wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:27 PM BST

PDB ID	:	3J80
EMDB ID:	:	EMD-2764
Title	:	CryoEM structure of 40S-eIF1-eIF1A preinitiation complex
Authors	:	Hussain, T.; Llacer, J.L.; Fernandez, I.S.; Savva, C.G.; Ramakrishnan, V.
Deposited on	:	2014-08-28
Resolution	:	3.75 Å(reported)
Based on PDB ID	:	3U5C, 3U5B

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

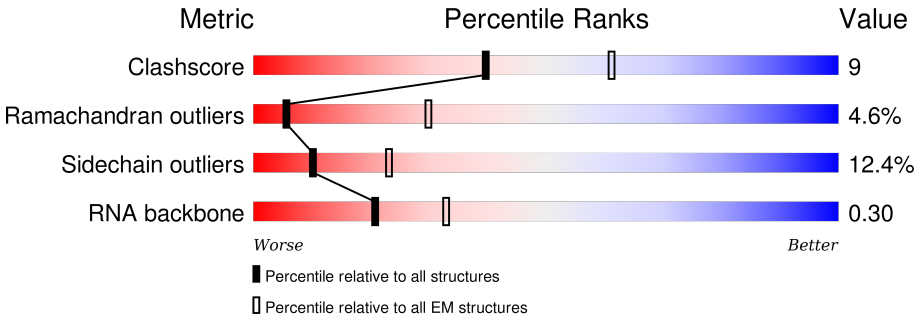
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 3.75 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	2	1799	29% 52% 17% •
2	A	254	52% 25% 5% 19%
3	B	255	59% 21% • • 16%
4	C	259	51% 27% 5% 16%
5	E	261	69% 25% 6%
6	G	236	69% 25% • •
7	H	190	63% 26% 7% •
8	I	201	59% 30% • • 6%

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Mol	Chain	Length	Quality of chain
9	J	188	56% 33% 8%
10	L	156	69% 25%
11	N	151	75% 21%
12	O	137	68% 22% 7%
13	V	87	63% 32% 5%
14	W	130	61% 31% 8%
15	X	145	67% 26% 6%
16	Y	135	67% 27%
17	a	119	58% 23% 18%
18	b	82	80% 17%
19	e	63	75% 10% 16%
20	D	237	67% 24% 6%
21	F	227	70% 19% 9%
22	K	106	68% 23% 9%
23	M	134	72% 18% 9%
24	P	140	69% 14% 12%
25	Q	143	69% 27%
26	R	136	65% 20% 12%
27	S	146	74% 23%
28	T	144	78% 19%
29	U	117	55% 32% 9%
30	Z	108	57% 5% 35%
31	c	67	85% 9% 6%
32	d	56	80% 14% 5%
33	f	150	37% 9% 54%

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Mol	Chain	Length	Quality of chain
34	g	326	91% 6%
35	h	25	88% 12%
36	i	153	58% 5% 37%
37	j	108	74% 6% 20%

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 77716 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1779	37775	16882	6653	12461	1779	0	0

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	206	1616	1035	285	294	2	0	0

- Molecule 3 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	214	1722	1089	313	317	3	0	0

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	217	1629	1041	287	297	4	0	0

- Molecule 5 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	260	2078	1322	393	359	4	0	0

- Molecule 6 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	226	1812	1134	348	326	4	0	0

- Molecule 7 is a protein called eS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	184	Total	C	N	O	0	0
			1483	950	270	263		

- Molecule 8 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	188	Total	C	N	O	S	0	0
			1493	926	301	265	1		

- Molecule 9 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 10 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 11 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	150	Total	C	N	O	S	0	0
			1187	756	223	206	2		

- Molecule 12 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	127	Total	C	N	O	S	0	0
			942	578	188	173	3		

- Molecule 13 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 14 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 15 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 16 is a protein called eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Y	134	Total	C	N	O	0	0
			1061	665	207	189		

- Molecule 17 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	97	Total	C	N	O	S	0	0
			770	475	163	127	5		

- Molecule 18 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	81	Total	C	N	O	S	0	0
			609	379	112	113	5		

- Molecule 19 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	53	Total	C	N	O	S	0	0
			428	268	87	72	1		

- Molecule 20 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 21 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 22 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 23 is a protein called eS12.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	M	122	Total	C	N	O	0	0
			922	575	167	180		

- Molecule 24 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	123	Total	C	N	O	S	0	0
			980	628	179	168	5		

- Molecule 25 is a protein called uS9.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Q	141	Total	C	N	O	0	0
			1105	709	204	192		

- Molecule 26 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	120	Total	C	N	O	S	0	0
			959	598	178	180	3		

- Molecule 27 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 28 is a protein called eS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 29 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 30 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	70	Total	C	N	O	S	0	0
			558	355	104	98	1		

- Molecule 31 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	63	Total	C	N	O	S	0	0
			494	305	98	90	1		

- Molecule 32 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	53	Total	C	N	O	S	0	0
			446	280	89	76	1		

- Molecule 33 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	69	Total	C	N	O	S	0	0
			549	352	102	91	4		

- Molecule 34 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 35 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 36 is a protein called eIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	96	Total	C	N	O	S	0	0
			778	482	144	147	5		

- Molecule 37 is a protein called eIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	86	Total	C	N	O	S	0	0
			695	439	128	124	4		

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

Mol	Chain	Residues	Atoms		AltConf
38	2	67	Total	Mg	0
			67	67	

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

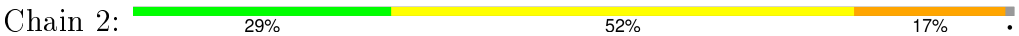
Mol	Chain	Residues	Atoms		AltConf
39	b	1	Total	Zn	0
			1	1	
39	a	1	Total	Zn	0
			1	1	
39	f	1	Total	Zn	0
			1	1	

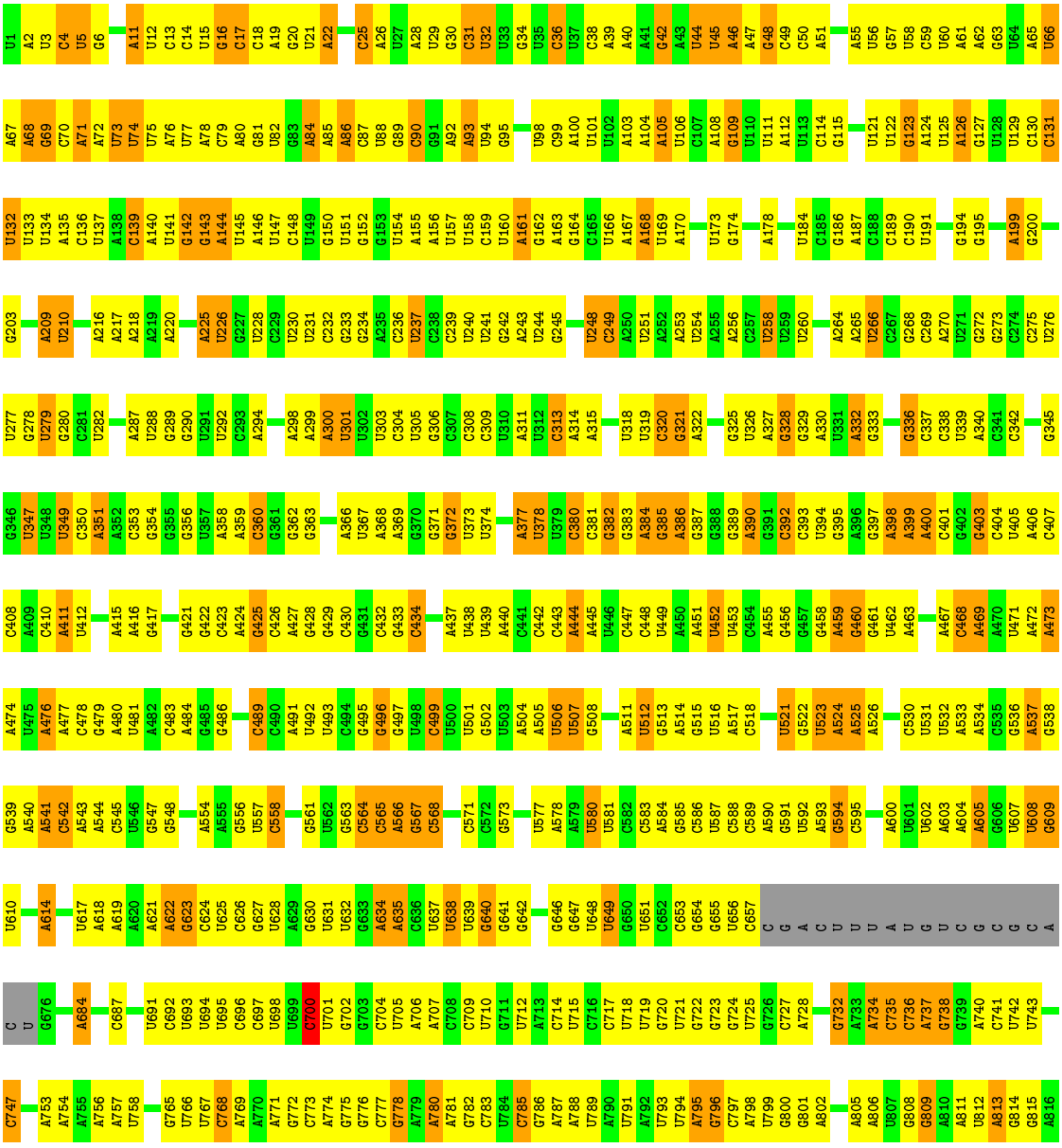
3 Residue-property plots (i)

