2450:A:OP2	2.37	0.57
3:A:1715:G:O2'	3:A:1743:G:O6	2.17	0.57
6:D:157:LYS:HD2	13:K:80:HIS:CE1	2.40	0.57
3:A:876:C:H2'	3:A:877:A:O4'	2.05	0.57
17:O:94:TYR:O	17:O:116:VAL:HG23	2.05	0.57
3:A:1063:G:H5'	12:J:77:ALA:HB1	1.87	0.57
5:C:166:ALA:HB3	5:C:173:THR:HB	1.86	0.57
3:A:849:A:H2'	3:A:850:U:H6	1.69	0.57
3:A:2216:G:H2'	3:A:2217:G:C8	2.40	0.57
3:A:1645:G:H5"	3:A:1646:C:H5'	1.85	0.57
24:V:18:ASP:OD2	24:V:40:ASN:N	2.37	0.57
3:A:839:U:H2'	3:A:840:C:C6	2.40	0.57
1:1:49:G:H1	1:1:60:A:N6	1.99	0.56
3:A:2602:A:H4'	3:A:2603:G:O5'	2.04	0.56
3:A:849:A:H2'	3:A:850:U:C6	2.39	0.56
7:E:112:LEU:HB3	7:E:118:LEU:HB2	1.87	0.56
6:D:148:GLN:HB2	6:D:152:PRO:HD2	1.85	0.56
3:A:1905:C:H2'	3:A:1930:G:C8	2.40	0.56
3:A:2430:A:N3	3:A:2430:A:H2'	2.21	0.56
9:G:30:ASN:HB3	9:G:79:VAL:HA	1.88	0.56
13:K:72:LYS:HE3	13:K:74:TYR:CE1	2.39	0.56
3:A:1790:C:H3'	3:A:1828:G:N2	2.21	0.56
3:A:812:C:H4'	20:R:13:ARG:NH1	2.21	0.56
3:A:2491:U:H5"	3:A:2570:G:H5"	1.88	0.56
6:D:1:MET:HG2	6:D:2:ILE:H	1.70	0.56
8:F:33:LYS:HG2	8:F:157:THR:HB	1.87	0.56
11:I:60:LEU:O	11:I:64:VAL:HB	2.06	0.56
4:B:42:C:C5	8:F:66:LEU:HD22	2.41	0.56
1:1:60:A:H2'	1:1:61:G:O4'	2.06	0.56
3:A:721:A:H2'	3:A:722:A:C8	2.41	0.56
3:A:1076:C:H2'	3:A:1077:A:H8	1.69	0.56
3:A:1796:U:H2'	3:A:1797:G:C8	2.40	0.56
12:J:73:THR:HB	12:J:112:THR:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1800:C:H5'	5:C:146:MET:HE1	1.88	0.56
3:A:2298:A:H2'	3:A:2299:U:O4'	2.05	0.56
3:A:26:G:C6	3:A:27:G:N1	2.73	0.56
10:H:37:VAL:HG22	10:H:38:PRO:HD2	1.86	0.56
3:A:388:G:N7	3:A:390:U:H2'	2.21	0.56
17:O:48:VAL:O	17:O:51:LEU:HB2	2.06	0.56
3:A:2584:U:H3'	3:A:2585:U:C5'	2.36	0.56
3:A:591:U:H2'	3:A:592:A:H8	1.71	0.56
18:P:16:ARG:HA	18:P:16:ARG:HH21	1.71	0.56
8:F:132:VAL:HG22	8:F:152:LEU:HB3	1.88	0.55
24:V:33:LYS:HB3	24:V:64:ALA:HB1	1.87	0.55
3:A:19:A:H2'	3:A:20:C:C6	2.41	0.55
12:J:53:LEU:HD22	12:J:78:VAL:HG13	1.87	0.55
23:U:56:GLU:HG3	23:U:88:LYS:HG2	1.88	0.55
25:W:62:THR:HG22	25:W:71:LYS:HG2	1.88	0.55
3:A:1442:U:H2'	3:A:1443:U:C6	2.41	0.55
12:J:79:LEU:HA	12:J:82:LYS:HG2	1.88	0.55
17:O:2:ARG:HB3	17:O:2:ARG:NH1	2.21	0.55
23:U:88:LYS:C	23:U:90:GLY:H	2.08	0.55
3:A:882:G:H1	3:A:894:U:H3	1.54	0.55
5:C:160:THR:HG22	5:C:177:ARG:HG2	1.89	0.55
3:A:184:C:H2'	3:A:185:G:C8	2.41	0.55
3:A:2783:U:H2'	3:A:2784:U:C6	2.42	0.55
10:H:7:ASP:OD1	10:H:8:LYS:N	2.40	0.55
3:A:2162:G:H5"	3:A:2171:A:H2'	1.86	0.55
12:J:127:ARG:HA	12:J:130:GLU:HB2	1.89	0.55
3:A:2171:A:H3'	3:A:2173:A:C8	2.42	0.55
3:A:621:A:OP2	15:M:99:ASN:ND2	2.40	0.55
18:P:69:ASP:N	18:P:69:ASP:OD1	2.40	0.55
3:A:2133:G:H2'	3:A:2157:G:H1	1.70	0.55
3:A:996:A:OP2	21:S:10:LYS:HD3	2.07	0.55
8:F:134:GLU:HB3	8:F:136:ILE:HG12	1.89	0.55
3:A:2070:A:H2'	3:A:2071:A:C8	2.42	0.55
3:A:833:A:H2'	3:A:834:G:H8	1.72	0.55
3:A:968:C:H2'	3:A:969:G:C8	2.42	0.55
3:A:2262:U:H2'	3:A:2263:C:H6	1.72	0.55
3:A:609:A:H2'	3:A:610:C:O4'	2.07	0.55
3:A:2591:C:H2'	3:A:2592:G:C8	2.41	0.54
3:A:2576:G:O2'	3:A:2579:C:OP2	2.23	0.54
6:D:8:LYS:HB2	6:D:201:LEU:HD11	1.88	0.54
21:S:20:VAL:HG13	21:S:96:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2267:A:H5"	3:A:2268:A:H5"	1.89	0.54
3:A:1837:C:H2'	3:A:1899:A:H61	1.73	0.54
3:A:586:A:H5'	7:E:84:THR:HG21	1.90	0.54
1:1:72:A:H2'	1:1:73:G:H8	1.72	0.54
3:A:172:A:H2'	3:A:173:A:C8	2.43	0.54
3:A:645:C:O2'	3:A:646:U:OP1	2.24	0.54
3:A:2619:C:H5"	6:D:157:LYS:HG3	1.89	0.54
1:1:45:U:H3	1:1:64:G:H1	1.54	0.54
13:K:34:ARG:HH22	13:K:40:HIS:HB3	1.71	0.54
12:J:56:PRO:HD3	12:J:75:PRO:HD3	1.90	0.54
7:E:88:ARG:HH21	7:E:88:ARG:HA	1.72	0.54
3:A:2424:C:H5"	3:A:2425:A:C5'	2.37	0.54
3:A:284:U:O2	3:A:356:G:N2	2.37	0.54
3:A:2845:U:H5"	19:Q:52:ASN:O	2.08	0.54
3:A:639:U:H2'	3:A:640:C:C6	2.42	0.54
23:U:88:LYS:O	23:U:90:GLY:N	2.41	0.54
3:A:2834:G:O6	3:A:2879:A:H2'	2.08	0.54
26:X:56:ASP:N	26:X:56:ASP:OD1	2.28	0.54
3:A:2443:C:H2'	3:A:2444:G:C8	2.43	0.54
3:A:1056:G:O2'	3:A:1103:A:N6	2.41	0.54
5:C:62:TYR:HA	5:C:86:ASN:HD21	1.73	0.53
11:I:54:VAL:HG22	11:I:81:LEU:HD13	1.90	0.53
4:B:93:C:OP2	25:W:18:ARG:NH1	2.42	0.53
14:L:38:ILE:HD11	14:L:112:PHE:HZ	1.73	0.53
3:A:720:U:H2'	3:A:721:A:H8	1.72	0.53
3:A:608:A:H2'	3:A:609:A:C8	2.44	0.53
17:O:36:THR:OG1	17:O:37:THR:N	2.42	0.53
17:O:36:THR:HG23	17:O:41:ALA:HB2	1.90	0.53
5:C:145:GLU:HB2	5:C:188:CYS:HB3	1.89	0.53
21:S:48:LYS:HE3	21:S:103:ALA:HB1	1.90	0.53
3:A:2579:C:O2'	6:D:136:ASN:ND2	2.41	0.53
23:U:68:LYS:HG3	23:U:77:ARG:NH2	2.23	0.53
3:A:2547:A:H4'	14:L:29:HIS:CD2	2.44	0.53
13:K:98:GLU:OE1	13:K:98:GLU:N	2.41	0.53
3:A:120:U:H4'	3:A:121:G:H5"	1.89	0.53
14:L:40:LYS:HE3	14:L:57:VAL:HG12	1.91	0.53
3:A:1923:U:H2'	3:A:1924:C:C6	2.43	0.53
9:G:104:ASN:ND2	9:G:114:ASP:OD1	2.41	0.53
11:I:88:HIS:ND1	11:I:89:PRO:O	2.42	0.53
3:A:653:U:H1'	3:A:654:A:H5"	1.91	0.53
3:A:2210:U:H4'	3:A:2211:A:H5'	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2171:A:H3'	3:A:2173:A:H8	1.74	0.53
7:E:28:VAL:O	7:E:32:VAL:HG13	2.09	0.52
3:A:1056:G:H5"	3:A:1057:A:H5'	1.90	0.52
3:A:2086:U:H2'	3:A:2087:G:C8	2.45	0.52
10:H:116:ARG:HH21	10:H:133:GLN:HB3	1.74	0.52
3:A:2637:U:C2'	3:A:2638:G:H5'	2.39	0.52
3:A:9:G:O2'	3:A:2800:A:N6	2.42	0.52
3:A:2808:G:O2'	3:A:2890:G:O6	2.21	0.52
13:K:3:THR:HB	20:R:57:PHE:HE1	1.75	0.52
25:W:55:GLU:CD	25:W:55:GLU:H	2.13	0.52
3:A:1069:A:C2	3:A:1096:A:H5"	2.44	0.52
3:A:90:U:H3'	3:A:91:A:H8	1.74	0.52
3:A:2127:G:H2'	3:A:2128:G:C8	2.45	0.52
1:1:68:A:O2'	1:1:69:G:OP1	2.27	0.52
8:F:99:PHE:HD1	8:F:102:ARG:HH22	1.57	0.52
3:A:1791:A:N6	3:A:1828:G:O2'	2.42	0.52
3:A:671:C:H2'	3:A:672:C:H6	1.74	0.52
21:S:52:PRO:HG2	21:S:53:PHE:CD2	2.45	0.52
3:A:1798:U:H5"	5:C:258:ARG:HB2	1.92	0.52
3:A:1428:C:C5	3:A:1569:A:H5"	2.45	0.52
1:1:42:A:N6	1:1:67:A:H62	2.05	0.52
3:A:256:A:H2'	3:A:257:C:H6	1.74	0.52
3:A:1425:G:H2'	3:A:1426:G:O4'	2.09	0.52
3:A:1993:U:H4'	6:D:133:THR:OG1	2.10	0.52
28:Z:38:GLN:HG3	28:Z:39:GLN:H	1.75	0.52
3:A:679:C:H2'	3:A:680:C:C6	2.44	0.52
3:A:2564:A:OP1	3:A:2648:G:O2'	2.20	0.52
6:D:114:LYS:HD3	6:D:196:ALA:HB2	1.92	0.52
3:A:68:G:H2'	3:A:69:C:O4'	2.10	0.52
17:O:55:ALA:HA	17:O:80:PHE:CE2	2.45	0.52
8:F:128:TYR:HE2	8:F:130:MET:HG2	1.76	0.51
3:A:1115:G:O2'	3:A:1116:G:H5"	2.10	0.51
3:A:1790:C:H2'	3:A:1791:A:C5	2.45	0.51
3:A:788:A:OP1	3:A:791:C:N4	2.41	0.51
3:A:1421:G:C2	3:A:1422:G:C8	2.98	0.51
7:E:41:GLN:HG2	7:E:43:THR:HG23	1.92	0.51
3:A:364:C:H2'	3:A:365:U:C6	2.45	0.51
3:A:845:A:H61	3:A:932:U:H3	1.58	0.51
3:A:2720:U:OP1	19:Q:53:ARG:NH2	2.41	0.51
16:N:30:SER:H	16:N:106:ASP:HB3	1.75	0.51
3:A:1289:C:H2'	3:A:1290:C:C6	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2133:G:H21	3:A:2158:A:H62	1.58	0.51
3:A:2647:U:H2'	3:A:2648:G:H8	1.76	0.51
15:M:4:ASN:OD1	15:M:4:ASN:N	2.39	0.51
21:S:28:ALA:HB3	21:S:31:GLU:HG3	1.93	0.51
3:A:1451:C:H1'	3:A:1452:G:C2	2.45	0.51
24:V:74:ASN:HD21	24:V:99:ASN:HD21	1.58	0.51
3:A:1410:G:H1	3:A:1592:C:H42	1.57	0.51
22:T:40:ASN:O	22:T:41:LYS:HG2	2.10	0.51
7:E:145:ASP:HA	7:E:166:LYS:HB3	1.93	0.51
6:D:184:ARG:NH1	19:Q:7:GLN:OE1	2.40	0.51
3:A:2439:A:H4'	3:A:2440:C:H5"	1.91	0.51
3:A:1437:C:H2'	3:A:1438:U:C6	2.46	0.51
3:A:1681:G:H21	3:A:1762:A:H3'	1.75	0.51
20:R:76:TYR:CZ	20:R:80:ILE:HG13	2.46	0.51
3:A:576:U:H2'	3:A:577:G:C8	2.46	0.51
3:A:1873:G:H2'	3:A:1874:C:H6	1.74	0.51
7:E:24:ASN:ND2	7:E:27:LEU:HB2	2.25	0.51
3:A:1405:U:H2'	3:A:1406:U:C6	2.46	0.51
3:A:499:U:H2'	3:A:500:G:O4'	2.10	0.51
28:Z:2:LYS:HG3	28:Z:5:GLU:OE1	2.10	0.51
3:A:1414:C:H2'	3:A:1415:U:O4'	2.11	0.51
3:A:1000:A:OP2	3:A:1154:G:N1	2.32	0.51
3:A:898:C:H2'	3:A:899:A:O4'	2.10	0.51
3:A:1132:U:H2'	3:A:1133:A:C8	2.46	0.51
3:A:2271:G:H5"	26:X:18:ALA:HB1	1.93	0.51
8:F:40:VAL:HG11	8:F:43:ALA:HB2	1.92	0.51
12:J:73:THR:OG1	12:J:113:LYS:NZ	2.40	0.51
3:A:2502:G:H5"	3:A:2503:A:H5"	1.93	0.51
3:A:2024:G:H2'	3:A:2025:C:H6	1.76	0.51
3:A:948:C:H2'	3:A:949:G:C8	2.45	0.51
3:A:1344:U:HO2'	3:A:1345:C:P	2.34	0.50
3:A:141:G:H2'	3:A:142:A:O4'	2.11	0.50
8:F:50:LEU:O	8:F:54:ALA:N	2.38	0.50
23:U:7:LEU:HD13	23:U:46:ALA:HA	1.92	0.50
3:A:95:A:O2'	28:Z:41:HIS:N	2.43	0.50
3:A:256:A:H2'	3:A:257:C:C6	2.46	0.50
12:J:113:LYS:HE3	12:J:116:ASP:HB3	1.92	0.50
3:A:1394:U:H4'	3:A:1603:A:H4'	1.92	0.50
16:N:1:MET:HA	16:N:47:GLU:HG3	1.94	0.50
3:A:1939:U:OP1	3:A:2604:U:O2'	2.28	0.50
13:K:32:LEU:O	13:K:36:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2282:G:C6	3:A:2425:A:C2	3.00	0.50
3:A:128:C:H2'	3:A:129:C:C6	2.46	0.50
20:R:65:ILE:HD11	20:R:95:LEU:HB2	1.93	0.50
27:Y:6:GLN:NE2	27:Y:76:GLU:OE2	2.39	0.50
3:A:90:U:C2	3:A:91:A:N7	2.80	0.50
3:A:2333:A:P	26:X:77:ARG:HH22	2.34	0.50
9:G:83:PHE:O	9:G:134:LYS:HA	2.12	0.50
15:M:36:LYS:O	15:M:40:SER:HB3	2.11	0.50
3:A:738:G:H1'	3:A:759:G:N2	2.27	0.50
14:L:64:ARG:NH1	14:L:102:PRO:O	2.44	0.50
3:A:1927:A:H2'	3:A:1928:A:C8	2.46	0.50
4:B:2:G:H2'	4:B:3:C:C6	2.47	0.50
3:A:878:A:N6	3:A:899:A:O2'	2.45	0.50
3:A:357:C:H2'	3:A:358:U:C6	2.47	0.50
1:1:37:U:H2'	1:1:38:U:C6	2.47	0.50
24:V:46:GLN:OE1	24:V:54:GLN:NE2	2.44	0.50
12:J:83:ALA:O	12:J:105:GLN:NE2	2.45	0.50
3:A:1327:A:N6	3:A:1647:U:O2	2.45	0.50
19:Q:23:GLY:O	19:Q:90:GLY:HA3	2.11	0.50
3:A:2171:A:H5'	3:A:2173:A:N7	2.26	0.50
5:C:175:ARG:HG3	5:C:181:MET:HE1	1.94	0.50
9:G:127:THR:HG22	9:G:128:GLN:H	1.77	0.50
3:A:1088:A:N6	12:J:135:SER:HB3	2.26	0.50
3:A:1638:C:H1'	3:A:2698:U:O2'	2.12	0.50
26:X:34:GLY:N	26:X:61:ALA:O	2.37	0.49
9:G:8:PRO:HB3	9:G:51:THR:HG22	1.94	0.49
7:E:184:ASP:N	7:E:184:ASP:OD1	2.44	0.49
3:A:2626:C:H2'	3:A:2627:G:O4'	2.12	0.49
15:M:23:ILE:HG12	21:S:82:HIS:CD2	2.47	0.49
3:A:1506:U:H2'	3:A:1507:C:C6	2.48	0.49
1:1:46:C:H42	1:1:61:G:H3'	1.77	0.49
3:A:2290:G:H2'	3:A:2291:U:O4'	2.12	0.49
3:A:2183:A:H2'	3:A:2184:A:C8	2.46	0.49
10:H:94:ILE:HB	10:H:122:LEU:HB2	1.94	0.49
18:P:30:ARG:HG3	18:P:35:ILE:HD12	1.94	0.49
25:W:75:GLN:HB2	25:W:92:VAL:HG12	1.94	0.49
3:A:2151:U:H2'	3:A:2152:G:H8	1.77	0.49
8:F:17:MET:SD	8:F:22:TYR:HB2	2.52	0.49
3:A:1790:C:H3'	3:A:1828:G:H22	1.77	0.49
3:A:27:G:N2	3:A:512:G:H1'	2.28	0.49
15:M:19:LEU:HD23	15:M:27:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:563:A:C4	3:A:2018:G:C2	3.01	0.49
21:S:65:ALA:HB3	21:S:95:ASP:HB2	1.94	0.49
3:A:2308:G:H3'	3:A:2310:C:OP2	2.11	0.49
3:A:239:C:HO2'	3:A:622:G:HO2'	1.58	0.49
5:C:132:MET:HG2	5:C:135:ILE:HD12	1.94	0.49
17:O:14:SER:HA	17:O:17:ARG:NH1	2.27	0.49
3:A:1243:C:H1'	15:M:4:ASN:O	2.13	0.49
3:A:2280:G:O2'	3:A:2388:A:N1	2.37	0.49
3:A:1005:C:H2'	3:A:1006:C:C6	2.47	0.49
3:A:2747:G:O2'	9:G:67:THR:HG23	2.12	0.49
9:G:101:ASN:ND2	9:G:116:GLN:OE1	2.46	0.49
3:A:1021:A:H3'	3:A:1021:A:N3	2.27	0.49
3:A:613:A:O2'	3:A:614:A:O5'	2.30	0.49
3:A:1093:G:C2'	3:A:1098:A:H61	2.26	0.49
20:R:24:TYR:N	20:R:24:TYR:CD1	2.78	0.49
3:A:1903:G:C2	3:A:1904:G:C8	3.00	0.49
3:A:1179:G:H2'	3:A:1180:U:C6	2.48	0.49
3:A:136:G:H2'	3:A:137:U:O4'	2.12	0.49
27:Y:17:ASN:OD1	27:Y:27:ARG:HD2	2.13	0.49
11:I:33:VAL:HG21	11:I:106:PHE:CE2	2.47	0.48
3:A:671:C:H2'	3:A:672:C:C6	2.48	0.48
3:A:1773:A:N7	3:A:1829:A:H1'	2.28	0.48
3:A:467:G:H2'	3:A:468:G:O4'	2.13	0.48
3:A:719:C:H2'	3:A:720:U:H6	1.78	0.48
12:J:113:LYS:O	12:J:117:MET:N	2.46	0.48
3:A:1132:U:H3'	3:A:1133:A:H5"	1.95	0.48
26:X:55:ARG:HE	26:X:55:ARG:HB2	1.45	0.48
8:F:7:TYR:CD1	8:F:11:GLU:HG3	2.48	0.48
4:B:116:G:H2'	4:B:117:G:C8	2.49	0.48
3:A:184:C:H2'	3:A:185:G:H8	1.77	0.48
3:A:156:A:H2'	3:A:157:C:O4'	2.13	0.48
1:1:72:A:H2'	1:1:73:G:C8	2.48	0.48
3:A:140:C:H4'	3:A:141:G:OP1	2.13	0.48
14:L:10:VAL:HG12	14:L:12:ASP:H	1.78	0.48
3:A:981:A:N1	3:A:2027:G:O2'	2.42	0.48
13:K:78:THR:HG23	13:K:83:GLY:O	2.13	0.48
5:C:260:ASN:OD1	5:C:262:ARG:N	2.37	0.48
14:L:73:ASP:OD1	14:L:73:ASP:N	2.39	0.48
6:D:25:THR:HG21	6:D:193:VAL:HG22	1.95	0.48
3:A:2834:G:H2'	3:A:2879:A:N6	2.29	0.48
5:C:145:GLU:HG2	5:C:151:GLY:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:957:C:C5	3:A:959:A:C5	3.01	0.48
8:F:73:SER:OG	8:F:81:GLN:N	2.33	0.48
3:A:2226:C:H2'	3:A:2227:A:O4'	2.13	0.48
10:H:115:VAL:HG22	10:H:132:PHE:CE2	2.48	0.48
3:A:910:A:H2'	3:A:911:A:C8	2.49	0.48
3:A:911:A:H2'	16:N:9:PHE:HZ	1.78	0.48
3:A:784:G:H5'	3:A:785:G:OP1	2.13	0.48
7:E:23:PHE:CD1	7:E:111:GLU:HG3	2.48	0.48
16:N:41:LEU:HG	16:N:96:ILE:HG13	1.95	0.48
3:A:1268:A:H2'	3:A:1269:A:O4'	2.13	0.48
3:A:1654:A:H2'	3:A:1655:A:H8	1.79	0.48
3:A:1386:C:H2'	3:A:1387:A:C8	2.49	0.48
3:A:208:C:H2'	3:A:209:C:H6	1.78	0.48
9:G:86:LYS:HG2	9:G:132:VAL:HG22	1.96	0.48
3:A:1187:G:HO2'	3:A:1188:U:H6	1.61	0.48
13:K:72:LYS:HE3	13:K:74:TYR:CZ	2.49	0.48
27:Y:17:ASN:HB2	27:Y:25:THR:OG1	2.13	0.48
3:A:995:C:OP2	20:R:54:LYS:NZ	2.44	0.48
3:A:813:U:H2'	3:A:814:C:C6	2.49	0.48
4:B:7:G:OP1	18:P:4:LYS:NZ	2.27	0.48
3:A:2433:A:H2	27:Y:21:ALA:HB1	1.79	0.48
3:A:175:G:N2	3:A:176:A:N3	2.62	0.48
16:N:11:LYS:HD3	16:N:86:LYS:HD3	1.96	0.48
3:A:1527:G:N1	3:A:1544:A:OP2	2.32	0.48
28:Z:14:LEU:HB3	28:Z:57:LEU:HD21	1.96	0.48
10:H:110:VAL:HG12	10:H:114:GLU:HB2	1.94	0.48
3:A:2158:A:H4'	3:A:2159:G:O5'	2.14	0.48
3:A:1007:C:H5"	13:K:37:ARG:NH2	2.28	0.48
3:A:2305:U:H5"	8:F:131:GLY:HA3	1.96	0.48
3:A:2809:A:H2'	3:A:2810:A:H8	1.75	0.48
3:A:2060:A:H3'	7:E:63:LYS:NZ	2.29	0.48
3:A:1085:A:H61	11:I:35:VAL:HG22	1.78	0.48
3:A:2073:C:H2'	3:A:2074:U:H6	1.77	0.48
10:H:93:SER:HB3	10:H:123:ARG:HG2	1.95	0.48
3:A:477:A:H2'	3:A:478:A:C8	2.49	0.48
9:G:80:THR:OG1	9:G:81:GLU:N	2.46	0.48
3:A:1873:G:H2'	3:A:1874:C:C6	2.49	0.48
9:G:102:VAL:HG22	9:G:116:GLN:HE22	1.78	0.48
18:P:51:ALA:HB3	18:P:78:VAL:HG13	1.95	0.48
26:X:40:GLN:NE2	26:X:43:THR:HA	2.29	0.48
22:T:7:HIS:CE1	22:T:10:ALA:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:58:ASN:ND2	13:K:128:ASN:OD1	2.42	0.48
3:A:1027:A:C6	3:A:1126:A:C4	3.02	0.48
8:F:25:VAL:O	8:F:28:VAL:HG12	2.14	0.47
3:A:1846:G:H5"	3:A:1847:A:OP2	2.14	0.47
3:A:2116:G:C5	3:A:2165:C:N4	2.82	0.47
3:A:2428:G:H21	15:M:60:ARG:NH2	2.12	0.47
3:A:1819:A:H5"	5:C:160:THR:HG21	1.94	0.47
12:J:42:PHE:O	12:J:46:THR:OG1	2.32	0.47
24:V:14:LEU:HD11	24:V:71:ALA:HB2	1.95	0.47
18:P:31:THR:HG23	18:P:32:PRO:HD2	1.96	0.47
23:U:68:LYS:HG3	23:U:77:ARG:HH21	1.79	0.47
3:A:1446:C:H2'	3:A:1447:C:C6	2.49	0.47
3:A:1606:C:H5'	3:A:1607:C:OP1	2.13	0.47
3:A:483:A:O4'	24:V:45:HIS:HB3	2.14	0.47
3:A:428:A:H2'	3:A:429:A:C8	2.49	0.47
3:A:160:A:N3	3:A:2208:C:O2'	2.42	0.47
3:A:2483:C:N3	16:N:123:LYS:NZ	2.60	0.47
3:A:914:G:H5'	3:A:915:C:OP2	2.14	0.47
7:E:125:SER:OG	7:E:126:VAL:N	2.46	0.47
15:M:55:MET:SD	15:M:56:PRO:HD2	2.55	0.47
23:U:58:VAL:HG22	23:U:85:VAL:HG22	1.96	0.47
17:O:38:LEU:HB3	17:O:39:PRO:HD3	1.96	0.47
9:G:35:ARG:CD	9:G:71:LEU:HD13	2.43	0.47
3:A:358:U:H2'	3:A:359:G:C8	2.44	0.47
3:A:2570:G:H2'	3:A:2571:U:O4'	2.14	0.47
3:A:782:A:N7	5:C:220:VAL:HG21	2.29	0.47
1:1:53:G:C6	1:1:55:A:OP2	2.68	0.47
11:I:85:VAL:HG22	11:I:92:ALA:HB2	1.96	0.47
18:P:30:ARG:HB3	18:P:97:PHE:CE1	2.50	0.47
3:A:2431:U:H5	3:A:2433:A:H5"	1.79	0.47
3:A:2419:U:O2'	3:A:2420:C:H5'	2.15	0.47
3:A:2592:G:C6	3:A:2593:U:N3	2.83	0.47
3:A:1808:A:H3'	3:A:1809:A:H8	1.79	0.47
3:A:1438:U:H2'	3:A:1439:A:H8	1.79	0.47
10:H:142:VAL:HG12	10:H:143:ILE:H	1.79	0.47
19:Q:106:LYS:O	19:Q:109:ARG:NH2	2.45	0.47
3:A:2786:U:H2'	3:A:2787:C:H6	1.79	0.47
12:J:40:LYS:N	12:J:40:LYS:HD2	2.30	0.47
24:V:41:LEU:HD22	24:V:62:GLU:HG2	1.96	0.47
12:J:28:LEU:HD11	12:J:33:VAL:HG11	1.97	0.47
6:D:121:THR:HB	6:D:127:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1672:A:C6	3:A:1673:G:C6	3.03	0.47
6:D:56:LYS:HB2	6:D:59:ARG:HB2	1.96	0.47
3:A:2209:G:H1	3:A:2215:C:N4	2.11	0.47
3:A:1420:A:N7	3:A:2211:A:N6	2.62	0.47
4:B:116:G:H2'	4:B:117:G:H8	1.80	0.47
3:A:1387:A:H5'	3:A:1469:A:H1'	1.97	0.47
27:Y:40:VAL:HG12	27:Y:43:GLU:H	1.80	0.47
8:F:4:LEU:HA	8:F:4:LEU:HD23	1.73	0.47
3:A:75:G:H4'	28:Z:48:ARG:CZ	2.45	0.47
25:W:25:LYS:HB3	25:W:25:LYS:HE2	1.71	0.47
3:A:247:G:H4'	3:A:386:G:C5	2.50	0.47
3:A:1097:U:H2'	3:A:1098:A:O4'	2.15	0.47
3:A:2444:G:OP2	7:E:63:LYS:HD2	2.14	0.47
3:A:871:U:H2'	3:A:872:U:C6	2.50	0.47
7:E:149:ILE:HB	7:E:188:MET:HG2	1.96	0.47
3:A:998:C:H2'	3:A:999:U:O4'	2.14	0.47
17:O:25:ALA:O	17:O:29:VAL:HG23	2.15	0.47
12:J:10:LYS:O	12:J:11:LEU:HD12	2.15	0.47
3:A:112:U:H5'	28:Z:58:ASN:HD21	1.80	0.47
18:P:43:ASN:ND2	18:P:43:ASN:H	2.13	0.47
5:C:252:THR:OG1	5:C:253:LYS:N	2.48	0.47
3:A:713:G:H2'	3:A:714:U:C6	2.50	0.47
3:A:2788:C:H2'	3:A:2789:C:C6	2.50	0.47
20:R:18:LEU:HD11	20:R:32:TYR:HA	1.97	0.47
3:A:795:C:H2'	3:A:796:C:C6	2.49	0.47
3:A:1028:A:N6	3:A:1125:G:H2'	2.30	0.47
13:K:114:LEU:O	13:K:118:MET:HG3	2.14	0.47
3:A:630:G:N2	3:A:633:A:OP2	2.43	0.47
3:A:1060:U:C2	3:A:1062:G:H5'	2.50	0.47
21:S:38:VAL:O	21:S:54:VAL:HG23	2.15	0.47
3:A:1416:G:N2	3:A:1582:C:O2	2.33	0.47
11:I:27:VAL:HG13	11:I:80:THR:HG23	1.97	0.46
3:A:911:A:H2'	16:N:9:PHE:CZ	2.50	0.46
3:A:323:C:C4	3:A:333:G:C8	3.03	0.46
25:W:2:PHE:HB3	25:W:50:MET:CE	2.44	0.46
10:H:29:PHE:O	10:H:32:PRO:HD2	2.15	0.46
27:Y:62:LYS:HE3	27:Y:66:THR:HG21	1.96	0.46
3:A:825:A:C2	3:A:833:A:C2	3.03	0.46
3:A:127:A:H5"	3:A:128:C:O4'	2.14	0.46
3:A:796:C:H2'	3:A:797:G:C8	2.51	0.46
3:A:1341:G:O2'	23:U:59:ASN:ND2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:975:A:H1'	3:A:990:A:C2	2.50	0.46
1:1:47:A:OP2	1:1:61:G:N1	2.48	0.46
11:I:39:THR:HG22	11:I:43:LYS:HE3	1.98	0.46
3:A:2126:A:H61	3:A:2163:A:H5'	1.80	0.46
3:A:1149:G:H2'	3:A:1150:C:C6	2.50	0.46
26:X:41:ARG:HA	26:X:41:ARG:HD3	1.53	0.46
3:A:532:A:H2'	3:A:532:A:N3	2.31	0.46
3:A:2339:C:H2'	3:A:2340:A:H8	1.81	0.46
3:A:1825:U:O2	5:C:253:LYS:NZ	2.31	0.46
12:J:75:PRO:HD2	12:J:78:VAL:HB	1.96	0.46
3:A:1062:G:N2	12:J:93:PRO:HG2	2.30	0.46
3:A:2557:G:H2'	3:A:2558:C:C6	2.49	0.46
20:R:49:ASP:HA	20:R:52:GLN:HB2	1.96	0.46
3:A:861:A:C6	3:A:917:A:C8	3.03	0.46
5:C:232:HIS:NE2	5:C:244:PRO:HA	2.30	0.46
3:A:1038:G:H2'	3:A:1039:A:C8	2.50	0.46
19:Q:88:ARG:NH2	19:Q:112:GLU:HB2	2.31	0.46
3:A:1689:A:C6	3:A:1700:A:C2	3.03	0.46
13:K:95:ARG:HG2	13:K:96:ARG:N	2.29	0.46
3:A:2039:U:H2'	3:A:2040:G:C8	2.50	0.46
3:A:1799:G:C5	5:C:176:LEU:HD13	2.50	0.46
3:A:857:G:H2'	3:A:858:G:O4'	2.16	0.46
3:A:880:G:N2	3:A:898:C:C2	2.84	0.46
3:A:1709:U:H2'	3:A:1710:G:H8	1.80	0.46
22:T:25:ARG:NH2	22:T:74:ILE:O	2.49	0.46
14:L:25:LEU:HD23	14:L:25:LEU:HA	1.67	0.46
3:A:144:A:H1'	23:U:3:ARG:HH22	1.80	0.46
18:P:53:THR:HB	18:P:65:THR:HB	1.98	0.46
3:A:1848:A:H3'	3:A:1849:G:H8	1.80	0.46
3:A:1946:U:H2'	3:A:1947:C:C6	2.51	0.46
9:G:148:LEU:HD23	9:G:148:LEU:HA	1.71	0.46
23:U:87:LEU:HD13	23:U:93:LEU:CD1	2.42	0.46
3:A:96:C:H4'	28:Z:41:HIS:CD2	2.50	0.46
11:I:30:SER:HB3	11:I:81:LEU:HB2	1.98	0.46
3:A:1342:A:C6	3:A:1397:U:C5	3.04	0.46
16:N:133:LYS:HE3	16:N:133:LYS:HB3	1.42	0.46
18:P:18:LEU:HD23	18:P:18:LEU:HA	1.71	0.46
3:A:1510:G:H2'	3:A:1511:G:H8	1.79	0.46
3:A:2821:A:H2'	3:A:2822:G:C8	2.51	0.46
5:C:33:LEU:HD23	5:C:33:LEU:HA	1.58	0.46
3:A:2069:G:N2	3:A:2443:C:C2	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:861:A:H2'	3:A:862:G:O4'	2.15	0.46
6:D:207:VAL:HG13	6:D:208:LYS:HG3	1.98	0.46
18:P:88:LYS:HG2	18:P:116:GLN:HB2	1.98	0.46
10:H:40:THR:HG22	10:H:41:LYS:H	1.80	0.46
3:A:2524:G:H2'	3:A:2525:G:O4'	2.16	0.46
11:I:53:ARG:O	11:I:81:LEU:HD12	2.16	0.46
3:A:1508:A:O2'	3:A:1509:A:O4'	2.19	0.46
24:V:81:ASP:OD2	24:V:96:PHE:HB3	2.16	0.46
4:B:95:U:H2'	4:B:96:G:H8	1.81	0.46
9:G:42:GLU:CG	9:G:55:ARG:HH21	2.29	0.46
3:A:1022:G:O2'	3:A:1024:G:O6	2.27	0.46
20:R:17:ILE:HD13	20:R:17:ILE:HA	1.63	0.46
14:L:79:PHE:CD1	19:Q:70:VAL:HG22	2.46	0.45
3:A:1869:G:N2	3:A:1873:G:C5	2.83	0.45
5:C:160:THR:O	5:C:195:VAL:HG23	2.17	0.45
3:A:1570:A:H5'	5:C:36:LYS:HB2	1.98	0.45
3:A:2327:A:H2'	3:A:2328:A:C8	2.51	0.45
16:N:66:ARG:HB2	16:N:101:VAL:O	2.16	0.45
14:L:66:LYS:HB3	14:L:66:LYS:HE2	1.64	0.45
6:D:184:ARG:HH11	19:Q:7:GLN:CD	2.20	0.45
3:A:141:G:H3'	3:A:141:G:C8	2.51	0.45
9:G:121:ILE:HD13	9:G:135:GLY:HA3	1.98	0.45
15:M:27:LEU:O	15:M:31:GLY:HA2	2.17	0.45
3:A:483:A:H5"	24:V:47:LYS:HG2	1.97	0.45
3:A:594:U:H2'	3:A:595:C:C6	2.51	0.45
3:A:1653:G:H3'	17:O:2:ARG:HG3	1.98	0.45
8:F:20:PHE:CZ	8:F:165:GLU:HA	2.51	0.45
3:A:1545:A:H2'	3:A:1546:G:O4'	2.17	0.45
3:A:772:C:H2'	3:A:773:U:C6	2.52	0.45
3:A:629:G:H5"	3:A:650:C:O2'	2.16	0.45
3:A:2052:A:OP1	6:D:146:ILE:HG12	2.17	0.45
27:Y:77:LYS:HD2	27:Y:77:LYS:HA	1.66	0.45
1:1:42:A:H61	1:1:67:A:N6	2.10	0.45
11:I:52:MET:HE3	11:I:81:LEU:HD11	1.99	0.45
3:A:878:A:H5'	3:A:879:G:OP2	2.16	0.45
3:A:111:A:H2'	3:A:112:U:O4'	2.16	0.45
3:A:1785:A:O2'	3:A:1786:A:H2'	2.16	0.45
3:A:1313:U:H2'	3:A:1610:A:C2	2.51	0.45
3:A:706:A:C2	3:A:707:G:H1'	2.52	0.45
22:T:13:SER:O	22:T:17:VAL:HG23	2.17	0.45
3:A:718:A:H2'	3:A:719:C:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2229:U:H2'	3:A:2230:G:C8	2.51	0.45
3:A:2230:G:H2'	3:A:2231:U:C6	2.51	0.45
3:A:77:G:H2'	3:A:78:U:O4'	2.16	0.45
3:A:831:G:H5"	15:M:37:GLY:HA2	1.97	0.45
3:A:2313:C:H5"	8:F:88:LYS:HD3	1.98	0.45
3:A:1706:C:O2'	3:A:1757:A:H5'	2.17	0.45
8:F:136:ILE:HG22	8:F:141:ILE:HG21	1.98	0.45
3:A:1086:A:H4'	3:A:1103:A:C2	2.52	0.45
6:D:49:GLN:HA	6:D:80:TRP:O	2.16	0.45
3:A:1972:G:H2'	3:A:1973:G:H8	1.81	0.45
26:X:23:VAL:HG22	26:X:38:VAL:HB	1.99	0.45
3:A:2646:C:OP2	3:A:2732:G:O2'	2.35	0.45
13:K:65:THR:O	13:K:68:LYS:HB2	2.17	0.45
3:A:2667:C:H1'	9:G:109:PHE:CD1	2.52	0.45
3:A:764:A:H5'	5:C:209:GLY:HA2	1.98	0.45
6:D:7:LYS:HB3	6:D:7:LYS:HE2	1.78	0.45
6:D:99:GLU:OE2	6:D:182:ALA:HB2	2.15	0.45
1:1:40:C:H3'	1:1:41:C:H5"	1.98	0.45
17:O:2:ARG:CZ	17:O:2:ARG:HB3	2.46	0.45
3:A:2683:C:H4'	6:D:13:ARG:HH12	1.81	0.45
28:Z:27:ASN:O	28:Z:31:GLN:HG3	2.16	0.45
21:S:4:VAL:HA	21:S:12:HIS:O	2.17	0.45
3:A:2165:C:H2'	3:A:2166:U:O4'	2.16	0.45
3:A:208:C:H2'	3:A:209:C:C6	2.52	0.45
12:J:80:LEU:HB3	12:J:138:LEU:CD1	2.46	0.45
3:A:2396:G:N3	3:A:2421:G:N2	2.64	0.45
25:W:83:LYS:HB3	25:W:85:LYS:HG3	1.98	0.45
3:A:1287:A:H3'	3:A:1288:G:N2	2.32	0.45
11:I:41:LEU:HB2	11:I:99:PHE:CE1	2.52	0.45
12:J:117:MET:HB2	12:J:125:MET:HG2	1.99	0.45
19:Q:53:ARG:HB2	19:Q:56:HIS:HB2	1.99	0.45
3:A:1848:A:N3	3:A:1849:G:C8	2.85	0.45
10:H:62:LEU:HD23	10:H:135:HIS:CD2	2.52	0.45
3:A:1177:G:H2'	3:A:1178:C:C6	2.51	0.45
3:A:181:A:H1'	3:A:435:C:O4'	2.17	0.45
3:A:2318:G:C6	3:A:2319:G:N1	2.85	0.45
22:T:28:LYS:HE2	22:T:28:LYS:HB2	1.41	0.45
1:1:54:G:H2'	1:1:55:A:O4'	2.17	0.45
3:A:2569:G:C2	3:A:2570:G:C8	3.05	0.45
21:S:27:ILE:HG22	21:S:28:ALA:O	2.17	0.45
3:A:499:U:H5"	24:V:43:LYS:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:17:ARG:HG2	17:O:21:PHE:HE2	1.82	0.45
12:J:86:ILE:CD1	12:J:138:LEU:HD21	2.46	0.45
15:M:10:GLU:OE2	15:M:11:GLY:N	2.50	0.45
3:A:1466:U:H5"	3:A:1467:U:H5'	1.98	0.45
13:K:69:ARG:O	13:K:89:PHE:HB3	2.17	0.45
3:A:1918:A:O2'	3:A:1920:C:N4	2.50	0.45
16:N:65:ILE:HG12	16:N:103:TYR:CD2	2.51	0.45
3:A:257:C:H2'	3:A:258:G:O4'	2.15	0.44
3:A:356:G:H2'	3:A:357:C:O4'	2.18	0.44
3:A:239:C:H2'	3:A:240:C:O4'	2.16	0.44
9:G:42:GLU:HG3	9:G:55:ARG:HH21	1.83	0.44
10:H:100:ALA:O	10:H:104:THR:HG23	2.17	0.44
3:A:2273:A:H2'	3:A:2274:A:C8	2.52	0.44
3:A:1563:U:H2'	3:A:1564:C:C6	2.51	0.44
3:A:657:U:H2'	3:A:658:U:C6	2.52	0.44
23:U:34:VAL:HG21	23:U:43:ILE:HD11	1.99	0.44
19:Q:100:LEU:HD23	19:Q:100:LEU:HA	1.67	0.44
25:W:21:ARG:HE	25:W:87:GLN:HA	1.83	0.44
3:A:2396:G:C2	3:A:2421:G:C2	3.05	0.44
9:G:155:GLU:OE1	9:G:157:TYR:N	2.45	0.44
9:G:155:GLU:OE2	9:G:158:LYS:N	2.48	0.44
5:C:141:VAL:HG12	5:C:192:LEU:HA	1.99	0.44
26:X:36:ILE:HG23	26:X:58:THR:HG23	2.00	0.44
14:L:99:ILE:HG12	14:L:118:LEU:HB2	1.98	0.44
3:A:2130:U:O2'	3:A:2133:G:O2'	2.32	0.44
19:Q:89:ARG:HB3	19:Q:113:ARG:NH1	2.32	0.44
12:J:130:GLU:HB3	12:J:134:ARG:NH2	2.32	0.44
9:G:117:LEU:HD13	9:G:121:ILE:HG22	1.99	0.44
3:A:198:C:O2'	3:A:199:A:H5'	2.17	0.44
3:A:154:U:H2'	3:A:155:A:C8	2.52	0.44
24:V:37:GLU:O	24:V:39:ILE:HG12	2.17	0.44
3:A:1858:A:H2'	3:A:1859:U:O4'	2.17	0.44
3:A:593:U:H2'	3:A:594:U:C6	2.52	0.44
16:N:90:GLU:HB3	16:N:91:TYR:CD1	2.52	0.44
3:A:2134:A:H1'	3:A:2159:G:H21	1.82	0.44
1:1:34:U:H2'	1:1:35:G:C8	2.52	0.44
3:A:2489:U:C4	3:A:2490:G:C6	3.06	0.44
3:A:2776:A:C8	3:A:2782:G:C5	3.05	0.44
3:A:1450:G:C6	3:A:1451:C:N4	2.86	0.44
3:A:2038:G:H2'	3:A:2039:U:O4'	2.17	0.44
3:A:1962:C:H4'	3:A:1963:U:C5	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:149:A:C2	3:A:150:U:C2	3.06	0.44
17:O:86:ARG:HD3	17:O:121:LYS:HG3	1.98	0.44
23:U:31:VAL:O	23:U:32:LEU:HD23	2.18	0.44
3:A:1082:U:O2'	11:I:39:THR:HG23	2.18	0.44
3:A:2683:C:H4'	6:D:13:ARG:NH1	2.33	0.44
3:A:620:G:H4'	3:A:621:A:O5'	2.17	0.44
3:A:172:A:H2'	3:A:173:A:H8	1.81	0.44
3:A:1420:A:N7	3:A:2211:A:C6	2.86	0.44
3:A:2433:A:H5'	3:A:2434:A:P	2.57	0.44
3:A:2667:C:H1'	9:G:109:PHE:HD1	1.82	0.44
3:A:566:U:H5"	15:M:29:LYS:HE3	1.99	0.44
3:A:1542:U:H2'	3:A:1543:G:O4'	2.18	0.44
3:A:1205:A:H2'	7:E:165:HIS:HE1	1.83	0.44
8:F:48:LYS:HE2	8:F:48:LYS:HB2	1.85	0.44
3:A:277:G:H4'	3:A:278:A:N7	2.33	0.44
3:A:2443:C:H2'	3:A:2444:G:H8	1.82	0.44
3:A:57:C:H2'	3:A:58:G:O4'	2.18	0.44
18:P:52:SER:O	18:P:58:ILE:HD12	2.18	0.44
3:A:2377:A:H2'	3:A:2378:A:C8	2.53	0.44
10:H:26:ALA:HA	10:H:30:LEU:HB2	1.98	0.44
3:A:2230:G:H1'	27:Y:32:ASN:HB2	1.99	0.44
3:A:2292:U:H2'	3:A:2293:G:C8	2.52	0.44
3:A:1056:G:H1'	3:A:1103:A:N6	2.33	0.44
3:A:1591:A:H2'	3:A:1592:C:C6	2.53	0.44
3:A:948:C:H1'	3:A:984:A:C8	2.52	0.44
3:A:463:G:N1	3:A:467:G:C6	2.86	0.44
14:L:114:LYS:HZ2	14:L:118:LEU:HD11	1.83	0.44
12:J:90:SER:HB2	12:J:136:MET:O	2.18	0.44
3:A:2678:C:H2'	3:A:2679:A:O4'	2.18	0.44
3:A:1198:U:H2'	3:A:1199:U:C6	2.52	0.44
3:A:2704:C:H2'	3:A:2705:A:O4'	2.17	0.44
14:L:17:ARG:HD3	14:L:17:ARG:HA	1.77	0.44
3:A:2654:A:OP1	3:A:2654:A:H8	2.01	0.44
21:S:91:GLN:NE2	21:S:92:TRP:H	2.16	0.44
3:A:1093:G:H1'	3:A:1099:G:N1	2.32	0.43
3:A:2786:U:H2'	3:A:2787:C:C6	2.53	0.43
3:A:2387:U:H1'	26:X:41:ARG:NH1	2.33	0.43
3:A:1710:G:H2'	3:A:1711:A:C8	2.53	0.43
3:A:870:U:OP1	16:N:6:ARG:NH1	2.51	0.43
7:E:121:VAL:O	7:E:189:THR:HA	2.18	0.43
7:E:128:ALA:O	7:E:130:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:28:LEU:O	17:O:32:GLU:N	2.45	0.43
10:H:46:PHE:HD1	10:H:50:ARG:NH2	2.16	0.43
3:A:746:U:HO2'	3:A:2611:C:HO2'	1.66	0.43
17:O:72:ASP:OD1	17:O:73:ASN:N	2.51	0.43
21:S:4:VAL:HG12	21:S:39:LEU:HB2	2.00	0.43
3:A:2533:U:OP1	3:A:2665:A:O2'	2.34	0.43
3:A:1853:A:N6	3:A:1888:G:O2'	2.51	0.43
8:F:67:ILE:HD12	8:F:84:PRO:HB3	2.00	0.43
3:A:2172:U:H4'	3:A:2173:A:H5'	2.00	0.43
3:A:1082:U:H4'	11:I:46:ARG:NH1	2.32	0.43
3:A:783:A:C5	3:A:785:G:H1'	2.53	0.43
3:A:677:A:O2'	3:A:2071:A:H5'	2.17	0.43
3:A:2024:G:H2'	3:A:2025:C:C6	2.53	0.43
3:A:11:C:H2'	3:A:12:U:H5'	2.00	0.43
3:A:1287:A:H5'	17:O:103:ARG:HD2	1.98	0.43
24:V:49:VAL:HA	24:V:50:PRO:HD3	1.84	0.43
3:A:14:A:C6	3:A:526:A:C2	3.07	0.43
19:Q:62:ARG:NH2	19:Q:101:ARG:HG2	2.32	0.43
6:D:131:ASP:O	6:D:140:HIS:HD2	2.02	0.43
3:A:1517:G:C2	3:A:1732:C:N3	2.86	0.43
27:Y:59:ILE:HG12	27:Y:67:VAL:HG21	1.99	0.43
3:A:2512:C:H5"	3:A:2513:A:OP2	2.17	0.43
5:C:205:LEU:HD23	5:C:205:LEU:HA	1.68	0.43
13:K:26:GLY:O	13:K:30:THR:HG23	2.18	0.43
3:A:834:G:C2	3:A:835:C:C2	3.06	0.43
3:A:1614:A:C2	22:T:93:ALA:HB2	2.52	0.43
8:F:128:TYR:CE2	8:F:130:MET:HG2	2.53	0.43
20:R:24:TYR:O	20:R:29:SER:HB3	2.19	0.43
5:C:176:LEU:HA	5:C:176:LEU:HD23	1.80	0.43
8:F:147:ASP:OD1	8:F:150:ARG:NH2	2.51	0.43
3:A:1354:A:H2'	3:A:1355:G:O4'	2.19	0.43
3:A:1266:G:N2	3:A:2012:G:H2'	2.33	0.43
3:A:997:G:H5"	20:R:92:ARG:NH1	2.33	0.43
3:A:1301:A:H2'	3:A:1301:A:N3	2.33	0.43
11:I:118:ILE:HA	11:I:119:PRO:HD2	1.84	0.43
5:C:251:GLN:HB2	5:C:251:GLN:HE21	1.58	0.43
3:A:195:A:H5"	15:M:47:ARG:HH22	1.84	0.43
3:A:969:G:H2'	3:A:970:U:C6	2.53	0.43
15:M:80:SER:O	15:M:84:LYS:HE3	2.19	0.43
3:A:464:U:C2	3:A:788:A:C6	3.07	0.43
19:Q:25:THR:HB	19:Q:88:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:34:VAL:HG11	23:U:43:ILE:HD13	2.01	0.43
3:A:1627:G:C2	3:A:1628:G:C8	3.07	0.43
3:A:2144:G:N2	3:A:2148:G:O6	2.52	0.43
3:A:493:G:H2'	3:A:494:G:O4'	2.19	0.43
3:A:819:A:H2'	3:A:819:A:N3	2.34	0.43
5:C:153:GLN:O	5:C:156:ARG:HG3	2.18	0.43
1:1:69:G:H2'	1:1:70:G:C1'	2.48	0.43
3:A:2114:A:C2	3:A:2166:U:H2'	2.54	0.43
3:A:1327:A:H2'	3:A:1328:A:O4'	2.19	0.43
3:A:112:U:H5'	28:Z:58:ASN:ND2	2.34	0.43
16:N:26:VAL:HB	16:N:133:LYS:HB2	2.00	0.43
10:H:104:THR:HA	10:H:108:VAL:O	2.18	0.43
3:A:307:G:N1	3:A:310:A:OP2	2.51	0.43
3:A:2047:C:O2'	3:A:2823:A:N1	2.42	0.43
12:J:110:ALA:O	12:J:114:ALA:HB2	2.18	0.43
3:A:543:G:H5'	3:A:544:C:OP2	2.18	0.43
3:A:1494:A:H2'	3:A:1495:A:H8	1.83	0.43
20:R:117:LEU:HD23	20:R:117:LEU:HA	1.77	0.43
28:Z:42:LEU:HD23	28:Z:42:LEU:HA	1.81	0.43
3:A:93:G:H2'	3:A:94:A:H8	1.84	0.43
3:A:1434:A:C2	3:A:1435:G:C5	3.07	0.43
10:H:8:LYS:HE3	10:H:8:LYS:HB3	1.87	0.43
3:A:141:G:C8	3:A:142:A:O4'	2.72	0.43
3:A:1387:A:H2'	3:A:1388:G:O4'	2.18	0.43
3:A:1230:A:H2'	3:A:1231:U:O4'	2.18	0.43
3:A:1515:A:H3'	3:A:1516:G:H8	1.84	0.43
3:A:1667:G:N2	3:A:1992:G:OP2	2.44	0.43
5:C:90:ASN:ND2	5:C:197:ASN:HB2	2.34	0.43
5:C:8:PRO:HB3	5:C:14:ARG:HG3	1.99	0.43
22:T:47:VAL:HG22	22:T:103:ILE:HD13	2.00	0.43
17:O:22:ARG:HE	17:O:22:ARG:HB2	1.49	0.43
3:A:2847:U:H2'	3:A:2848:G:O4'	2.18	0.43
20:R:24:TYR:HD1	20:R:24:TYR:N	2.17	0.43
3:A:973:A:OP2	21:S:81:LYS:HE3	2.18	0.43
3:A:1735:A:H2'	3:A:1736:U:O4'	2.18	0.43
3:A:2790:U:H5'	3:A:2893:A:N7	2.34	0.43
3:A:1759:A:C2	3:A:2697:G:H1'	2.54	0.43
3:A:2518:A:N3	3:A:2518:A:H2'	2.34	0.43
3:A:1400:U:H2'	3:A:1401:G:O4'	2.19	0.43
5:C:245:VAL:HA	5:C:252:THR:HG22	2.01	0.43
3:A:2292:U:H2'	3:A:2293:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2184:A:H2'	3:A:2185:U:C6	2.53	0.43