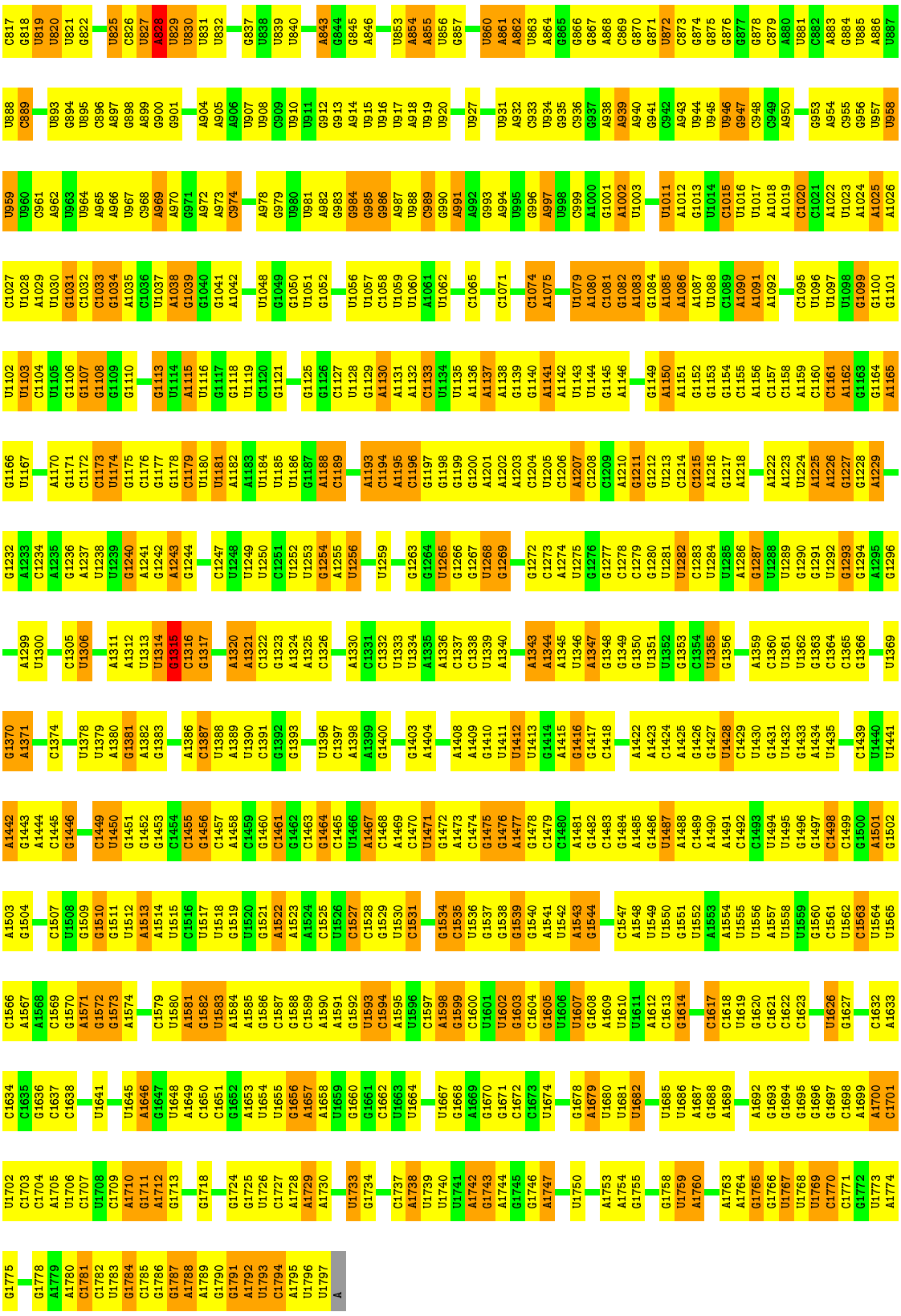
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: 18S rRNA

Chain 2:

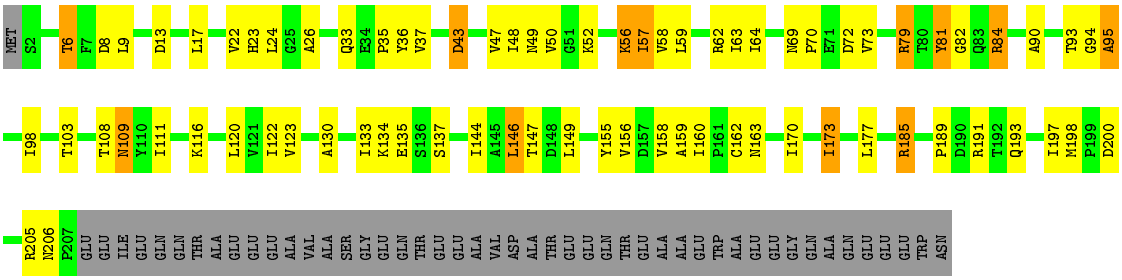






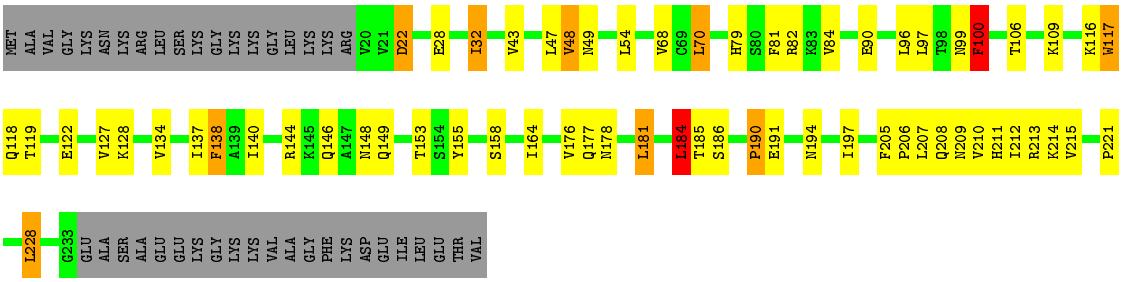
- Molecule 2: uS2

Chain A:



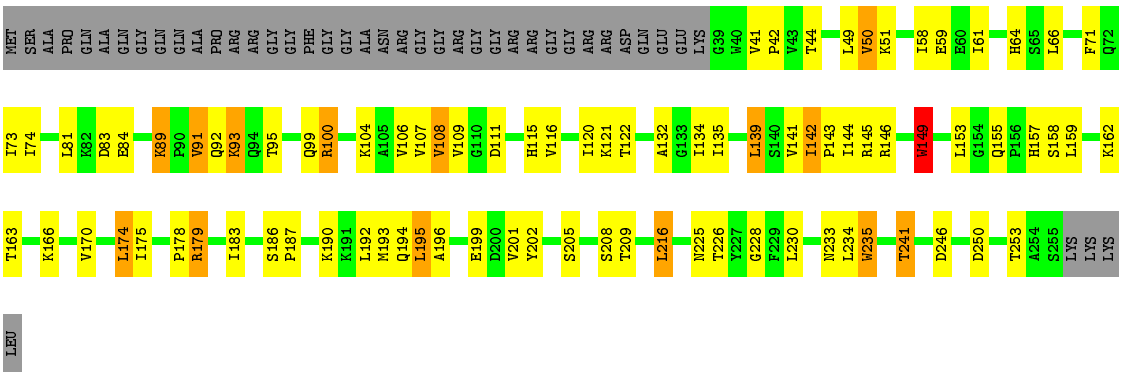
• Molecule 3: eS1

Chain B:



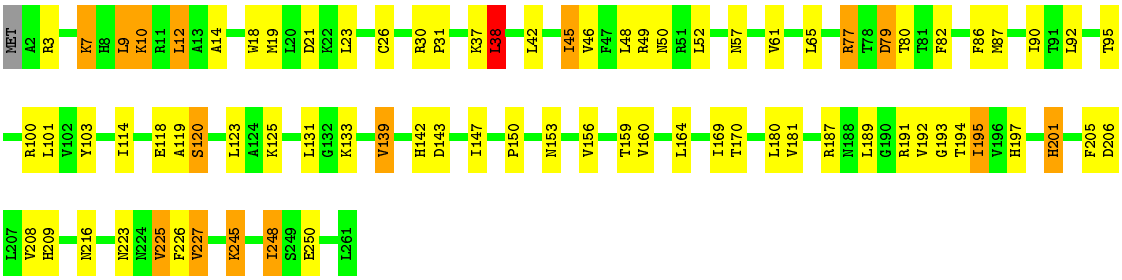
• Molecule 4: uS5

Chain C:



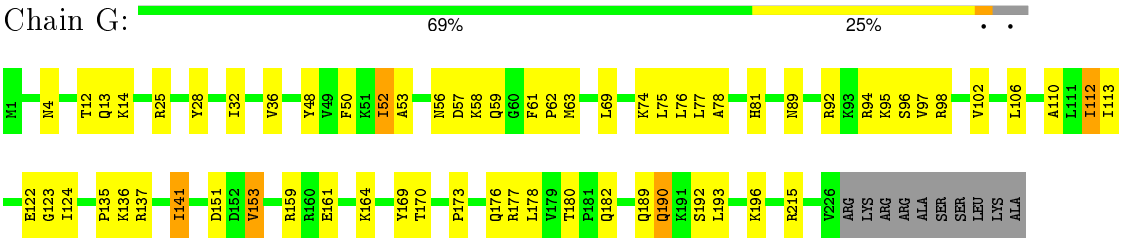
• Molecule 5: eS4

Chain E:



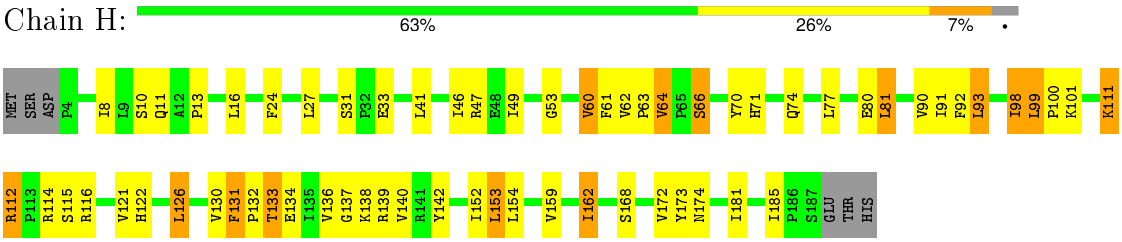
• Molecule 6: eS6

Chain G:



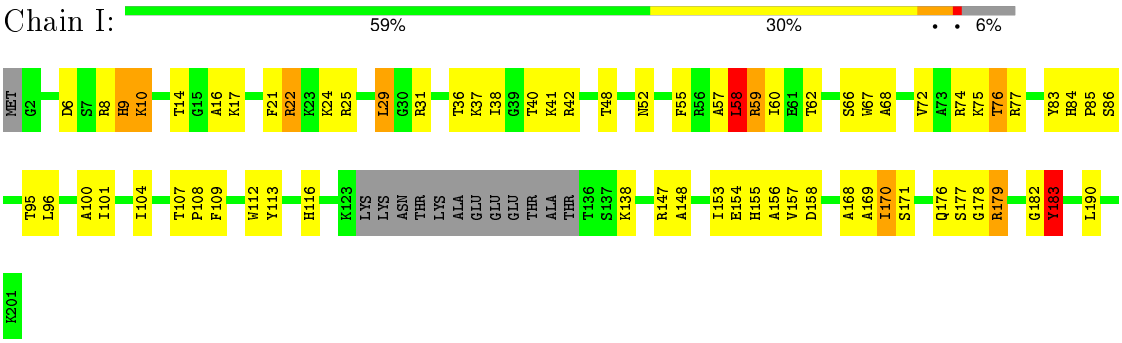
- Molecule 7: eS7

Chain H:



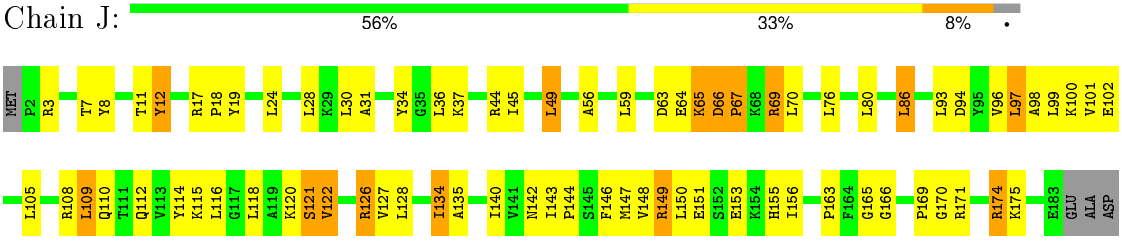
- Molecule 8: eS8

Chain I:



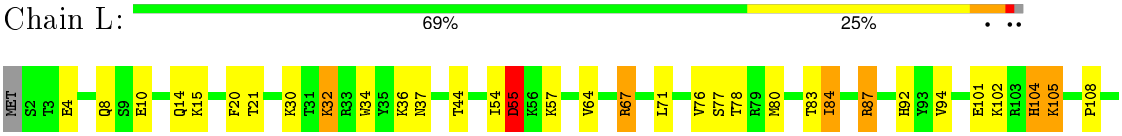
- Molecule 9: uS4

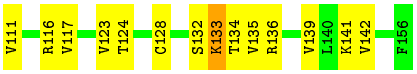
Chain J:



- Molecule 10: uS17

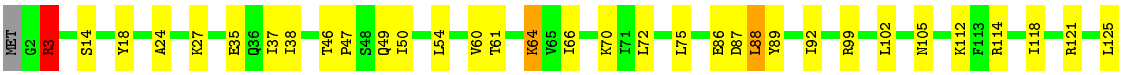
Chain L:





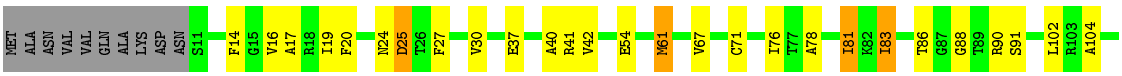
- Molecule 11: uS15

Chain N:



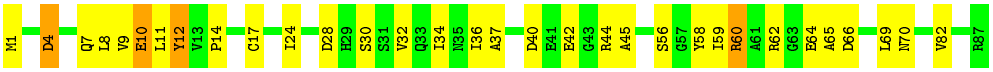
- Molecule 12: uS11

Chain O:



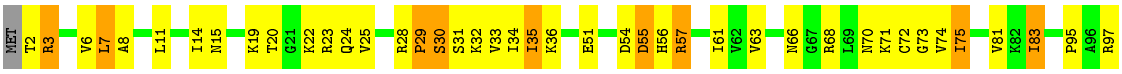
- Molecule 13: eS21

Chain V:



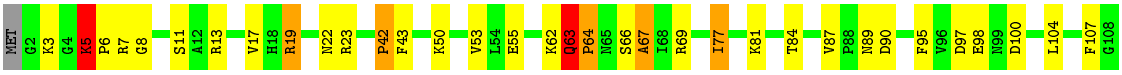
- Molecule 14: uS8

Chain W:



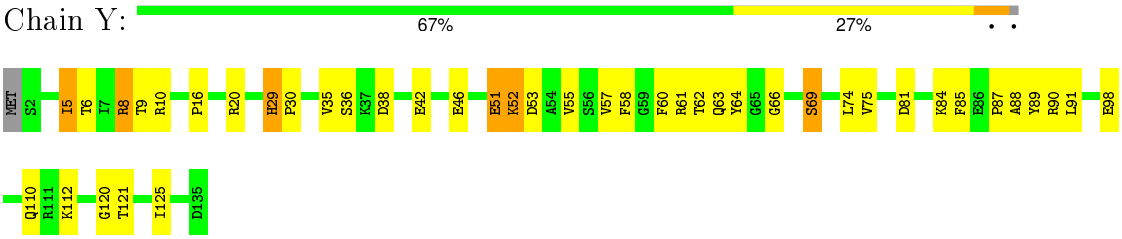
- Molecule 15: uS12

Chain X:



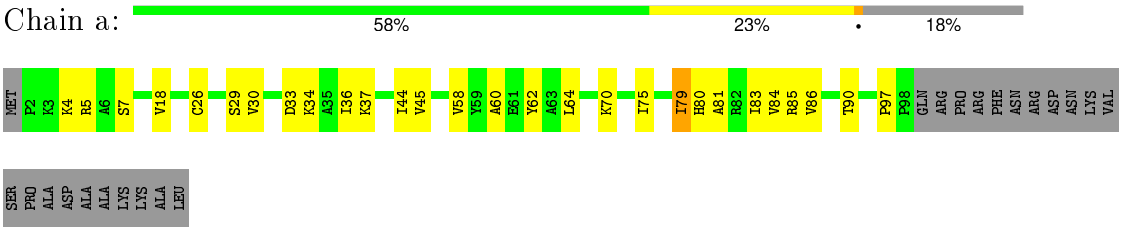
- Molecule 16: eS24

Chain Y:



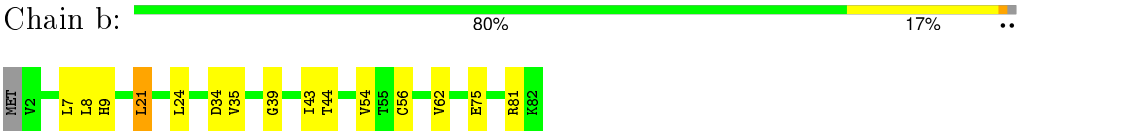
- Molecule 17: eS26

Chain a:



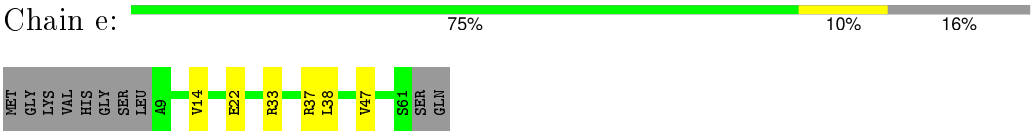
- Molecule 18: eS27

Chain b:



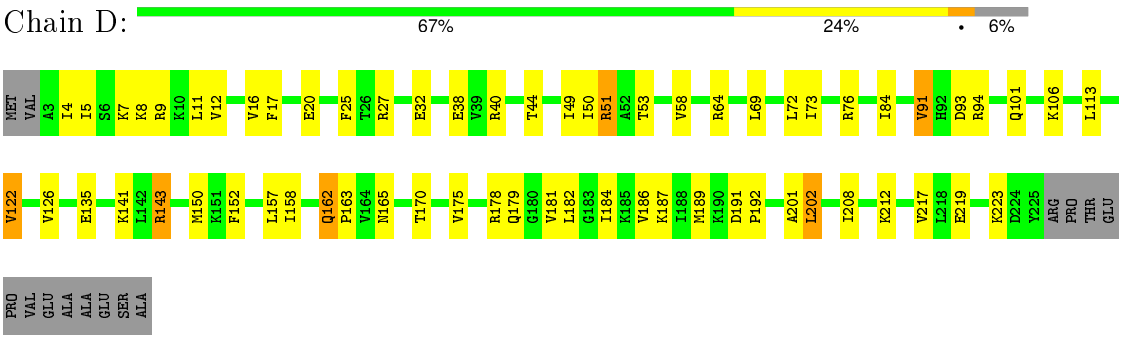
- Molecule 19: eS30

Chain e:



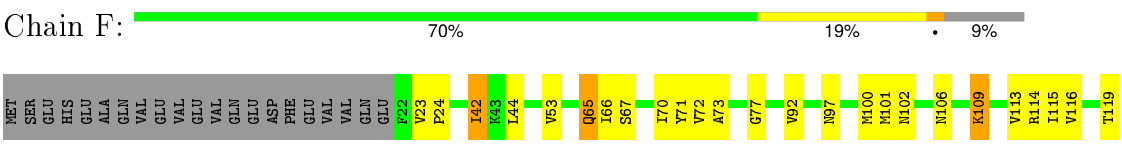
- Molecule 20: uS3

Chain D:



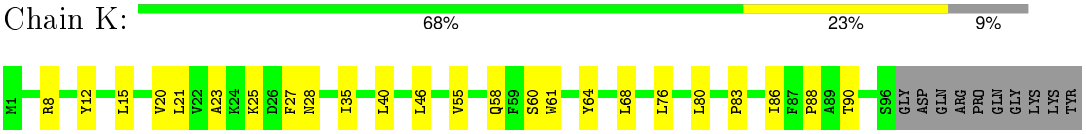
- Molecule 21: uS7

Chain F:



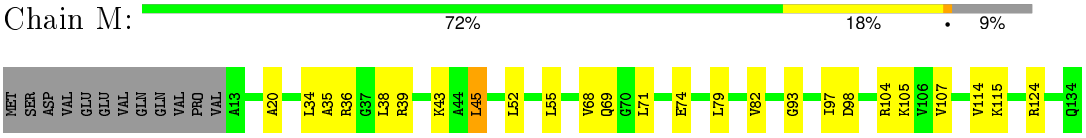
- Molecule 22: eS10

Chain K:



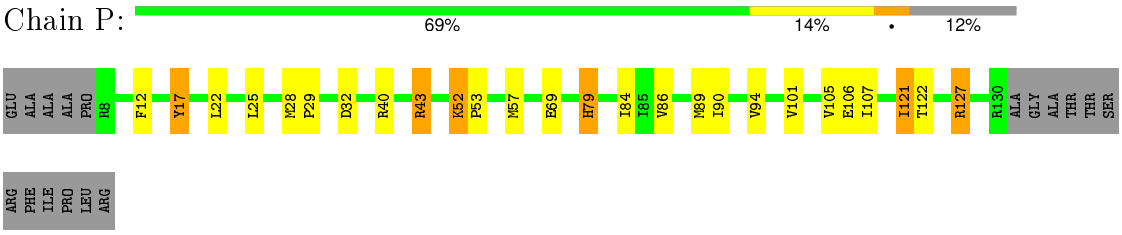
- Molecule 23: eS12

Chain M:



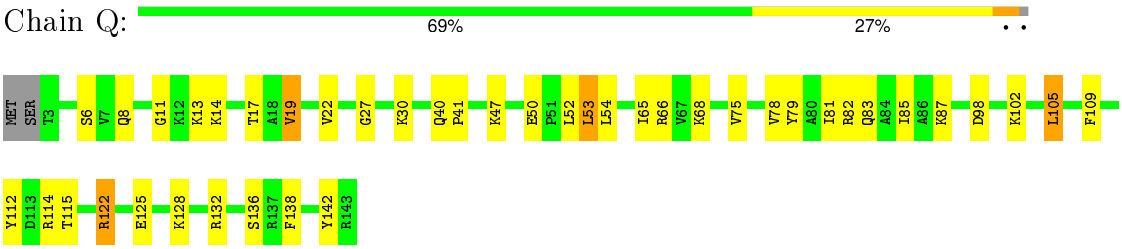
- Molecule 24: uS19

Chain P:



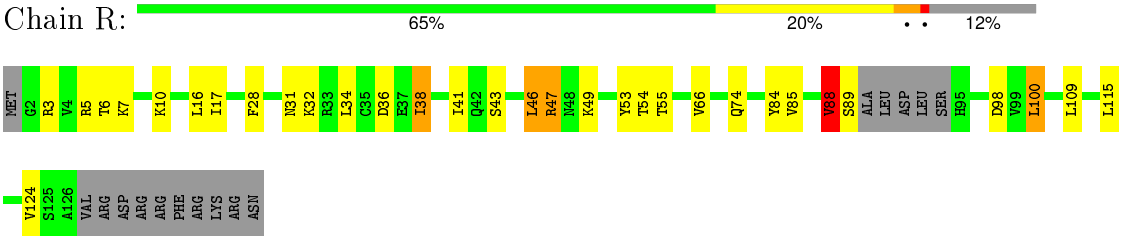
- Molecule 25: uS9

Chain Q:



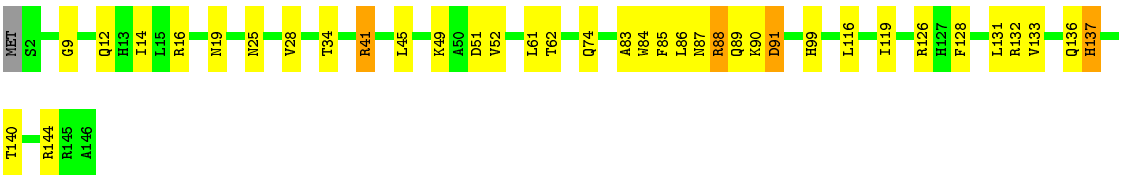
- Molecule 26: eS17

Chain R:



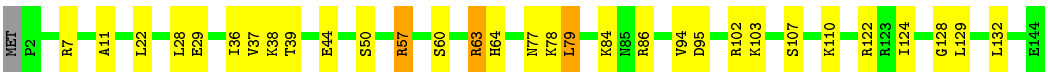
- Molecule 27: uS13

Chain S:



- Molecule 28: eS19

Chain T:



- Molecule 29: uS10

Chain U:

- Molecule 30: eS25

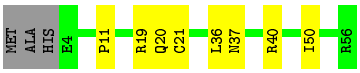
Chain Z:

- Molecule 31: eS28

Chain c:

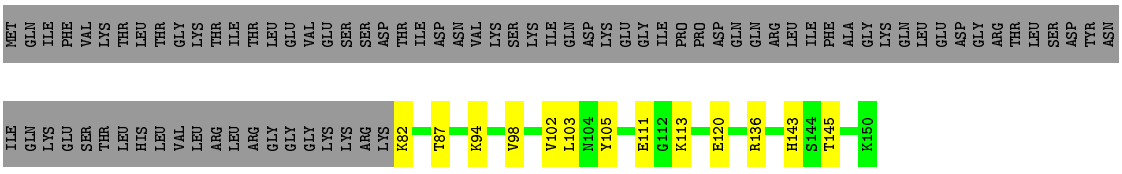
- Molecule 32: uS14

Chain d:



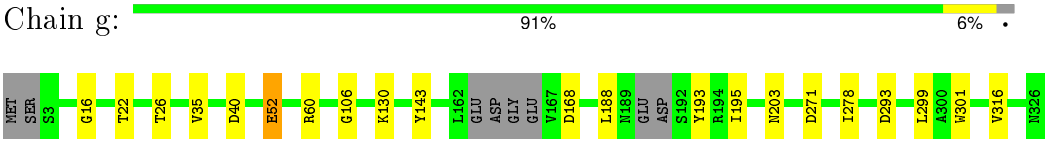
- Molecule 33: eS31

Chain f:



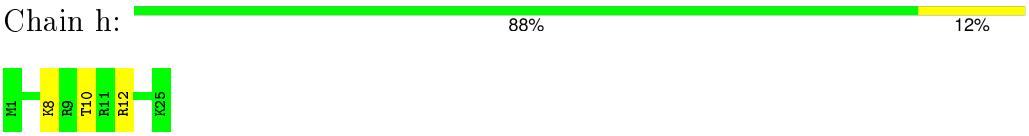
- Molecule 34: RACK1

Chain g:



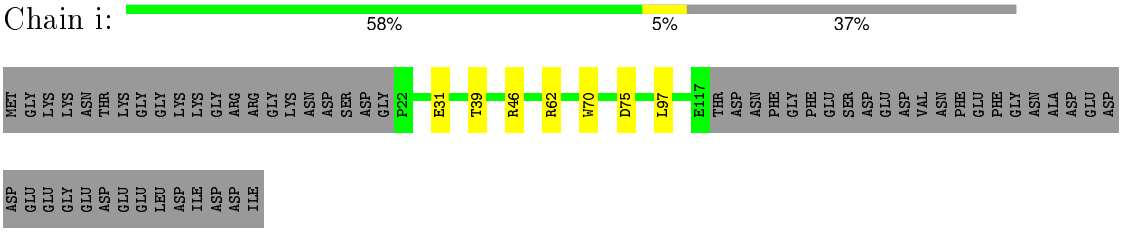
- Molecule 35: eL41

Chain h:



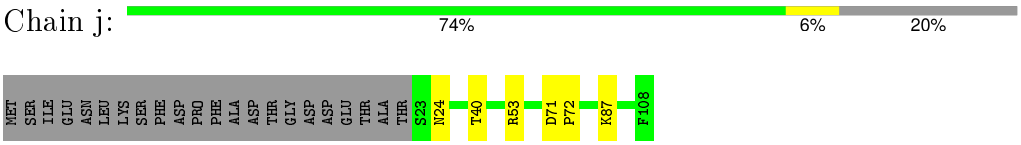
- Molecule 36: eIF1A

Chain i:



- Molecule 37: eIF1

Chain j:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	100709	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	2	0.30	0/42244	0.70	5/65823 (0.0%)
10	L	0.45	0/1276	0.70	0/1718
11	N	0.45	0/1210	0.78	1/1628 (0.1%)
12	O	0.40	0/953	0.72	0/1279
13	V	0.43	0/696	0.73	0/938
14	W	0.50	0/1039	0.82	0/1399
15	X	0.48	0/1137	0.80	0/1516
16	Y	0.42	0/1075	0.72	0/1433
17	a	0.44	0/782	0.82	0/1047
18	b	0.40	0/619	0.70	0/837
19	e	0.39	0/435	0.70	0/579
2	A	0.43	0/1656	0.78	0/2264
20	D	0.43	0/1769	0.70	0/2378
21	F	0.40	0/1628	0.71	0/2198
22	K	0.46	0/831	0.67	0/1123
23	M	0.40	0/929	0.69	0/1255
24	P	0.43	0/1000	0.65	0/1343
25	Q	0.41	0/1125	0.69	0/1510
26	R	0.44	0/969	0.73	0/1299
27	S	0.39	0/1212	0.68	0/1629
28	T	0.39	0/1129	0.68	0/1520
29	U	0.43	0/857	0.73	0/1158
3	B	0.40	0/1747	0.72	1/2353 (0.0%)
30	Z	0.43	0/567	0.64	0/762
31	c	0.39	0/496	0.72	0/666
32	d	0.47	0/457	0.66	0/607
33	f	0.47	0/562	0.65	0/751
34	g	0.41	0/2521	0.61	0/3431
35	h	0.39	0/234	0.81	0/300
36	i	0.38	0/788	0.62	0/1051
37	j	0.41	0/703	0.66	0/938
4	C	0.45	0/1659	0.79	3/2252 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
5	E	0.41	0/2122	0.71	1/2861 (0.0%)
6	G	0.39	0/1835	0.68	0/2451
7	H	0.43	0/1507	0.74	0/2028
8	I	0.44	0/1519	0.74	2/2033 (0.1%)
9	J	0.45	0/1495	0.82	2/2001 (0.1%)
All	All	0.37	0/82783	0.71	15/120359 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	W	0	1
15	X	0	2
16	Y	0	1
17	a	0	1
25	Q	0	1
7	H	0	1
9	J	0	1
All	All	0	8