3:A:558:U:OP1	13:K:114:LEU:N	2.46	0.43
3:A:1501:G:H2'	3:A:1502:A:H8	1.84	0.43
3:A:1351:C:H4'	3:A:1572:A:O4'	2.18	0.43
3:A:2588:G:O6	3:A:2607:G:C6	2.72	0.43
3:A:475:C:N4	3:A:476:G:C6	2.87	0.43
3:A:76:C:H6	3:A:76:C:O5'	2.02	0.43
25:W:29:ILE:O	25:W:91:PHE:HB2	2.19	0.43
4:B:49:C:H2'	4:B:50:A:C8	2.54	0.43
7:E:108:ILE:O	7:E:112:LEU:HG	2.18	0.43
12:J:113:LYS:HA	12:J:116:ASP:HB2	2.01	0.43
3:A:1088:A:H61	12:J:135:SER:HB3	1.82	0.43
10:H:62:LEU:HD22	10:H:137:GLU:OE1	2.19	0.43
3:A:1047:G:OP1	11:I:56:ARG:NH1	2.52	0.43
3:A:976:G:HO2'	3:A:1155:A:HO2'	1.61	0.43
3:A:2304:G:H22	3:A:2312:U:H3	1.67	0.43
12:J:103:ARG:H	12:J:103:ARG:HD2	1.83	0.43
3:A:5:A:H2'	3:A:6:A:C8	2.54	0.42
12:J:74:PRO:HA	12:J:75:PRO:HD3	1.89	0.42
12:J:38:PHE:CD1	12:J:59:ILE:HD11	2.54	0.42
7:E:29:HIS:O	7:E:32:VAL:HG22	2.19	0.42
3:A:2843:G:H2'	3:A:2844:G:C8	2.54	0.42
3:A:1751:U:H2'	3:A:1752:C:C6	2.54	0.42
3:A:2700:A:H2'	3:A:2701:U:C6	2.54	0.42
3:A:1044:C:O2'	3:A:1111:A:N1	2.45	0.42
8:F:170:LEU:HD23	8:F:170:LEU:HA	1.75	0.42
20:R:9:ILE:HD12	20:R:9:ILE:H	1.84	0.42
22:T:46:LEU:HA	22:T:46:LEU:HD23	1.82	0.42
4:B:114:C:H2'	4:B:115:A:H8	1.83	0.42
3:A:2293:G:OP1	18:P:94:ARG:NH1	2.46	0.42
3:A:1736:U:H2'	3:A:1737:G:O4'	2.18	0.42
3:A:1759:A:H2'	3:A:1760:C:C6	2.54	0.42
3:A:1780:A:H3'	3:A:1781:U:H2'	2.01	0.42
9:G:149:ARG:HG3	9:G:162:VAL:O	2.19	0.42
28:Z:12:GLU:O	28:Z:16:THR:N	2.53	0.42
3:A:461:C:H2'	3:A:462:C:H6	1.84	0.42
3:A:380:G:H2'	3:A:381:G:O4'	2.18	0.42
4:B:106:G:H2'	4:B:107:G:O4'	2.19	0.42
3:A:1614:A:H8	3:A:1614:A:O5'	2.02	0.42
3:A:1922:G:H2'	3:A:1923:U:O4'	2.18	0.42
10:H:94:ILE:HG23	10:H:98:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:33:VAL:HG13	12:J:67:PHE:CD2	2.54	0.42
3:A:794:A:H2'	3:A:795:C:C6	2.55	0.42
3:A:2339:C:O3'	4:B:41:G:N2	2.53	0.42
3:A:2776:A:C2	3:A:2778:A:C4	3.07	0.42
4:B:66:A:H61	4:B:107:G:H2'	1.84	0.42
16:N:33:LEU:HD11	16:N:128:THR:HB	2.00	0.42
3:A:2079:U:O2'	27:Y:23:ASN:OD1	2.31	0.42
3:A:674:G:H2'	3:A:804:A:H61	1.83	0.42
3:A:2586:U:OP2	3:A:2608:G:N1	2.48	0.42
3:A:1473:G:H2'	3:A:1474:U:O4'	2.19	0.42
16:N:42:THR:N	16:N:45:GLN:OE1	2.47	0.42
8:F:145:LYS:HA	8:F:145:LYS:HD3	1.89	0.42
6:D:148:GLN:N	6:D:148:GLN:OE1	2.51	0.42
4:B:57:A:C4	8:F:26:MET:HB3	2.54	0.42
24:V:61:LYS:HG2	24:V:62:GLU:H	1.85	0.42
25:W:2:PHE:HE1	25:W:53:LYS:HD2	1.84	0.42
3:A:1141:U:H4'	3:A:1142:A:O4'	2.19	0.42
3:A:1064:C:H5"	12:J:88:SER:HB2	2.02	0.42
3:A:1524:G:H2'	3:A:1525:A:O4'	2.20	0.42
3:A:729:G:C5	5:C:207:LYS:HB2	2.55	0.42
3:A:669:G:N2	3:A:670:A:C2	2.88	0.42
5:C:200:HIS:C	5:C:200:HIS:CD2	2.92	0.42
17:O:75:ILE:HD12	17:O:75:ILE:HA	1.82	0.42
3:A:2119:A:H62	3:A:2167:U:H1'	1.85	0.42
8:F:79:ILE:HG21	8:F:85:ILE:HD11	2.01	0.42
3:A:123:G:N2	3:A:129:C:C2	2.87	0.42
3:A:1637:A:H2'	3:A:1638:C:C6	2.54	0.42
3:A:1039:A:H2'	3:A:1040:A:O4'	2.20	0.42
12:J:22:PRO:HB2	12:J:23:PRO:HD3	2.02	0.42
26:X:47:ALA:HB1	26:X:51:VAL:O	2.19	0.42
4:B:48:U:H4'	18:P:100:HIS:HD2	1.84	0.42
10:H:1:MET:O	10:H:20:ASN:HA	2.20	0.42
14:L:3:GLN:HB3	14:L:3:GLN:HE21	1.65	0.42
9:G:44:LYS:HB2	9:G:44:LYS:HE3	1.80	0.42
3:A:571:U:H3'	21:S:80:ARG:NH2	2.33	0.42
3:A:812:C:C2	3:A:1250:G:N1	2.87	0.42
3:A:1463:C:H2'	3:A:1464:G:H8	1.85	0.42
3:A:1880:U:H2'	3:A:1881:C:C6	2.55	0.42
3:A:2138:G:C6	3:A:2154:A:C2	3.06	0.42
3:A:393:C:H2'	3:A:394:C:H6	1.85	0.42
3:A:2322:A:C4	3:A:2323:G:C8	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:73:ASN:O	9:G:77:ILE:HG13	2.20	0.42
23:U:88:LYS:H	23:U:91:GLN:HE22	1.67	0.42
3:A:1590:A:H2'	3:A:1591:A:C8	2.54	0.42
3:A:910:A:C6	3:A:911:A:C6	3.08	0.42
3:A:729:G:H2'	3:A:1775:U:H1'	2.01	0.42
5:C:210:ALA:HA	5:C:213:TRP:CE3	2.53	0.42
16:N:36:VAL:HG13	25:W:82:TYR:CD2	2.55	0.42
3:A:647:G:H2'	3:A:648:G:C8	2.55	0.42
14:L:65:THR:HB	14:L:68:GLY:H	1.84	0.42
20:R:74:ILE:HG12	20:R:75:SER:N	2.34	0.42
6:D:109:VAL:HG12	6:D:201:LEU:HD22	2.01	0.42
9:G:97:ALA:HB3	9:G:104:ASN:HB2	2.01	0.42
5:C:133:ARG:HD2	10:H:123:ARG:NH1	2.35	0.42
3:A:1482:G:H2'	3:A:1483:G:H8	1.83	0.42
15:M:41:ARG:H	15:M:41:ARG:HG2	1.62	0.42
3:A:1509:A:O2'	3:A:1510:G:H8	2.03	0.42
3:A:1057:A:N7	3:A:1086:A:H2'	2.35	0.42
3:A:1709:U:H2'	3:A:1710:G:C8	2.55	0.42
3:A:1048:A:N1	3:A:1112:G:O2'	2.36	0.42
3:A:1417:C:H2'	3:A:1418:G:C8	2.55	0.42
3:A:799:G:C6	3:A:800:A:C6	3.08	0.42
3:A:1631:G:N2	3:A:1634:A:OP2	2.32	0.42
3:A:1821:A:H2'	3:A:1822:C:C6	2.55	0.42
3:A:2771:C:H2'	3:A:2772:C:C6	2.54	0.42
11:I:43:LYS:HE2	12:J:118:THR:HA	2.02	0.42
3:A:2209:G:C2	3:A:2216:G:C2	3.08	0.42
3:A:1065:U:H2'	3:A:1066:U:O4'	2.19	0.42
11:I:15:VAL:HG11	11:I:60:LEU:CD2	2.50	0.42
8:F:70:ALA:HB3	8:F:81:GLN:HA	2.02	0.42
19:Q:106:LYS:O	19:Q:109:ARG:HD3	2.20	0.42
3:A:1946:U:H2'	3:A:1947:C:H6	1.84	0.42
3:A:2286:G:C8	3:A:2287:A:N6	2.88	0.42
3:A:1902:C:H4'	5:C:242:LYS:O	2.19	0.42
3:A:297:G:H2'	3:A:298:G:O4'	2.20	0.42
3:A:2706:A:C2	3:A:2707:U:C2	3.08	0.42
3:A:1597:A:C5'	3:A:1598:A:H5'	2.47	0.41
3:A:2365:G:H4'	26:X:60:PHE:CE2	2.55	0.41
3:A:2433:A:H5'	3:A:2434:A:OP2	2.19	0.41
28:Z:14:LEU:HA	28:Z:14:LEU:HD23	1.79	0.41
17:O:103:ARG:HB3	17:O:106:ASP:OD1	2.20	0.41
3:A:2812:G:H2'	3:A:2813:A:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:73:VAL:HG11	6:D:93:GLY:HA2	2.02	0.41
3:A:848:C:H42	3:A:930:G:H1	1.68	0.41
13:K:12:LYS:HA	13:K:12:LYS:HD2	1.81	0.41
23:U:87:LEU:HD11	23:U:93:LEU:HD12	2.01	0.41
3:A:877:A:C6	3:A:899:A:C6	3.08	0.41
3:A:1432:G:H2'	3:A:1433:A:C8	2.55	0.41
8:F:79:ILE:O	8:F:79:ILE:HD12	2.20	0.41
3:A:335:C:H5"	24:V:82:ARG:HD2	2.02	0.41
3:A:1056:G:H5'	11:I:35:VAL:HG21	2.02	0.41
3:A:678:C:H2'	3:A:679:C:H6	1.84	0.41
3:A:1078:U:O2	3:A:1088:A:H3'	2.20	0.41
3:A:1068:G:N2	3:A:1095:A:O3'	2.44	0.41
8:F:57:LEU:HD12	8:F:87:CYS:SG	2.61	0.41
3:A:2796:U:HO2'	3:A:2797:U:H6	1.63	0.41
3:A:908:C:O2'	16:N:70:ASP:OD2	2.30	0.41
3:A:1449:G:N2	3:A:1463:C:C2	2.88	0.41
3:A:1463:C:H2'	3:A:1464:G:C8	2.55	0.41
3:A:1324:G:C4	3:A:1328:A:N6	2.88	0.41
3:A:1877:A:H2'	3:A:1878:G:O4'	2.19	0.41
18:P:85:LYS:HB3	18:P:85:LYS:HE2	1.79	0.41
3:A:2352:A:N1	26:X:34:GLY:HA3	2.35	0.41
10:H:128:HIS:O	10:H:143:ILE:HA	2.20	0.41
3:A:2343:U:H2'	3:A:2344:U:C6	2.55	0.41
3:A:648:G:C2	3:A:649:G:C5	3.08	0.41
3:A:328:U:H4'	24:V:66:GLN:HE21	1.86	0.41
3:A:2895:G:H2'	3:A:2896:C:C6	2.56	0.41
3:A:1484:U:H2'	3:A:1485:U:C6	2.55	0.41
7:E:181:ILE:H	7:E:181:ILE:HG13	1.70	0.41
3:A:2578:G:OP2	3:A:2578:G:H4'	2.19	0.41
3:A:1365:A:N3	3:A:1365:A:H2'	2.36	0.41
3:A:2229:U:H2'	3:A:2230:G:H8	1.85	0.41
3:A:653:U:C1'	3:A:654:A:H5"	2.49	0.41
3:A:1798:U:OP2	5:C:271:ARG:NH2	2.52	0.41
3:A:948:C:H2'	3:A:949:G:H8	1.85	0.41
5:C:176:LEU:HB2	5:C:180:GLU:O	2.20	0.41
3:A:1499:C:H2'	3:A:1500:G:H8	1.85	0.41
3:A:465:G:C6	3:A:466:A:N6	2.89	0.41
15:M:78:ARG:HG2	15:M:113:ALA:HB3	2.03	0.41
9:G:83:PHE:HB2	9:G:135:GLY:O	2.20	0.41
3:A:75:G:H4'	28:Z:48:ARG:NH2	2.35	0.41
3:A:1972:G:H2'	3:A:1973:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:71:C:C2	4:B:106:G:C2	3.08	0.41
20:R:31:VAL:HG12	20:R:34:VAL:H	1.85	0.41
27:Y:54:LYS:O	27:Y:58:VAL:HG23	2.19	0.41
27:Y:3:ARG:NE	27:Y:30:LEU:HD13	2.35	0.41
3:A:561:G:H4'	20:R:48:ARG:HH22	1.86	0.41
11:I:100:ALA:HB2	11:I:106:PHE:CE1	2.56	0.41
3:A:2209:G:N2	3:A:2215:C:N3	2.60	0.41
17:O:65:LEU:HD12	17:O:65:LEU:HA	1.85	0.41
3:A:2102:G:C2	3:A:2187:U:O2	2.74	0.41
3:A:2627:G:H1'	3:A:2777:G:N2	2.36	0.41
4:B:7:G:H5"	18:P:29:HIS:CE1	2.56	0.41
3:A:2785:C:H2'	3:A:2786:U:H6	1.85	0.41
3:A:681:G:C2	3:A:797:G:C2	3.09	0.41
3:A:1770:G:C6	3:A:1983:G:C6	3.07	0.41
3:A:449:A:C4	3:A:450:G:C8	3.08	0.41
3:A:779:U:H2'	3:A:780:G:C8	2.56	0.41
3:A:565:C:H4'	3:A:1253:A:C6	2.55	0.41
3:A:118:A:N3	3:A:178:G:H1'	2.36	0.41
3:A:205:G:HO2'	3:A:206:U:P	2.43	0.41
1:1:72:A:C4	1:1:73:G:C8	3.08	0.41
11:I:85:VAL:HG21	11:I:90:GLY:O	2.20	0.41
3:A:1275:A:OP2	3:A:1646:C:N4	2.53	0.41
4:B:95:U:H2'	4:B:96:G:C8	2.56	0.41
16:N:6:ARG:HB2	16:N:6:ARG:CZ	2.50	0.41
8:F:34:ILE:HB	8:F:96:MET:HG3	2.02	0.41
8:F:36:LEU:HA	8:F:153:ASP:O	2.21	0.41
5:C:84:ASP:HA	5:C:85:PRO:HD2	1.85	0.41
3:A:1807:G:N2	3:A:1811:G:C5	2.89	0.41
28:Z:46:VAL:O	28:Z:50:VAL:HG23	2.21	0.41
22:T:109:ASP:OD1	22:T:110:ARG:N	2.54	0.41
14:L:93:GLN:HA	14:L:94:PRO:HD3	1.88	0.41
1:1:42:A:OP1	1:1:42:A:H4'	2.20	0.41
1:1:67:A:C4	1:1:68:A:C8	3.08	0.41
3:A:2847:U:C5	3:A:2848:G:C5	3.09	0.41
11:I:48:ALA:HB3	11:I:50:VAL:HG23	2.02	0.41
3:A:1073:A:H2'	3:A:1074:G:O4'	2.21	0.41
3:A:2267:A:H5"	3:A:2268:A:C5'	2.50	0.41
3:A:811:U:C2	3:A:1251:C:C5	3.09	0.41
17:O:72:ASP:O	17:O:76:VAL:HG13	2.21	0.41
3:A:1789:A:H2'	3:A:1790:C:O4'	2.21	0.41
3:A:2431:U:O2	3:A:2431:U:O4'	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:76:VAL:O	9:G:80:THR:HG23	2.20	0.41
12:J:42:PHE:CE1	12:J:57:VAL:HB	2.56	0.41
3:A:1672:A:N6	3:A:1673:G:C6	2.89	0.41
3:A:31:C:O3'	3:A:1238:G:H5'	2.21	0.41
3:A:601:C:O2'	3:A:605:G:H5"	2.21	0.41
3:A:53:A:H2'	3:A:54:G:O4'	2.21	0.41
8:F:65:PRO:HA	8:F:89:VAL:HG22	2.02	0.41
9:G:154:PRO:HA	9:G:160:LYS:O	2.21	0.41
3:A:2061:G:H2'	3:A:2501:C:O2'	2.21	0.41
3:A:528:A:C8	3:A:2042:A:C2	3.09	0.41
3:A:1071:G:O2'	3:A:1089:A:OP2	2.36	0.41
3:A:2663:G:H2'	3:A:2664:G:O4'	2.21	0.41
3:A:2860:A:H5"	3:A:2861:U:OP2	2.21	0.41
22:T:96:ILE:HD13	22:T:96:ILE:HA	1.73	0.41
3:A:1374:G:H8	3:A:1374:G:OP2	2.04	0.41
3:A:807:U:H2'	3:A:808:G:H8	1.85	0.41
3:A:1341:G:C2	3:A:1398:C:H4'	2.56	0.41
3:A:1024:G:C6	3:A:1025:G:C6	3.09	0.41
16:N:65:ILE:HG12	16:N:103:TYR:HD2	1.86	0.41
3:A:2143:C:H2'	3:A:2144:G:O4'	2.21	0.41
3:A:2550:G:C6	3:A:2551:C:C4	3.09	0.41
3:A:2838:G:H2'	3:A:2839:G:O4'	2.20	0.41
3:A:1127:A:N7	3:A:2488:G:O2'	2.55	0.41
3:A:1366:A:H2'	3:A:1367:A:O4'	2.21	0.41
3:A:743:A:OP1	6:D:135:GLY:HA2	2.21	0.41
3:A:1838:C:H4'	3:A:1839:G:H8	1.85	0.41
3:A:339:U:O5'	3:A:339:U:H6	2.04	0.41
11:I:99:PHE:HD2	11:I:106:PHE:HZ	1.69	0.40
3:A:1869:G:C2	3:A:1873:G:C6	3.09	0.40
8:F:13:VAL:O	8:F:17:MET:HB2	2.21	0.40
6:D:13:ARG:HD2	6:D:15:PHE:CE2	2.57	0.40
24:V:96:PHE:O	24:V:100:SER:HA	2.21	0.40
3:A:396:G:H1'	27:Y:29:PHE:HB3	2.02	0.40
5:C:157:SER:O	5:C:160:THR:OG1	2.38	0.40
3:A:729:G:C6	5:C:207:LYS:HB2	2.56	0.40
3:A:118:A:C8	3:A:119:A:C8	3.09	0.40
3:A:520:G:H2'	3:A:521:U:C6	2.56	0.40
3:A:2682:A:C2	6:D:23:PRO:HB3	2.56	0.40
3:A:64:A:C6	3:A:65:U:C4	3.09	0.40
3:A:717:C:C5	3:A:718:A:C8	3.10	0.40
3:A:247:G:H4'	3:A:386:G:C4	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2603:G:C6	3:A:2604:U:C4	3.10	0.40
3:A:1005:C:H2'	3:A:1006:C:H6	1.84	0.40
3:A:2365:G:P	26:X:55:ARG:HG2	2.61	0.40
25:W:2:PHE:HB3	25:W:50:MET:HE3	2.03	0.40
3:A:2667:C:O5'	3:A:2667:C:H6	2.04	0.40
15:M:79:LEU:HB2	15:M:113:ALA:O	2.21	0.40
27:Y:3:ARG:O	27:Y:12:PRO:HD3	2.21	0.40
3:A:501:A:H2'	3:A:502:A:C8	2.56	0.40
3:A:33:C:N4	3:A:446:G:O2'	2.45	0.40
27:Y:36:HIS:O	27:Y:48:THR:HA	2.21	0.40
16:N:38:ARG:HB2	16:N:98:PRO:HD3	2.02	0.40
4:B:68:C:H2'	4:B:69:G:O4'	2.21	0.40
3:A:1423:G:N2	3:A:1576:U:O2	2.54	0.40
6:D:125:TRP:CE2	6:D:160:LYS:HB3	2.57	0.40
23:U:49:LYS:HG3	23:U:50:LEU:HD23	2.03	0.40
13:K:9:GLU:H	13:K:9:GLU:HG2	1.66	0.40
3:A:258:G:H1'	15:M:104:GLN:NE2	2.31	0.40
8:F:22:TYR:HB3	8:F:27:GLN:HB2	2.04	0.40
3:A:776:G:HO2'	3:A:777:G:P	2.41	0.40
3:A:2647:U:H2'	3:A:2648:G:C8	2.54	0.40
15:M:27:LEU:HD23	15:M:27:LEU:HA	1.66	0.40
3:A:199:A:N6	3:A:2434:A:C5	2.90	0.40
3:A:125:A:H2	6:D:9:VAL:HG12	91.24	0.40
24:V:36:VAL:HB	24:V:39:ILE:HB	2.03	0.40
3:A:445:C:H2'	3:A:446:G:O4'	2.22	0.40
5:C:34:LEU:HD21	5:C:63:ARG:HG3	2.04	0.40
3:A:2563:U:O2	3:A:2566:A:C5	2.75	0.40
3:A:2394:C:H42	3:A:2422:C:N4	2.19	0.40
8:F:103:LEU:HA	8:F:107:ALA:HB3	2.02	0.40
21:S:22:LEU:HA	21:S:22:LEU:HD23	1.94	0.40
5:C:13:ARG:HD2	5:C:13:ARG:HA	1.82	0.40
3:A:1818:U:C5	5:C:156:ARG:NH2	2.90	0.40
3:A:277:G:H4'	3:A:278:A:C5	2.56	0.40
4:B:49:C:H2'	4:B:50:A:H8	1.87	0.40
3:A:1869:G:C6	3:A:1871:A:OP2	2.75	0.40
3:A:1607:C:O2'	3:A:1608:A:OP1	2.37	0.40
3:A:871:U:H4'	16:N:68:PHE:CD2	2.57	0.40
3:A:2052:A:C6	3:A:2053:G:N7	2.90	0.40
3:A:778:G:H5"	3:A:779:U:OP2	2.21	0.40
3:A:2804:U:H2'	3:A:2805:C:C6	2.56	0.40
11:I:61:ARG:HG2	11:I:73:LYS:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1803:A:C8	3:A:1804:C:C6	3.10	0.40
10:H:60:GLU:HA	10:H:63:ALA:HB3	2.04	0.40
3:A:42:A:C6	3:A:43:G:C5	3.10	0.40
26:X:70:GLU:HG3	26:X:72:LYS:HE2	2.04	0.40
3:A:1139:G:OP2	3:A:1139:G:H8	2.05	0.40
15:M:81:ASP:HB3	15:M:100:ILE:HD13	2.02	0.40
3:A:856:G:H2'	3:A:857:G:C8	2.57	0.40
9:G:90:VAL:HG21	9:G:163:ARG:NH1	2.37	0.40
3:A:1707:G:C5	3:A:1756:G:C6	3.10	0.40
3:A:1258:U:C2	3:A:1259:G:C8	3.09	0.40
3:A:353:C:H2'	3:A:354:A:O4'	2.22	0.40
3:A:822:G:H2'	3:A:823:C:C6	2.57	0.40
3:A:2048:G:H2'	3:A:2049:G:O4'	2.22	0.40
3:A:1113:U:H2'	3:A:1114:C:H6	1.86	0.40
2:2:74:C:O5'	2:2:74:C:H6	2.04	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	
5	C	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
6	D	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
7	E	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
8	F	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
9	G	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
10	H	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	26	72
11	I	123/165 (74%)	113 (92%)	9 (7%)	1 (1%)	24	70
12	J	132/142 (93%)	126 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	K	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
14	L	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
15	M	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
17	O	123/127 (97%)	118 (96%)	5 (4%)	0	100	100
18	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	Q	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
20	R	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
21	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	T	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
23	U	93/100 (93%)	89 (96%)	3 (3%)	1 (1%)	17	65
24	V	100/104 (96%)	99 (99%)	1 (1%)	0	100	100
25	W	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
26	X	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
27	Y	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
28	Z	56/63 (89%)	54 (96%)	2 (4%)	0	100	100
29	a	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
30	b	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
31	c	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
32	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
33	e	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
34	f	36/38 (95%)	36 (100%)	0	0	100	100
35	i	378/450 (84%)	361 (96%)	17 (4%)	0	100	100
36	k	16/18 (89%)	11 (69%)	5 (31%)	0	100	100
37	l	196/497 (39%)	189 (96%)	7 (4%)	0	100	100
All	All	4018/4539 (88%)	3876 (96%)	139 (4%)	3 (0%)	59	90