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1315	G	C2'-C3'-O3'	7.15	125.23	109.50
9	J	49	LEU	CA-CB-CG	7.12	131.67	115.30
4	C	139	LEU	CA-CB-CG	6.41	130.05	115.30
3	B	184	LEU	CA-CB-CG	6.33	129.86	115.30
8	I	29	LEU	CA-CB-CG	6.22	129.61	115.30
1	2	1243	A	C2'-C3'-O3'	5.86	123.07	113.70
4	C	192	LEU	CA-CB-CG	5.75	128.51	115.30
1	2	279	U	C2'-C3'-O3'	5.60	122.66	113.70
1	2	828	A	C2'-C3'-O3'	5.43	122.39	113.70
5	E	38	LEU	CA-CB-CG	5.26	127.41	115.30
1	2	700	C	C2'-C3'-O3'	5.24	122.09	113.70
11	N	128	TYR	CB-CA-C	5.21	120.83	110.40
4	C	216	LEU	CA-CB-CG	-5.13	103.49	115.30
8	I	183	TYR	CA-CB-CG	-5.13	103.65	113.40
9	J	24	LEU	CA-CB-CG	5.12	127.09	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	H	131	PHE	Peptide
9	J	12	TYR	Peptide
25	Q	40	GLN	Peptide
14	W	75	ILE	Peptide
15	X	11	SER	Peptide
15	X	63	GLN	Peptide
16	Y	29	HIS	Peptide
17	a	79	ILE	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	2	37775	0	19004	704	0
2	A	1616	0	1636	35	0
3	B	1722	0	1795	27	0
4	C	1629	0	1710	41	0
5	E	2078	0	2157	37	0
6	G	1812	0	1911	32	0
7	H	1483	0	1579	29	0
8	I	1493	0	1515	29	0
9	J	1471	0	1554	43	0
10	L	1248	0	1311	25	0
11	N	1187	0	1251	17	0
12	O	942	0	979	16	0
13	V	687	0	682	14	0
14	W	1021	0	1056	34	0
15	X	1119	0	1198	21	0
16	Y	1061	0	1111	17	0
17	a	770	0	822	0	0
18	b	609	0	631	0	0
19	e	428	0	468	0	0
20	D	1744	0	1826	27	0
21	F	1609	0	1679	18	0
22	K	809	0	810	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	M	922	0	953	9	0
24	P	980	0	1026	10	0
25	Q	1105	0	1170	20	0
26	R	959	0	1006	12	0
27	S	1193	0	1217	19	0
28	T	1110	0	1124	16	0
29	U	845	0	913	14	0
30	Z	558	0	585	2	0
31	c	494	0	534	0	0
32	d	446	0	436	0	0
33	f	549	0	564	0	0
34	g	2466	0	2406	0	0
35	h	233	0	284	0	0
36	i	778	0	779	0	0
37	j	695	0	729	0	0
38	2	67	0	0	0	0
39	a	1	0	0	0	0
39	b	1	0	0	0	0
39	f	1	0	0	0	0
All	All	77716	0	60411	1161	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 (1161) 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)
1:2:1037:U:H3	1:2:1091:A:N6	1.23	1.32
1:2:1290:G:N2	1:2:1323:G:H22	1.28	1.28
1:2:991:A:N1	1:2:1011:U:O4	1.78	1.15
1:2:991:A:N1	1:2:1011:U:C4	2.17	1.12
1:2:1290:G:H22	1:2:1323:G:N2	1.56	1.03
1:2:813:A:N6	1:2:856:U:N3	2.09	0.99
1:2:1079:U:O4	1:2:1090:A:N1	1.97	0.97
1:2:1290:G:N2	1:2:1323:G:N2	2.13	0.95
1:2:1598:A:H1'	1:2:1599:G:H5"	1.46	0.94
1:2:1541:A:C6	1:2:1542:U:C5	2.56	0.93
1:2:1292:U:C4	1:2:1321:A:N1	2.37	0.92
1:2:4:C:H4'	4:C:186:SER:HB3	1.52	0.90
1:2:1541:A:C2	1:2:1542:U:C5	2.60	0.89
1:2:1542:U:O4	1:2:1565:U:O2	1.89	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1170:A:H2'	1:2:1171:G:C8	2.08	0.89
1:2:991:A:C2	1:2:1011:U:O4	2.25	0.88
1:2:1542:U:H4'	27:S:132:ARG:NH1	1.89	0.88
1:2:813:A:N6	1:2:856:U:H3	1.71	0.87
8:I:57:ALA:HB2	8:I:178:GLY:HA2	1.58	0.86
1:2:826:C:O2	1:2:826:C:H2'	1.75	0.85
1:2:1159:A:H2'	1:2:1160:C:C6	2.11	0.85
1:2:1037:U:O4	1:2:1091:A:N1	2.09	0.85
1:2:548:G:H1	1:2:588:C:H5	1.23	0.84
1:2:1481:A:H2'	1:2:1482:G:C8	2.13	0.83
1:2:1541:A:C2	1:2:1542:U:C6	2.67	0.83
1:2:1541:A:N1	1:2:1542:U:C5	2.47	0.82
1:2:1486:G:H3'	1:2:1513:A:H61	1.44	0.81
14:W:6:VAL:HG12	14:W:34:ILE:HD11	1.61	0.81
1:2:1292:U:O4	1:2:1321:A:N1	2.14	0.80
1:2:1370:G:H2'	1:2:1371:A:C8	2.15	0.80
1:2:1186:U:H3	1:2:1197:G:H1	1.26	0.80
1:2:1188:A:H3'	1:2:1189:C:H5"	1.63	0.80
1:2:938:A:H2'	1:2:939:A:C8	2.18	0.79
1:2:1176:C:H5"	1:2:1188:A:H61	1.46	0.79
1:2:392:C:H2'	1:2:393:C:C6	2.18	0.78
1:2:1604:C:H2'	1:2:1605:G:C8	2.19	0.78
1:2:1450:U:H2'	1:2:1451:G:H8	1.46	0.78
1:2:537:A:H2	1:2:541:A:H62	1.32	0.77
1:2:1583:U:O4	1:2:1609:A:C6	2.37	0.77
1:2:1290:G:H22	1:2:1323:G:H22	0.77	0.77
1:2:864:A:N1	1:2:964:U:H5	1.81	0.77
1:2:1193:A:H2'	1:2:1194:C:H5'	1.67	0.77
1:2:1590:A:H2'	1:2:1591:A:C8	2.21	0.76
1:2:867:G:H1	1:2:959:U:H3	1.31	0.76
3:B:164:ILE:HD11	3:B:205:PHE:HB3	1.66	0.76
1:2:1679:A:H2	1:2:1718:G:H21	1.33	0.76
1:2:1560:G:C2	1:2:1561:C:N3	2.54	0.75
1:2:98:U:H2'	1:2:99:C:C6	2.20	0.75
14:W:75:ILE:HD11	14:W:125:ILE:HG21	1.67	0.75
1:2:870:G:H2'	1:2:871:G:C8	2.21	0.75
6:G:78:ALA:H	6:G:81:HIS:HD2	1.32	0.74
1:2:1619:U:H2'	1:2:1620:G:C8	2.22	0.74
1:2:813:A:N1	1:2:856:U:O4	2.20	0.74
1:2:144:A:H62	6:G:137:ARG:HH12	1.35	0.74
9:J:31:ALA:HA	9:J:36:LEU:HD12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:168:SER:O	7:H:172:VAL:HG23	1.88	0.74
1:2:1522:A:H2'	1:2:1523:A:C8	2.23	0.74
1:2:1589:C:H2'	1:2:1590:A:C8	2.23	0.73
1:2:299:A:H2'	1:2:300:A:C8	2.23	0.73
1:2:1477:A:H2'	1:2:1478:G:H8	1.53	0.73
1:2:1598:A:H1'	1:2:1599:G:C5'	2.19	0.73
20:D:27:ARG:HD3	22:K:60:SER:HB3	1.69	0.72
1:2:1085:A:H3'	1:2:1086:A:C8	2.24	0.72
1:2:163:A:H2'	1:2:164:G:C8	2.24	0.72
10:L:117:VAL:HG22	10:L:142:VAL:HG21	1.72	0.72
1:2:86:A:H2'	1:2:87:C:C6	2.23	0.72
6:G:135:PRO:HB2	6:G:141:ILE:HG13	1.71	0.72
1:2:1583:U:O2	1:2:1583:U:H2'	1.89	0.71
11:N:142:GLU:HG2	11:N:143:SER:H	1.55	0.71
1:2:1450:U:H2'	1:2:1451:G:C8	2.24	0.71
1:2:353:C:H5"	8:I:16:ALA:HB2	1.72	0.71
1:2:605:A:H1'	1:2:608:U:OP1	1.89	0.71
1:2:1541:A:C5	1:2:1542:U:H5	2.07	0.71
1:2:617:U:H5	1:2:1086:A:N1	1.88	0.71
1:2:1541:A:N1	1:2:1542:U:C4	2.58	0.71
1:2:1542:U:H4'	27:S:132:ARG:HH12	1.54	0.71
1:2:236:C:H5"	1:2:237:U:H5'	1.72	0.71
1:2:1451:G:H2'	1:2:1452:G:H8	1.56	0.71
1:2:395:G:H22	1:2:398:A:H5"	1.56	0.71
1:2:1174:U:H2'	1:2:1175:G:H8	1.57	0.70
1:2:1560:G:C6	1:2:1561:C:N4	2.59	0.70
1:2:1207:A:H1'	1:2:1268:U:H1'	1.74	0.70
14:W:11:LEU:HD12	14:W:74:VAL:HG22	1.74	0.70
1:2:1541:A:C5	1:2:1542:U:C5	2.78	0.70
1:2:1608:G:H5"	21:F:109:LYS:HB2	1.73	0.70
1:2:86:A:H2'	1:2:87:C:H6	1.56	0.70
1:2:1593:U:H3	1:2:1598:A:H2	1.39	0.70
1:2:1170:A:H2'	1:2:1171:G:H8	1.54	0.70
1:2:1598:A:H4'	1:2:1599:G:OP1	1.91	0.70
1:2:1501:A:N6	27:S:84:TRP:HB2	2.06	0.69
1:2:1783:U:H2'	1:2:1784:G:H8	1.56	0.69
1:2:1528:C:H2'	1:2:1529:G:C8	2.28	0.69
1:2:1584:A:C2	1:2:1609:A:N7	2.61	0.69
1:2:392:C:H2'	1:2:393:C:H6	1.58	0.69
1:2:1541:A:C6	1:2:1542:U:C4	2.80	0.69
1:2:898:G:H2'	1:2:899:A:C8	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:W:72:CYS:SG	14:W:129:VAL:HG12	2.33	0.69
6:G:14:LYS:HB2	6:G:124:ILE:HD12	1.73	0.68
1:2:893:U:H2'	1:2:894:G:H8	1.58	0.68
22:K:25:LYS:HA	22:K:64:TYR:HE1	1.58	0.68
1:2:452:U:O2	1:2:452:U:H2'	1.91	0.68
29:U:53:LYS:HB2	29:U:92:ASP:HB2	1.75	0.68
1:2:1583:U:O4	1:2:1609:A:N1	2.27	0.68
1:2:1332:C:H2'	1:2:1333:U:C6	2.28	0.68
1:2:1037:U:N3	1:2:1091:A:N6	2.01	0.68
1:2:1338:C:O2'	1:2:1340:A:N7	2.27	0.68
1:2:991:A:C6	1:2:1011:U:O4	2.46	0.68
1:2:1562:U:H2'	1:2:1563:C:C6	2.29	0.68
5:E:95:THR:HG22	16:Y:16:PRO:HD2	1.76	0.67
20:D:20:GLU:HG2	22:K:61:TRP:CZ3	2.30	0.67