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	U	89	GLU
10	H	118	PRO
11	I	108	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	C	216/218 (99%)	192 (89%)	24 (11%)	8 39
6	D	164/164 (100%)	154 (94%)	10 (6%)	23 65
7	E	165/165 (100%)	152 (92%)	13 (8%)	15 55
8	F	148/150 (99%)	130 (88%)	18 (12%)	6 34
9	G	137/138 (99%)	129 (94%)	8 (6%)	25 67
10	H	114/114 (100%)	100 (88%)	14 (12%)	6 34
11	I	95/123 (77%)	89 (94%)	6 (6%)	22 64
12	J	104/110 (94%)	93 (89%)	11 (11%)	8 42
13	K	116/116 (100%)	105 (90%)	11 (10%)	11 47
14	L	104/104 (100%)	94 (90%)	10 (10%)	10 46
15	M	103/103 (100%)	94 (91%)	9 (9%)	13 51
16	N	109/109 (100%)	100 (92%)	9 (8%)	14 53
17	O	102/103 (99%)	95 (93%)	7 (7%)	19 61
18	P	87/87 (100%)	75 (86%)	12 (14%)	4 30
19	Q	99/100 (99%)	90 (91%)	9 (9%)	12 49
20	R	89/90 (99%)	82 (92%)	7 (8%)	15 55
21	S	84/84 (100%)	76 (90%)	8 (10%)	11 47
22	T	93/93 (100%)	88 (95%)	5 (5%)	27 69
23	U	82/84 (98%)	76 (93%)	6 (7%)	17 59
24	V	83/85 (98%)	76 (92%)	7 (8%)	14 53
25	W	78/78 (100%)	72 (92%)	6 (8%)	16 56
26	X	57/63 (90%)	51 (90%)	6 (10%)	8 42
27	Y	67/68 (98%)	63 (94%)	4 (6%)	24 66
28	Z	54/55 (98%)	48 (89%)	6 (11%)	8 39
29	a	48/49 (98%)	46 (96%)	2 (4%)	36 75
30	b	47/48 (98%)	35 (74%)	12 (26%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
31	c	45/49 (92%)	40 (89%)	5 (11%)	8 39
32	d	38/38 (100%)	32 (84%)	6 (16%)	3 23
33	e	51/52 (98%)	47 (92%)	4 (8%)	16 56
34	f	34/34 (100%)	31 (91%)	3 (9%)	12 51
35	i	311/313 (99%)	298 (96%)	13 (4%)	36 75
36	k	17/17 (100%)	15 (88%)	2 (12%)	6 36
37	l	156/405 (38%)	153 (98%)	3 (2%)	65 88
All	All	3297/3609 (91%)	3021 (92%)	276 (8%)	18 53

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	3	VAL
5	C	24	LEU
5	C	35	GLU
5	C	51	THR
5	C	72	ASP
5	C	74	ILE
5	C	120	VAL
5	C	130	LEU
5	C	134	ASN
5	C	156	ARG
5	C	180	GLU
5	C	185	GLU
5	C	189	ARG
5	C	195	VAL
5	C	203	ARG
5	C	204	VAL
5	C	228	VAL
5	C	242	LYS
5	C	250	VAL
5	C	251	GLN
5	C	257	THR
5	C	261	LYS
5	C	265	LYS
5	C	271	ARG
6	D	12	THR
6	D	13	ARG
6	D	18	ASP
6	D	28	GLU

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Mol	Chain	Res	Type
6	D	73	VAL
6	D	84	LEU
6	D	128	ARG
6	D	139	SER
6	D	160	LYS
6	D	168	GLU
7	E	84	THR
7	E	85	PHE
7	E	94	GLN
7	E	97	ASN
7	E	105	LEU
7	E	115	GLN
7	E	119	ILE
7	E	127	GLU
7	E	148	ILE
7	E	173	THR
7	E	179	SER
7	E	184	ASP
7	E	196	VAL
8	F	3	LYS
8	F	4	LEU
8	F	14	LYS
8	F	25	VAL
8	F	49	LEU
8	F	51	ASP
8	F	52	ASN
8	F	72	LYS
8	F	81	GLN
8	F	104	ILE
8	F	106	ILE
8	F	130	MET
8	F	141	ILE
8	F	144	ASP
8	F	149	VAL
8	F	150	ARG
8	F	153	ASP
8	F	162	SER
9	G	10	VAL
9	G	11	VAL
9	G	49	THR
9	G	87	LEU
9	G	114	ASP