1:2:1670:G:H2'	1:2:1671:G:C8	2.30	0.67
1:2:590:A:H2'	1:2:591:G:C8	2.29	0.67
1:2:605:A:N3	1:2:605:A:H5'	2.09	0.67
15:X:6:PRO:C	15:X:8:GLY:H	1.98	0.67
3:B:116:LYS:O	3:B:117:TRP:HB2	1.93	0.67
14:W:6:VAL:HG13	14:W:29:PRO:HG2	1.77	0.67
1:2:634:A:H2'	1:2:635:A:O4'	1.95	0.67
1:2:1408:A:H2'	1:2:1409:A:C8	2.30	0.67
1:2:1589:C:H2'	1:2:1590:A:H8	1.59	0.67
1:2:1193:A:C2'	1:2:1194:C:H5'	2.25	0.67
1:2:209:A:H4'	8:I:183:TYR:CE2	2.30	0.67
1:2:1238:U:H1'	1:2:1247:C:H42	1.60	0.66
25:Q:22:VAL:HG12	25:Q:65:ILE:HG13	1.77	0.66
1:2:16:G:C2	1:2:17:C:N3	2.63	0.66
1:2:434:C:H5'	15:X:50:LYS:HG3	1.77	0.66
1:2:1033:C:HO2'	14:W:2:THR:N	1.94	0.66
9:J:122:VAL:HG12	9:J:126:ARG:HH22	1.59	0.66
11:N:114:ARG:O	11:N:118:ILE:HG12	1.97	0.65
1:2:991:A:C6	1:2:1011:U:C4	2.85	0.65
6:G:76:LEU:HD11	6:G:92:ARG:HD3	1.78	0.65
1:2:1165:A:H5"	21:F:106:ASN:HD21	1.60	0.65
4:C:162:LYS:HE2	14:W:95:PRO:HA	1.79	0.65
1:2:916:U:H1'	12:O:41:ARG:HH21	1.61	0.65
1:2:1471:U:H5'	21:F:192:ILE:HD11	1.78	0.65
1:2:384:A:H5'	8:I:25:ARG:HH22	1.60	0.65
1:2:1079:U:N3	1:2:1090:A:N6	2.45	0.65
1:2:1442:A:N3	1:2:1442:A:H2'	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:248:U:H3'	1:2:249:C:H5'	1.79	0.65
1:2:1156:A:H2'	1:2:1159:A:N7	2.11	0.65
11:N:64:LYS:HE2	11:N:70:LYS:HA	1.78	0.64
1:2:1726:U:H2'	1:2:1727:C:C6	2.32	0.64
14:W:95:PRO:HD2	14:W:130:TYR:HB3	1.78	0.64
5:E:31:PRO:HG2	5:E:38:LEU:HD22	1.79	0.64
3:B:106:THR:H	3:B:109:LYS:HD2	1.62	0.64
3:B:176:VAL:HG12	3:B:177:GLN:H	1.61	0.64
1:2:1174:U:H2'	1:2:1175:G:C8	2.32	0.64
1:2:537:A:C8	1:2:542:C:N4	2.65	0.64
3:B:122:GLU:HG2	3:B:140:ILE:HG12	1.78	0.64
15:X:126:LYS:HA	15:X:131:SER:HA	1.78	0.64
1:2:366:A:H2'	1:2:367:U:O4'	1.97	0.63
4:C:106:VAL:HG11	4:C:216:LEU:HD13	1.81	0.63
1:2:1403:G:H2'	1:2:1404:A:C8	2.34	0.63
1:2:1312:A:H2'	1:2:1314:U:H5'	1.80	0.63
6:G:76:LEU:HB2	6:G:94:ARG:HE	1.64	0.63
1:2:1773:U:H2'	1:2:1774:A:C8	2.33	0.63
1:2:506:U:H3'	1:2:507:U:H5"	1.79	0.63
6:G:14:LYS:HZ1	6:G:123:GLY:H	1.45	0.63
9:J:66:ASP:HB3	9:J:67:PRO:HD3	1.79	0.63
1:2:1582:G:N2	1:2:1608:G:H2'	2.12	0.63
1:2:1277:G:C6	1:2:1278:C:N3	2.66	0.63
1:2:1477:A:H2'	1:2:1478:G:C8	2.34	0.63
1:2:737:A:HO2'	1:2:738:G:H8	1.47	0.63
1:2:1768:U:H2'	1:2:1769:U:C6	2.34	0.62
1:2:1332:C:H2'	1:2:1333:U:H6	1.64	0.62
1:2:1214:C:H2'	1:2:1215:C:C6	2.34	0.62
1:2:1712:A:H2'	1:2:1713:G:C8	2.34	0.62
1:2:42:G:H1	1:2:432:C:H42	1.46	0.62
1:2:395:G:N2	1:2:397:G:H3'	2.15	0.62
1:2:1286:A:H4'	1:2:1287:G:OP1	2.00	0.62
15:X:42:PRO:HA	15:X:81:LYS:HD2	1.81	0.62
1:2:917:U:H2'	1:2:918:A:C8	2.35	0.62
20:D:38:GLU:HB3	20:D:49:ILE:HB	1.82	0.62
4:C:193:MET:HG3	4:C:201:VAL:HG11	1.82	0.62
14:W:30:SER:HB2	14:W:61:ILE:HD12	1.80	0.62
9:J:128:LEU:HB3	9:J:134:ILE:CD1	2.30	0.62
2:A:6:THR:HG21	2:A:191:ARG:HD3	1.81	0.62
3:B:181:LEU:HA	3:B:184:LEU:HB3	1.82	0.61
1:2:428:G:H2'	1:2:429:G:H8	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:151:U:H3	1:2:161:A:H61	1.46	0.61
1:2:1173:C:HO2'	1:2:1174:U:H6	1.47	0.61
1:2:31:C:H3'	1:2:32:U:H5"	1.82	0.61
9:J:56:ALA:HA	9:J:59:LEU:HD12	1.82	0.61
1:2:1497:G:C6	1:2:1498:C:N4	2.68	0.61
1:2:1229:A:H61	1:2:1254:G:H1'	1.66	0.61
1:2:28:A:H2'	1:2:29:U:O4'	2.00	0.61
1:2:126:A:H62	1:2:290:G:H21	1.49	0.61
1:2:1541:A:C4	1:2:1542:U:C5	2.88	0.61
2:A:156:VAL:HG11	2:A:159:ALA:HB2	1.83	0.61
1:2:868:A:H61	1:2:957:U:H5	1.47	0.61
1:2:1583:U:H5"	1:2:1608:G:H22	1.64	0.61
1:2:94:U:H2'	1:2:95:G:O4'	2.00	0.61
1:2:1195:A:H4'	1:2:1196:C:H5"	1.82	0.61
1:2:1534:G:H4'	1:2:1535:C:OP1	2.00	0.61
1:2:1173:C:O2'	1:2:1174:U:H6	1.84	0.61
2:A:155:TYR:HA	13:V:60:ARG:HG2	1.82	0.61
1:2:826:C:C2'	1:2:826:C:O2	2.46	0.61
1:2:168:A:H5'	6:G:176:GLN:HG2	1.82	0.61
1:2:394:U:H2'	1:2:395:G:C8	2.35	0.60
1:2:1269:G:C2	1:2:1439:C:O2	2.54	0.60
1:2:1538:G:H1	1:2:1569:C:H42	1.49	0.60
15:X:63:GLN:HB3	15:X:64:PRO:CD	2.31	0.60
25:Q:83:GLN:HB3	25:Q:87:LYS:HZ2	1.66	0.60
1:2:624:C:H2'	1:2:625:U:C6	2.35	0.60
1:2:1113:G:N2	1:2:1129:G:H2'	2.16	0.60
1:2:15:U:H2'	1:2:16:G:O4'	2.01	0.60
1:2:1164:G:H2'	1:2:1165:A:C8	2.36	0.60
10:L:132:SER:O	10:L:134:THR:N	2.34	0.60
1:2:1481:A:H2'	1:2:1482:G:H8	1.64	0.60
1:2:1472:G:H1	1:2:1531:C:H42	1.49	0.60
26:R:10:LYS:HG2	26:R:53:TYR:CE2	2.37	0.60
6:G:36:VAL:HB	6:G:50:PHE:HB2	1.82	0.60
1:2:1619:U:H2'	1:2:1620:G:H8	1.64	0.60
1:2:985:G:H2'	1:2:986:G:O4'	2.02	0.60
5:E:45:ILE:HA	5:E:61:VAL:HG11	1.84	0.59
1:2:93:A:H2'	1:2:397:G:N2	2.17	0.59
1:2:471:U:O2'	1:2:769:A:N3	2.34	0.59
1:2:325:G:H2'	1:2:326:U:C6	2.37	0.59
4:C:149:TRP:HB3	4:C:178:PRO:HA	1.83	0.59
1:2:1451:G:H2'	1:2:1452:G:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:D:106:LYS:HG3	20:D:175:VAL:HG22	1.84	0.59
29:U:34:LEU:HD11	29:U:89:ARG:HG3	1.84	0.59
1:2:884:G:H2'	1:2:885:U:C6	2.38	0.59
1:2:626:C:H2'	1:2:627:G:O4'	2.03	0.59
1:2:1176:C:H2'	1:2:1177:G:O4'	2.03	0.59
7:H:173:TYR:CD1	7:H:181:ILE:HD11	2.38	0.59
1:2:1474:C:H2'	1:2:1475:G:C8	2.38	0.59
20:D:53:THR:HG22	20:D:94:ARG:HG2	1.84	0.59
1:2:1656:G:H2'	1:2:1656:G:N3	2.18	0.59
1:2:768:C:C2	9:J:143:ILE:HG12	2.37	0.58
1:2:25:C:H42	9:J:8:TYR:H	1.51	0.58
1:2:991:A:N6	1:2:1011:U:N3	2.51	0.58
8:I:168:ALA:HA	8:I:183:TYR:O	2.02	0.58
1:2:1581:A:C6	1:2:1609:A:H2	2.21	0.58
1:2:1227:G:OP1	23:M:38:LEU:HG	2.02	0.58
1:2:1543:A:OP1	27:S:133:VAL:N	2.28	0.58
1:2:1084:G:C3'	1:2:1085:A:H5"	2.33	0.58
1:2:1085:A:H5'	1:2:1086:A:OP2	2.03	0.58
1:2:827:U:HO2'	1:2:828:A:H8	1.51	0.58
24:P:52:LYS:HB2	24:P:53:PRO:HD3	1.85	0.58
1:2:854:A:H3'	1:2:855:A:H5"	1.85	0.58
9:J:110:GLN:HG2	9:J:126:ARG:NE	2.19	0.58
1:2:353:C:H2'	1:2:354:G:O4'	2.04	0.58
2:A:123:VAL:HG11	2:A:133:ILE:HD11	1.86	0.58
1:2:12:U:H2'	1:2:13:C:C6	2.39	0.58
5:E:181:VAL:HG23	5:E:227:VAL:HA	1.84	0.58
1:2:1037:U:C4	1:2:1091:A:N1	2.71	0.58
1:2:1180:U:H2'	1:2:1181:U:O4'	2.03	0.58
1:2:548:G:N1	1:2:588:C:H5	1.99	0.58
10:L:37:ASN:HA	10:L:44:THR:HG21	1.86	0.58
1:2:1452:G:H4'	24:P:122:THR:HG21	1.86	0.58
1:2:885:U:H2'	1:2:886:A:O4'	2.04	0.58
1:2:155:A:H2'	1:2:156:A:O4'	2.02	0.58
1:2:112:A:O2'	10:L:67:ARG:NH1	2.36	0.58
1:2:1583:U:O4	1:2:1609:A:C2	2.57	0.57
2:A:73:VAL:HG22	2:A:120:LEU:HB3	1.85	0.57
1:2:377:A:OP2	1:2:378:U:OP2	2.22	0.57
1:2:979:G:H4'	1:2:1774:A:H4'	1.86	0.57
1:2:108:A:H2'	1:2:109:G:C8	2.39	0.57
1:2:5:U:H2'	1:2:6:G:H8	1.70	0.57
1:2:425:G:N2	1:2:426:C:C2	2.73	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:825:U:N3	1:2:846:A:C2	2.72	0.57
1:2:1541:A:N3	1:2:1542:U:C6	2.73	0.57
1:2:105:A:H2'	1:2:106:U:O4'	2.04	0.57
1:2:1626:U:H2'	1:2:1627:G:C8	2.40	0.57
6:G:141:ILE:HG21	6:G:153:VAL:HG13	1.85	0.57
6:G:192:SER:O	6:G:196:LYS:HG2	2.05	0.57