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Mol	Chain	Res	Type
9	G	125	CYS
9	G	127	THR
9	G	153	ARG
10	H	15	LEU
10	H	17	ASP
10	H	25	TYR
10	H	37	VAL
10	H	58	LEU
10	H	60	GLU
10	H	76	GLU
10	H	77	THR
10	H	78	VAL
10	H	86	ASP
10	H	87	GLU
10	H	110	VAL
10	H	112	LYS
10	H	116	ARG
11	I	16	SER
11	I	36	ASP
11	I	58	THR
11	I	85	VAL
11	I	96	PHE
11	I	109	LYS
12	J	9	VAL
12	J	21	SER
12	J	28	LEU
12	J	31	GLN
12	J	55	ILE
12	J	66	SER
12	J	111	GLN
12	J	112	THR
12	J	113	LYS
12	J	116	ASP
12	J	128	SER
13	K	5	THR
13	K	7	LYS
13	K	34	ARG
13	K	40	HIS
13	K	44	TYR
13	K	69	ARG
13	K	70	THR
13	K	88	THR

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Mol	Chain	Res	Type
13	K	103	ILE
13	K	122	LEU
13	K	131	ASN
14	L	1	MET
14	L	21	CYS
14	L	42	THR
14	L	49	ARG
14	L	56	ASP
14	L	58	LEU
14	L	65	THR
14	L	84	CYS
14	L	106	GLU
14	L	116	ILE
15	M	2	ARG
15	M	14	LYS
15	M	46	VAL
15	M	47	ARG
15	M	55	MET
15	M	59	ARG
15	M	86	GLU
15	M	91	ASP
15	M	126	ARG
16	N	6	ARG
16	N	7	THR
16	N	12	MET
16	N	25	ASP
16	N	54	THR
16	N	58	LYS
16	N	115	GLU
16	N	133	LYS
16	N	135	VAL
17	O	2	ARG
17	O	14	SER
17	O	36	THR
17	O	69	ARG
17	O	74	GLU
17	O	75	ILE
17	O	100	CYS
18	P	2	ASP
18	P	5	SER
18	P	19	GLN
18	P	20	GLU

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Mol	Chain	Res	Type
18	P	31	THR
18	P	36	TYR
18	P	43	ASN
18	P	55	GLU
18	P	61	GLN
18	P	69	ASP
18	P	78	VAL
18	P	98	GLN
19	Q	3	ASN
19	Q	7	GLN
19	Q	21	ARG
19	Q	26	VAL
19	Q	51	ARG
19	Q	65	SER
19	Q	68	GLU
19	Q	92	VAL
19	Q	115	ASN
20	R	6	ARG
20	R	13	ARG
20	R	17	ILE
20	R	24	TYR
20	R	51	ARG
20	R	52	GLN
20	R	109	LEU
21	S	20	VAL
21	S	25	LEU
21	S	38	VAL
21	S	45	GLU
21	S	71	LYS
21	S	72	VAL
21	S	83	TYR
21	S	101	ILE
22	T	12	SER
22	T	28	LYS
22	T	74	ILE
22	T	95	ARG
22	T	98	LYS
23	U	7	LEU
23	U	16	VAL
23	U	17	SER
23	U	48	GLN
23	U	72	GLN

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Mol	Chain	Res	Type
23	U	91	GLN
24	V	7	ARG
24	V	34	VAL
24	V	41	LEU
24	V	42	VAL
24	V	68	SER
24	V	83	VAL
24	V	102	THR
25	W	7	GLU
25	W	12	GLN
25	W	61	LEU
25	W	78	GLN
25	W	90	ASP
25	W	92	VAL
26	X	11	ARG
26	X	12	ASN
26	X	21	LEU
26	X	35	SER
26	X	41	ARG
26	X	56	ASP
27	Y	2	SER
27	Y	4	VAL
27	Y	42	SER
27	Y	74	ARG
28	Z	2	LYS
28	Z	16	THR
28	Z	44	LYS
28	Z	45	GLN
28	Z	48	ARG
28	Z	56	LEU
29	a	36	VAL
29	a	56	LYS
30	b	4	GLN
30	b	9	THR
30	b	15	MET
30	b	18	SER
30	b	25	VAL
30	b	26	THR
30	b	28	LEU
30	b	32	LYS
30	b	36	GLU
30	b	40	ARG

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Mol	Chain	Res	Type
30	b	46	ASP
30	b	52	ARG
31	c	5	ILE
31	c	6	ARG
31	c	10	LYS
31	c	22	THR
31	c	47	VAL
32	d	1	MET
32	d	12	ARG
32	d	24	THR
32	d	25	LYS
32	d	34	ARG
32	d	41	ARG
33	e	8	ARG
33	e	31	HIS
33	e	32	ILE
33	e	51	SER
34	f	2	LYS
34	f	12	ARG
34	f	36	ARG
35	i	5	LEU
35	i	16	ILE
35	i	19	ARG
35	i	21	ARG
35	i	30	THR
35	i	92	THR
35	i	141	ARG
35	i	185	ASP
35	i	242	LEU
35	i	261	SER
35	i	290	ILE
35	i	411	GLN
35	i	425	ARG
36	k	27	MET
36	k	44	VAL
37	l	295	VAL
37	l	325	MET
37	l	359	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
5	C	86	ASN
5	C	90	ASN
5	C	200	HIS
5	C	251	GLN
6	D	136	ASN
6	D	140	HIS
7	E	165	HIS
8	F	81	GLN
8	F	127	ASN
10	H	11	ASN
10	H	33	GLN
10	H	43	ASN
10	H	66	ASN
12	J	31	GLN
13	K	80	HIS
13	K	86	GLN
14	L	3	GLN
14	L	89	ASN
15	M	104	GLN
16	N	3	GLN
17	O	18	GLN
18	P	100	HIS
19	Q	52	ASN
19	Q	66	ASN
20	R	81	ASN
21	S	82	HIS
22	T	7	HIS
23	U	48	GLN
23	U	59	ASN
24	V	53	ASN
26	X	46	HIS
28	Z	31	GLN
28	Z	39	GLN
28	Z	58	ASN
32	d	26	ASN
32	d	29	GLN
35	i	62	HIS
35	i	72	GLN
35	i	196	HIS
35	i	209	HIS
35	i	337	GLN
35	i	411	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	42/113 (37%)	18 (42%)	1 (2%)
2	2	2/3 (66%)	1 (50%)	0
3	A	2878/2903 (99%)	521 (18%)	19 (0%)
4	B	119/120 (99%)	13 (10%)	0
All	All	3041/3139 (96%)	553 (18%)	20 (0%)

All (553) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	33	C
1	1	34	U
1	1	37	U
1	1	39	A
1	1	41	C
1	1	42	A
1	1	43	G
1	1	46	C
1	1	54	G
1	1	55	A
1	1	57	G
1	1	58	G
1	1	67	A
1	1	69	G
1	1	70	G
1	1	71	C
1	1	72	A
1	1	74	A
2	2	76	A
3	A	10	A
3	A	12	U
3	A	33	C
3	A	34	U
3	A	35	G
3	A	45	G
3	A	46	G
3	A	49	A
3	A	50	U
3	A	51	G
3	A	62	U
3	A	63	A
3	A	65	U

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Mol	Chain	Res	Type
3	A	71	A
3	A	72	U
3	A	74	A
3	A	75	G
3	A	84	A
3	A	93	G
3	A	96	C
3	A	101	A
3	A	102	U
3	A	103	A
3	A	110	G
3	A	118	A
3	A	119	A
3	A	120	U
3	A	136	G
3	A	137	U
3	A	138	U
3	A	139	U
3	A	142	A
3	A	156	A
3	A	162	U
3	A	181	A
3	A	188	G
3	A	196	A
3	A	199	A
3	A	215	G
3	A	216	A
3	A	220	G
3	A	221	A
3	A	222	A
3	A	226	A
3	A	248	G
3	A	266	G
3	A	272	A
3	A	275	C
3	A	276	U
3	A	285	G
3	A	291	G
3	A	302	C
3	A	311	A
3	A	329	G
3	A	330	A

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Mol	Chain	Res	Type
3	A	335	C
3	A	349	U
3	A	353	C
3	A	356	G
3	A	361	G
3	A	362	A
3	A	372	G
3	A	386	G
3	A	396	G
3	A	399	U
3	A	411	G
3	A	419	U
3	A	424	G
3	A	454	A
3	A	455	C
3	A	473	G
3	A	475	C
3	A	477	A
3	A	479	A
3	A	480	A
3	A	481	G
3	A	491	G
3	A	504	A
3	A	505	A
3	A	509	C
3	A	510	C
3	A	513	A
3	A	518	G
3	A	529	A
3	A	531	C
3	A	532	A
3	A	533	G
3	A	543	G
3	A	544	C
3	A	550	C
3	A	552	U
3	A	558	U
3	A	563	A
3	A	567	U
3	A	568	U
3	A	573	U
3	A	575	A