1:2:1403:G:H2'	1:2:1404:A:H8	1.68	0.57
1:2:1085:A:H3'	1:2:1086:A:H8	1.67	0.57
12:O:17:ALA:HB3	12:O:81:ILE:HA	1.86	0.57
4:C:190:LYS:O	4:C:194:GLN:HG2	2.05	0.57
1:2:380:C:H5"	5:E:10:LYS:HD3	1.86	0.56
1:2:162:G:H2'	1:2:163:A:H8	1.71	0.56
1:2:1113:G:H22	1:2:1129:G:H2'	1.71	0.56
1:2:829:U:HO2'	1:2:830:U:H6	1.53	0.56
1:2:871:G:H2'	1:2:872:U:O4'	2.05	0.56
1:2:589:C:H2'	1:2:590:A:C8	2.40	0.56
9:J:128:LEU:HB3	9:J:134:ILE:HD11	1.87	0.56
24:P:127:ARG:H	24:P:127:ARG:HD2	1.70	0.56
8:I:107:THR:N	8:I:108:PRO:HD2	2.19	0.56
7:H:98:ILE:HG12	7:H:121:VAL:HG21	1.87	0.56
1:2:68:A:N3	1:2:68:A:H2'	2.19	0.56
20:D:73:ILE:HG22	20:D:84:ILE:HD13	1.87	0.56
1:2:85:A:O3'	16:Y:120:GLY:HA2	2.06	0.56
1:2:966:A:H2'	1:2:967:U:C6	2.40	0.56
1:2:266:U:H5"	1:2:266:U:H6	1.68	0.56
1:2:18:C:H2'	1:2:19:A:H8	1.69	0.56
4:C:175:ILE:HB	4:C:202:TYR:HB2	1.86	0.56
9:J:109:LEU:HB2	9:J:146:PHE:HB3	1.88	0.56
11:N:102:LEU:HD11	11:N:112:LYS:HA	1.87	0.56
14:W:35:ILE:HG13	14:W:61:ILE:HD11	1.88	0.56
1:2:139:C:H42	1:2:174:G:H21	1.53	0.56
27:S:86:LEU:HA	27:S:99:HIS:HD2	1.71	0.56
16:Y:87:PRO:HB2	16:Y:89:TYR:CE1	2.41	0.56
1:2:609:G:N3	1:2:609:G:H2'	2.20	0.56
12:O:71:CYS:SG	12:O:76:ILE:HB	2.45	0.56
1:2:946:U:HO2'	1:2:947:G:H8	1.52	0.56
6:G:57:ASP:HA	6:G:106:LEU:HA	1.87	0.56
5:E:114:ILE:HG23	5:E:119:ALA:HB2	1.88	0.55
1:2:1178:G:C6	1:2:1179:C:N3	2.74	0.55
1:2:16:G:C6	1:2:17:C:N4	2.74	0.55
5:E:46:VAL:HA	5:E:50:ASN:HD22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:58:VAL:HG22	12:O:111:ARG:HD3	83.92	0.55
1:2:988:U:H2'	1:2:989:C:O4'	2.07	0.55
1:2:1593:U:H5"	1:2:1594:C:O2	2.06	0.55
1:2:1549:U:H2'	1:2:1550:U:C6	2.40	0.55
1:2:405:U:H2'	1:2:406:A:C8	2.41	0.55
15:X:95:PHE:HB3	15:X:135:LEU:HD13	1.88	0.55
1:2:1079:U:C4	1:2:1090:A:N1	2.73	0.55
1:2:1320:A:H4'	1:2:1321:A:OP1	2.06	0.55
1:2:68:A:H4'	1:2:69:G:OP2	2.06	0.55
6:G:78:ALA:H	6:G:81:HIS:CD2	2.20	0.55
20:D:73:ILE:HA	20:D:76:ARG:HD2	1.89	0.55
21:F:178:THR:HB	21:F:182:ARG:HH21	1.71	0.55
1:2:1427:G:H2'	1:2:1428:U:C6	2.41	0.55
1:2:1349:G:C6	1:2:1374:C:N3	2.75	0.55
1:2:588:C:O4'	1:2:588:C:O2	2.24	0.55
4:C:145:ARG:NH1	4:C:226:THR:O	2.38	0.55
7:H:101:LYS:HA	7:H:112:ARG:NH2	2.21	0.55
23:M:93:GLY:HA2	23:M:104:ARG:HH12	1.72	0.54
1:2:1782:C:H2'	1:2:1783:U:C6	2.42	0.54
7:H:99:LEU:H	7:H:116:ARG:HB3	1.72	0.54
5:E:197:HIS:HB2	5:E:209:HIS:CD2	2.43	0.54
1:2:248:U:H5	10:L:34:TRP:CE2	2.24	0.54
1:2:5:U:H2'	1:2:6:G:C8	2.42	0.54
1:2:444:A:H1'	1:2:524:A:H5'	1.88	0.54
8:I:171:SER:H	8:I:182:GLY:HA2	1.71	0.54
22:K:58:GLN:O	22:K:64:TYR:HA	2.08	0.54
1:2:1583:U:C2'	1:2:1583:U:O2	2.53	0.54
2:A:146:LEU:HG	2:A:173:ILE:HG21	1.89	0.54
1:2:778:G:H22	16:Y:10:ARG:NE	2.06	0.54
1:2:1547:C:H42	1:2:1560:G:H1	1.55	0.54
8:I:76:THR:HG21	8:I:104:ILE:HG23	1.88	0.54
1:2:1581:A:N6	1:2:1609:A:H2	2.06	0.54
1:2:805:A:H2'	1:2:806:A:O4'	2.08	0.54
1:2:864:A:N1	1:2:964:U:C5	2.71	0.54
1:2:700:C:H42	1:2:738:G:H1	1.55	0.54
1:2:747:C:H42	1:2:801:G:H1	1.55	0.54
14:W:55:ASP:C	14:W:57:ARG:H	2.10	0.54
1:2:1161:C:H3'	1:2:1162:A:H8	1.73	0.54
28:T:60:SER:O	28:T:63:ARG:HG3	2.07	0.53
1:2:19:A:C2	1:2:20:G:C4	2.96	0.53
1:2:384:A:H5"	1:2:384:A:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:142:ILE:HG12	4:C:143:PRO:HD2	1.90	0.53
1:2:1417:G:H2'	1:2:1418:C:O4'	2.07	0.53
20:D:150:MET:HB3	20:D:152:PHE:CE2	2.43	0.53
1:2:209:A:H4'	8:I:183:TYR:HE2	1.72	0.53
1:2:390:A:H61	1:2:405:U:H3	1.56	0.53
4:C:179:ARG:HB2	9:J:97:LEU:HD13	1.89	0.53
1:2:974:C:H2'	1:2:974:C:O2	2.08	0.53
1:2:959:U:O2	1:2:959:U:H2'	2.07	0.53
1:2:1475:G:H2'	1:2:1476:G:O4'	2.08	0.53
1:2:1477:A:OP1	28:T:57:ARG:HG2	2.09	0.53
28:T:63:ARG:HD2	28:T:64:HIS:CD2	2.43	0.53
20:D:69:LEU:HA	20:D:72:LEU:HD12	1.89	0.53
4:C:157:HIS:HB3	4:C:199:GLU:HB3	1.91	0.53
1:2:1185:U:H2'	1:2:1186:U:O4'	2.07	0.53
1:2:380:C:H2'	1:2:381:C:C6	2.43	0.53
1:2:1381:G:H2'	1:2:1382:A:C8	2.44	0.53
25:Q:54:LEU:HD11	25:Q:114:ARG:NH2	2.23	0.53
23:M:45:LEU:HD13	23:M:71:LEU:HB3	1.90	0.53
1:2:898:G:H2'	1:2:899:A:H8	1.71	0.53
28:T:128:GLY:O	28:T:132:LEU:HG	2.08	0.53
7:H:46:ILE:HG12	7:H:60:VAL:HG12	1.89	0.53
1:2:1282:U:H5'	1:2:1283:C:H2'	1.90	0.53
14:W:15:ASN:HD21	14:W:71:LYS:HE2	1.74	0.53
1:2:1178:G:H2'	1:2:1179:C:O4'	2.09	0.53
8:I:9:HIS:CG	8:I:10:LYS:H	2.26	0.53
20:D:162:GLN:N	20:D:163:PRO:HD2	2.23	0.53
1:2:1099:G:H2'	1:2:1099:G:N3	2.22	0.53
27:S:86:LEU:HD22	27:S:99:HIS:HB2	1.91	0.53
1:2:1103:U:H2'	1:2:1104:C:O4'	2.08	0.53
1:2:999:C:O2	1:2:999:C:O4'	2.27	0.53
1:2:585:G:C2	1:2:586:C:C2	2.97	0.53
23:M:35:ALA:HB2	23:M:115:LYS:HE3	1.90	0.53
5:E:139:VAL:HB	5:E:150:PRO:HG3	1.91	0.53
9:J:170:GLY:H	9:J:174:ARG:HD2	1.72	0.53
1:2:1155:C:H42	1:2:1620:G:H1	1.56	0.53
1:2:732:G:H1'	1:2:734:A:H61	1.74	0.53
7:H:81:LEU:HD22	7:H:90:VAL:HG21	1.91	0.53
1:2:958:U:H2'	1:2:958:U:O2	2.08	0.53
7:H:63:PRO:O	7:H:64:VAL:HB	2.09	0.53
28:T:77:ASN:HB3	28:T:95:ASP:HB3	1.91	0.53
13:V:58:TYR:HB3	13:V:62:ARG:CZ	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:9:LEU:HB2	5:E:30:ARG:HB2	1.90	0.52
22:K:8:ARG:O	22:K:12:TYR:HD1	1.92	0.52
1:2:1581:A:O4'	1:2:1583:U:H1'	2.10	0.52
1:2:617:U:C5	1:2:1086:A:N1	2.74	0.52
1:2:89:G:C6	1:2:90:C:C4	2.97	0.52
1:2:1415:A:H2'	1:2:1416:G:O4'	2.09	0.52
1:2:1622:C:H2'	1:2:1623:C:C6	2.44	0.52
1:2:377:A:H2'	1:2:378:U:H5'	1.90	0.52
1:2:405:U:H2'	1:2:406:A:H8	1.73	0.52
1:2:1417:G:C6	1:2:1418:C:N3	2.77	0.52
1:2:1240:G:H1'	24:P:79:HIS:ND1	2.24	0.52
1:2:1785:C:H2'	1:2:1786:G:C8	2.44	0.52
1:2:780:A:C8	16:Y:8:ARG:HD2	2.44	0.52
13:V:9:VAL:HG12	13:V:10:GLU:H	1.75	0.52
1:2:1279:C:H2'	1:2:1280:G:H8	1.74	0.52
5:E:120:SER:O	5:E:164:LEU:HB3	2.09	0.52
14:W:30:SER:HA	14:W:34:ILE:HD12	1.90	0.52
1:2:326:U:H2'	1:2:327:A:C8	2.44	0.52
8:I:42:ARG:HB3	8:I:58:LEU:O	2.10	0.52
1:2:649:U:H3	1:2:684:A:H61	1.56	0.52
1:2:1482:G:N2	1:2:1483:C:C2	2.77	0.52
1:2:327:A:H2'	1:2:328:G:C8	2.45	0.52
1:2:1279:C:O2'	29:U:70:THR:HG22	2.09	0.52
2:A:162:CYS:SG	2:A:163:ASN:N	2.82	0.52
1:2:1130:A:H2'	1:2:1131:A:O4'	2.09	0.52
1:2:1150:A:H2'	1:2:1151:A:C8	2.45	0.52
1:2:1781:C:H2'	1:2:1782:C:C6	2.44	0.52
9:J:66:ASP:HB3	9:J:67:PRO:CD	2.40	0.52
1:2:468:C:H2'	1:2:469:A:O4'	2.10	0.52
28:T:84:LYS:HD2	28:T:94:VAL:HB	1.91	0.52
10:L:84:ILE:HB	10:L:111:VAL:CG2	2.39	0.52
1:2:1291:G:N1	1:2:1292:U:C4	2.78	0.52
1:2:363:G:C2	1:2:380:C:C2	2.97	0.52
1:2:1649:A:H61	1:2:1747:A:H61	1.58	0.52
1:2:1602:U:H2'	1:2:1602:U:O2	2.09	0.52
1:2:1671:G:C2	1:2:1672:C:C2	2.98	0.52
1:2:151:U:H2'	1:2:152:G:O4'	2.10	0.52
1:2:1180:U:H4'	24:P:127:ARG:HD3	1.91	0.52
1:2:638:U:C5	7:H:100:PRO:HA	2.45	0.52
1:2:398:A:O2'	1:2:400:A:H5"	2.09	0.51