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Mol	Chain	Res	Type
3	A	586	A
3	A	603	A
3	A	613	A
3	A	614	A
3	A	615	U
3	A	627	A
3	A	632	A
3	A	634	C
3	A	637	A
3	A	645	C
3	A	646	U
3	A	647	G
3	A	653	U
3	A	654	A
3	A	655	A
3	A	668	A
3	A	669	G
3	A	685	A
3	A	686	U
3	A	711	G
3	A	712	G
3	A	713	G
3	A	718	A
3	A	730	A
3	A	747	U
3	A	753	A
3	A	757	G
3	A	763	G
3	A	764	A
3	A	765	C
3	A	775	G
3	A	777	G
3	A	782	A
3	A	784	G
3	A	785	G
3	A	788	A
3	A	789	A
3	A	790	U
3	A	791	C
3	A	793	A
3	A	794	A
3	A	801	G

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Mol	Chain	Res	Type
3	A	805	G
3	A	812	C
3	A	827	U
3	A	828	U
3	A	831	G
3	A	846	U
3	A	859	G
3	A	865	C
3	A	869	G
3	A	878	A
3	A	896	A
3	A	897	C
3	A	899	A
3	A	907	G
3	A	910	A
3	A	914	G
3	A	915	C
3	A	932	U
3	A	933	A
3	A	946	C
3	A	953	G
3	A	957	C
3	A	961	C
3	A	974	G
3	A	983	A
3	A	990	A
3	A	996	A
3	A	999	U
3	A	1005	C
3	A	1009	A
3	A	1012	U
3	A	1013	C
3	A	1022	G
3	A	1023	U
3	A	1027	A
3	A	1033	U
3	A	1040	A
3	A	1046	A
3	A	1056	G
3	A	1057	A
3	A	1070	A
3	A	1071	G

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Mol	Chain	Res	Type
3	A	1073	A
3	A	1083	U
3	A	1087	G
3	A	1088	A
3	A	1090	A
3	A	1101	U
3	A	1111	A
3	A	1112	G
3	A	1116	G
3	A	1129	A
3	A	1130	U
3	A	1132	U
3	A	1133	A
3	A	1135	C
3	A	1136	G
3	A	1139	G
3	A	1142	A
3	A	1143	A
3	A	1155	A
3	A	1173	U
3	A	1179	G
3	A	1182	G
3	A	1206	G
3	A	1212	G
3	A	1218	G
3	A	1236	G
3	A	1238	G
3	A	1247	A
3	A	1249	U
3	A	1252	G
3	A	1253	A
3	A	1256	G
3	A	1262	A
3	A	1271	G
3	A	1272	A
3	A	1294	U
3	A	1300	G
3	A	1301	A
3	A	1302	A
3	A	1308	A
3	A	1329	U
3	A	1332	G

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Mol	Chain	Res	Type
3	A	1337	G
3	A	1338	G
3	A	1345	C
3	A	1346	G
3	A	1365	A
3	A	1379	U
3	A	1383	A
3	A	1395	A
3	A	1403	A
3	A	1416	G
3	A	1417	C
3	A	1424	G
3	A	1428	C
3	A	1434	A
3	A	1437	C
3	A	1449	G
3	A	1451	C
3	A	1452	G
3	A	1453	A
3	A	1482	G
3	A	1489	C
3	A	1491	G
3	A	1493	C
3	A	1494	A
3	A	1495	A
3	A	1497	U
3	A	1498	C
3	A	1509	A
3	A	1510	G
3	A	1515	A
3	A	1524	G
3	A	1529	G
3	A	1533	C
3	A	1535	A
3	A	1536	C
3	A	1537	G
3	A	1554	U
3	A	1560	G
3	A	1566	A
3	A	1569	A
3	A	1576	U
3	A	1578	U

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Mol	Chain	Res	Type
3	A	1581	G
3	A	1583	A
3	A	1585	C
3	A	1606	C
3	A	1607	C
3	A	1608	A
3	A	1616	A
3	A	1634	A
3	A	1639	C
3	A	1647	U
3	A	1648	U
3	A	1649	G
3	A	1660	G
3	A	1674	G
3	A	1677	A
3	A	1715	G
3	A	1722	A
3	A	1725	U
3	A	1729	U
3	A	1730	C
3	A	1738	G
3	A	1744	A
3	A	1757	A
3	A	1764	C
3	A	1773	A
3	A	1782	U
3	A	1786	A
3	A	1791	A
3	A	1800	C
3	A	1801	A
3	A	1802	A
3	A	1808	A
3	A	1809	A
3	A	1811	G
3	A	1816	C
3	A	1829	A
3	A	1847	A
3	A	1849	G
3	A	1850	G
3	A	1870	C
3	A	1871	A
3	A	1872	A

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Mol	Chain	Res	Type
3	A	1876	A
3	A	1896	G
3	A	1906	G
3	A	1920	C
3	A	1927	A
3	A	1929	G
3	A	1930	G
3	A	1931	U
3	A	1934	C
3	A	1936	A
3	A	1937	A
3	A	1939	U
3	A	1955	U
3	A	1956	U
3	A	1960	A
3	A	1962	C
3	A	1966	A
3	A	1967	C
3	A	1970	A
3	A	1971	U
3	A	1972	G
3	A	1974	C
3	A	1982	U
3	A	1991	U
3	A	1992	G
3	A	1993	U
3	A	1997	C
3	A	2021	C
3	A	2023	C
3	A	2030	A
3	A	2031	A
3	A	2033	A
3	A	2043	C
3	A	2050	C
3	A	2054	A
3	A	2055	C
3	A	2056	G
3	A	2060	A
3	A	2061	G
3	A	2062	A
3	A	2069	G
3	A	2072	C

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Mol	Chain	Res	Type
3	A	2093	G
3	A	2097	A
3	A	2101	A
3	A	2103	C
3	A	2104	C
3	A	2105	U
3	A	2106	U
3	A	2111	U
3	A	2112	G
3	A	2113	U
3	A	2116	G
3	A	2117	A
3	A	2118	U
3	A	2119	A
3	A	2120	G
3	A	2123	G
3	A	2126	A
3	A	2128	G
3	A	2131	U
3	A	2132	U
3	A	2133	G
3	A	2134	A
3	A	2145	C
3	A	2146	C
3	A	2147	A
3	A	2148	G
3	A	2159	G
3	A	2160	C
3	A	2161	C
3	A	2163	A
3	A	2164	C
3	A	2165	C
3	A	2167	U
3	A	2168	G
3	A	2169	A
3	A	2170	A
3	A	2171	A
3	A	2172	U
3	A	2173	A
3	A	2174	C
3	A	2177	C
3	A	2178	C

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Mol	Chain	Res	Type
3	A	2185	U
3	A	2187	U
3	A	2190	G
3	A	2198	A
3	A	2203	U
3	A	2204	G
3	A	2211	A
3	A	2212	A
3	A	2225	A
3	A	2238	G
3	A	2239	G
3	A	2250	G
3	A	2268	A
3	A	2278	A
3	A	2280	G
3	A	2283	C
3	A	2287	A
3	A	2288	A
3	A	2297	A
3	A	2305	U
3	A	2308	G
3	A	2322	A
3	A	2325	G
3	A	2331	G
3	A	2336	A
3	A	2345	G
3	A	2347	C
3	A	2350	C
3	A	2354	C
3	A	2357	G
3	A	2366	A
3	A	2383	G
3	A	2385	C
3	A	2402	U
3	A	2403	C
3	A	2406	A
3	A	2420	C
3	A	2421	G
3	A	2422	C
3	A	2423	U
3	A	2424	C
3	A	2425	A

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Mol	Chain	Res	Type
3	A	2427	C
3	A	2429	G
3	A	2430	A
3	A	2431	U
3	A	2432	A
3	A	2434	A
3	A	2435	A
3	A	2440	C
3	A	2441	U
3	A	2445	G
3	A	2448	A
3	A	2464	G
3	A	2475	C
3	A	2476	A
3	A	2478	A
3	A	2491	U
3	A	2492	U
3	A	2497	A
3	A	2502	G
3	A	2504	U
3	A	2505	G
3	A	2506	U
3	A	2507	C
3	A	2513	A
3	A	2514	U
3	A	2518	A
3	A	2520	C
3	A	2529	G
3	A	2566	A
3	A	2567	G
3	A	2578	G
3	A	2582	G
3	A	2585	U
3	A	2586	U
3	A	2602	A
3	A	2603	G
3	A	2609	U
3	A	2613	U
3	A	2615	U
3	A	2621	G
3	A	2623	G
3	A	2624	G

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Mol	Chain	Res	Type
3	A	2629	U
3	A	2630	G
3	A	2636	C
3	A	2638	G
3	A	2669	G
3	A	2682	A
3	A	2689	U
3	A	2690	U
3	A	2714	G
3	A	2716	C
3	A	2726	A
3	A	2733	A
3	A	2739	U
3	A	2744	G
3	A	2748	A
3	A	2757	A
3	A	2765	A
3	A	2778	A
3	A	2779	U
3	A	2780	G
3	A	2787	C
3	A	2791	G
3	A	2792	A
3	A	2798	U
3	A	2799	A
3	A	2801	G
3	A	2820	A
3	A	2821	A
3	A	2825	G
3	A	2833	U
3	A	2835	A
3	A	2836	U
3	A	2849	U
3	A	2860	A
3	A	2861	U
3	A	2867	G
3	A	2870	C
3	A	2873	A
3	A	2879	A
3	A	2880	C
3	A	2883	A
3	A	2884	U

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Mol	Chain	Res	Type
3	A	2885	G
3	A	2886	A
3	A	2888	C
3	A	2891	U
4	B	24	G
4	B	25	U
4	B	35	C
4	B	41	G
4	B	45	A
4	B	56	G
4	B	66	A
4	B	67	G
4	B	71	C
4	B	88	C
4	B	89	U
4	B	90	C
4	B	109	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	68	A
3	A	100	U
3	A	613	A
3	A	645	C
3	A	653	U
3	A	784	G
3	A	827	U
3	A	830	G
3	A	1110	G
3	A	1344	U
3	A	1494	A
3	A	1721	G
3	A	1939	U
3	A	2127	G
3	A	2158	A
3	A	2422	C
3	A	2424	C
3	A	2430	A
3	A	2602	A
3	A	2756	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 436 ligands modelled in this entry, 434 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
40	GNP	i	1400	38	29,34,34	2.18	8 (27%)	29,54,54	2.66	12 (41%)
40	GNP	l	1400	38	29,34,34	1.98	8 (27%)	29,54,54	2.54	11 (37%)

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
40	GNP	i	1400	38	-	0/13/38/38	0/3/3/3
40	GNP	l	1400	38	-	0/13/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	i	1400	GNP	PG-O3G	-3.01	1.48	1.56
40	i	1400	GNP	PB-O2B	-3.00	1.48	1.56
40	l	1400	GNP	PG-O3G	-2.58	1.49	1.56
40	i	1400	GNP	PG-O2G	-2.54	1.49	1.56
40	l	1400	GNP	PG-O2G	-2.45	1.50	1.56
40	l	1400	GNP	PB-O2B	-2.28	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	l	1400	GNP	PG-N3B	2.29	1.69	1.63
40	i	1400	GNP	C6-C5	2.72	1.46	1.41
40	l	1400	GNP	C6-C5	2.88	1.47	1.41
40	l	1400	GNP	PG-O1G	3.29	1.49	1.46
40	i	1400	GNP	O4'-C1'	3.40	1.46	1.41
40	i	1400	GNP	PG-O1G	4.18	1.50	1.46
40	i	1400	GNP	PB-O1B	4.44	1.50	1.46
40	l	1400	GNP	PB-O1B	4.76	1.51	1.46
40	l	1400	GNP	C4-N3	5.21	1.44	1.35
40	i	1400	GNP	C4-N3	5.89	1.45	1.35

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	i	1400	GNP	C6-C5-C4	-5.55	114.51	120.86
40	l	1400	GNP	C6-C5-C4	-5.21	114.91	120.86
40	i	1400	GNP	N3-C2-N1	-4.57	121.34	127.56
40	i	1400	GNP	O3'-C3'-C4'	-4.18	98.54	111.01
40	l	1400	GNP	N3-C2-N1	-3.80	122.39	127.56
40	l	1400	GNP	O3'-C3'-C2'	-3.61	100.19	111.86
40	l	1400	GNP	C5-C6-N1	-3.11	119.45	123.52
40	i	1400	GNP	C5-C6-N1	-2.91	119.72	123.52
40	i	1400	GNP	O3'-C3'-C2'	-2.85	102.65	111.86
40	l	1400	GNP	C1'-N9-C4	-2.76	123.72	126.81
40	i	1400	GNP	C1'-N9-C4	-2.10	124.46	126.81
40	l	1400	GNP	O2'-C2'-C1'	2.02	117.95	111.61
40	l	1400	GNP	C2'-C1'-N9	2.14	119.19	113.47
40	i	1400	GNP	O2'-C2'-C1'	2.51	119.45	111.61
40	i	1400	GNP	O2'-C2'-C3'	2.52	119.99	111.86
40	l	1400	GNP	C2'-C3'-C4'	2.56	107.87	102.64
40	i	1400	GNP	C2'-C1'-N9	3.03	121.56	113.47
40	i	1400	GNP	C2'-C3'-C4'	3.50	109.80	102.64
40	l	1400	GNP	O4'-C1'-N9	3.74	115.17	108.11
40	i	1400	GNP	O2B-PB-O1B	3.83	117.56	110.02
40	l	1400	GNP	O2B-PB-O1B	4.53	118.94	110.02
40	l	1400	GNP	C6-N1-C2	6.66	123.69	115.88
40	i	1400	GNP	C6-N1-C2	6.98	124.06	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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
28	Z	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	15:ASN	C	16:THR	N	3.07
1	Z	40:SER	C	41:HIS	N	2.90