12:O:122:PRO:HG2	12:O:125:SER:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1581:A:N6	1:2:1609:A:C2	2.78	0.51
7:H:138:LYS:HB2	14:W:54:ASP:HB3	1.91	0.51
16:Y:55:VAL:HG22	16:Y:75:VAL:HG22	1.92	0.51
1:2:1292:U:O4	1:2:1321:A:C6	2.62	0.51
1:2:1581:A:C6	1:2:1609:A:C2	2.98	0.51
1:2:1584:A:H5"	25:Q:136:SER:HB3	1.91	0.51
1:2:883:A:H2'	1:2:884:G:C8	2.46	0.51
1:2:819:U:H2'	1:2:820:U:H4'	1.93	0.51
26:R:41:ILE:HG22	26:R:43:SER:H	1.75	0.51
1:2:347:U:H4'	8:I:14:THR:HG22	1.91	0.51
14:W:6:VAL:HG12	14:W:34:ILE:CD1	2.37	0.51
9:J:30:LEU:HD11	9:J:102:GLU:HG2	1.91	0.51
1:2:1671:G:C6	1:2:1672:C:C4	2.99	0.51
4:C:234:LEU:HD11	13:V:14:PRO:HG2	1.93	0.51
1:2:166:U:H5"	6:G:135:PRO:HA	1.91	0.51
2:A:52:LYS:HG2	13:V:82:VAL:HA	1.92	0.51
1:2:1176:C:H5"	1:2:1188:A:N6	2.22	0.51
1:2:363:G:N2	1:2:380:C:C2	2.79	0.51
3:B:90:GLU:HG3	3:B:228:LEU:HD13	1.93	0.51
1:2:1510:G:H2'	1:2:1511:G:H8	1.76	0.51
1:2:242:G:H2'	1:2:243:A:C8	2.45	0.51
1:2:393:C:H4'	6:G:92:ARG:HH21	1.76	0.51
1:2:1712:A:H2'	1:2:1713:G:H8	1.73	0.51
27:S:89:GLN:C	27:S:91:ASP:H	2.14	0.51
1:2:1038:A:N7	1:2:1090:A:C8	2.79	0.51
1:2:1543:A:OP2	27:S:136:GLN:NE2	2.44	0.51
2:A:36:TYR:HB2	2:A:149:LEU:HD21	1.92	0.51
20:D:16:VAL:O	20:D:20:GLU:HG3	2.11	0.51
29:U:26:LEU:HB2	29:U:89:ARG:HB2	1.91	0.51
1:2:69:G:H1	1:2:82:U:H3	1.57	0.51
1:2:946:U:O2'	1:2:947:G:H8	1.93	0.51
1:2:1281:U:H3	1:2:1423:A:H61	1.59	0.51
3:B:119:THR:HG23	3:B:155:TYR:HD2	1.76	0.51
8:I:37:LYS:HD3	8:I:95:THR:HG22	1.93	0.51
1:2:1074:C:H2'	1:2:1075:A:O4'	2.11	0.51
1:2:737:A:O2'	1:2:738:G:H8	1.94	0.51
1:2:326:U:H2'	1:2:327:A:H8	1.75	0.51
7:H:126:LEU:HG	7:H:173:TYR:CE2	2.46	0.51
1:2:44:U:H3'	1:2:45:U:H5'	1.93	0.51
9:J:64:GLU:O	9:J:65:LYS:HB2	2.11	0.51
1:2:1540:G:H4'	1:2:1541:A:H5'	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:403:G:C2	1:2:404:C:N3	2.79	0.51
20:D:150:MET:HB3	20:D:152:PHE:HE2	1.75	0.51
1:2:1586:G:N1	1:2:1587:C:C2	2.79	0.51
29:U:50:LEU:HD11	29:U:99:ILE:HG12	1.92	0.51
1:2:1449:C:H2'	1:2:1450:U:C6	2.46	0.50
1:2:1783:U:H2'	1:2:1784:G:C8	2.42	0.50
8:I:55:PHE:HB2	8:I:177:SER:O	2.10	0.50
9:J:163:PRO:C	9:J:165:GLY:H	2.14	0.50
9:J:126:ARG:HD3	9:J:144:PRO:HB3	1.93	0.50
6:G:161:GLU:HG2	6:G:170:THR:HG22	1.93	0.50
14:W:8:ALA:HA	14:W:74:VAL:HG21	1.93	0.50
1:2:1668:G:O2'	1:2:1729:A:N6	2.44	0.50
2:A:70:PRO:HB2	2:A:94:GLY:HA3	1.93	0.50
2:A:57:ILE:HG13	2:A:160:ILE:HG12	1.92	0.50
9:J:80:LEU:HB3	9:J:86:LEU:HB2	1.93	0.50
22:K:25:LYS:HA	22:K:64:TYR:CE1	2.43	0.50
2:A:122:ILE:HA	2:A:144:ILE:O	2.11	0.50
11:N:46:THR:HB	11:N:86:GLU:HG3	1.92	0.50
23:M:52:LEU:HB3	23:M:114:VAL:HB	1.92	0.50
5:E:125:LYS:HB2	5:E:226:PHE:HD2	1.75	0.50
1:2:1269:G:N1	1:2:1439:C:C2	2.80	0.50
1:2:568:C:H41	15:X:69:ARG:HH22	1.58	0.50
1:2:799:U:H2'	1:2:800:G:C8	2.46	0.50
1:2:1025:A:N3	1:2:1788:A:O2'	2.36	0.50
26:R:88:VAL:HG12	26:R:89:SER:H	1.77	0.50
1:2:1084:G:N2	1:2:1087:A:OP2	2.32	0.50
1:2:471:U:H2'	1:2:472:A:H8	1.77	0.50
11:N:54:LEU:HD13	11:N:60:VAL:HG21	1.93	0.50
22:K:15:LEU:HD22	22:K:68:LEU:HD21	1.94	0.50
1:2:1210:A:H2'	1:2:1211:G:O4'	2.12	0.50
14:W:20:THR:OG1	14:W:22:LYS:HG2	2.12	0.50
9:J:169:PRO:HB2	9:J:174:ARG:HG3	1.94	0.50
4:C:84:GLU:HB2	4:C:108:VAL:HG23	1.93	0.50
3:B:90:GLU:HB2	3:B:97:LEU:HB2	1.94	0.50
26:R:34:LEU:O	26:R:38:ILE:HG13	2.12	0.50
1:2:1542:U:H2'	1:2:1542:U:O2	2.11	0.49
8:I:74:ARG:HG2	8:I:112:TRP:CD2	2.47	0.49
1:2:462:U:H2'	1:2:463:A:H8	1.76	0.49
1:2:1544:G:H21	27:S:87:ASN:HA	1.76	0.49
1:2:1573:G:H2'	1:2:1574:A:H8	1.76	0.49
1:2:955:C:H2'	1:2:956:G:C8	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:338:C:H2'	1:2:339:U:C6	2.47	0.49
1:2:647:G:N3	1:2:647:G:H2'	2.26	0.49
1:2:1563:C:H5"	27:S:41:ARG:HD2	1.93	0.49
1:2:73:U:H4'	1:2:74:U:OP1	2.12	0.49
12:O:20:PHE:HB3	12:O:27:PHE:HB2	1.93	0.49
1:2:1088:U:H6	1:2:1088:U:H5"	1.77	0.49
1:2:1159:A:H2'	1:2:1160:C:H6	1.73	0.49
1:2:589:C:H2'	1:2:590:A:H8	1.76	0.49
1:2:151:U:H3	1:2:161:A:N6	2.10	0.49
21:F:179:ILE:O	21:F:182:ARG:HG2	2.12	0.49
20:D:25:PHE:CE2	20:D:50:ILE:HG12	2.48	0.49
3:B:138:PHE:CD1	3:B:138:PHE:N	2.78	0.49
1:2:1293:G:H21	1:2:1320:A:H8	1.61	0.49
1:2:321:G:C2	1:2:336:G:C5	3.00	0.49
1:2:350:C:H5	1:2:630:G:H5"	1.76	0.49
1:2:360:C:C2	1:2:383:G:C2	3.00	0.49
7:H:154:LEU:HB2	7:H:185:ILE:HG13	1.94	0.49
16:Y:58:PHE:CB	16:Y:90:ARG:HH21	2.25	0.49
1:2:1482:G:C2	1:2:1483:C:N3	2.80	0.49
25:Q:6:SER:HA	25:Q:22:VAL:O	2.12	0.49
22:K:55:VAL:HG22	22:K:68:LEU:HD23	1.94	0.49
13:V:17:CYS:HB2	13:V:56:SER:HB3	1.95	0.49
1:2:1558:U:O2	1:2:1558:U:O4'	2.31	0.49
1:2:327:A:H2'	1:2:328:G:H8	1.78	0.49
1:2:627:G:N1	1:2:969:A:OP2	2.27	0.49
1:2:900:G:H2'	1:2:901:G:O4'	2.13	0.49
4:C:89:LYS:HZ3	4:C:104:LYS:HB3	1.78	0.49
1:2:621:A:H4'	1:2:622:A:H5"	1.94	0.49
1:2:1164:G:H2'	1:2:1165:A:H8	1.75	0.49
1:2:1349:G:C2	1:2:1374:C:O2	2.66	0.49
1:2:1138:A:C2	1:2:1139:G:H1'	2.47	0.49
22:K:23:ALA:HB3	22:K:64:TYR:HB2	1.95	0.49
1:2:1742:A:H3'	1:2:1743:G:H5'	1.95	0.49
1:2:1325:A:H2'	1:2:1326:C:C6	2.47	0.49
1:2:1598:A:H2'	1:2:1598:A:N3	2.27	0.49
1:2:1543:A:OP1	27:S:132:ARG:HA	2.12	0.49
7:H:91:ILE:HD13	7:H:172:VAL:HG21	1.93	0.49
25:Q:50:GLU:HA	25:Q:53:LEU:HD23	1.95	0.49
14:W:115:GLU:HA	14:W:118:ARG:HE	1.78	0.49
15:X:43:PHE:HZ	15:X:104:LEU:HB2	1.77	0.49
1:2:305:U:H2'	1:2:306:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1292:U:C4	1:2:1321:A:C2	3.00	0.48
8:I:9:HIS:CD2	8:I:10:LYS:H	2.31	0.48
4:C:42:PRO:HG3	4:C:51:LYS:HD2	1.95	0.48
1:2:989:C:H5	1:2:1013:G:H1	1.58	0.48
1:2:93:A:H2'	1:2:397:G:H21	1.77	0.48
1:2:1497:G:C2	1:2:1498:C:N3	2.80	0.48
1:2:449:U:H3	1:2:455:A:H61	1.61	0.48
1:2:1651:C:C2	1:2:1746:G:C2	3.01	0.48
1:2:225:A:H3'	1:2:226:U:H5'	1.94	0.48
6:G:53:ALA:HB3	6:G:112:ILE:HD11	1.94	0.48
1:2:143:G:H2'	1:2:144:A:C8	2.48	0.48
1:2:1529:G:H2'	1:2:1530:U:C6	2.48	0.48
1:2:868:A:H2'	1:2:869:C:O4'	2.14	0.48
22:K:27:PHE:O	22:K:28:ASN:HB2	2.13	0.48
1:2:210:U:H5'	10:L:20:PHE:HB3	1.95	0.48
1:2:460:G:H2'	1:2:461:G:O4'	2.14	0.48
9:J:63:ASP:O	9:J:69:ARG:HD3	2.12	0.48
1:2:1127:C:H2'	1:2:1128:U:O4'	2.14	0.48
1:2:775:G:C6	1:2:785:C:N4	2.81	0.48
1:2:1080:A:H4'	1:2:1081:C:OP1	2.12	0.48
1:2:1541:A:N6	1:2:1542:U:O4	2.47	0.48
1:2:542:C:O2	1:2:542:C:O4'	2.28	0.48
9:J:148:VAL:HG11	9:J:156:ILE:HD11	1.94	0.48
1:2:1607:U:H3'	1:2:1608:G:H8	1.79	0.48
1:2:1609:A:O2'	21:F:97:ASN:HB3	2.13	0.48
9:J:109:LEU:CB	9:J:146:PHE:HB3	2.43	0.48
1:2:243:A:H2'	1:2:244:U:C6	2.49	0.48
29:U:31:VAL:HG22	29:U:87:HIS:NE2	2.29	0.48
1:2:382:G:H5"	1:2:382:G:C8	2.48	0.48
4:C:116:VAL:HG13	4:C:196:ALA:HA	1.95	0.48
1:2:561:G:C2	1:2:583:C:C2	3.02	0.48
1:2:1522:A:H5"	28:T:78:LYS:HE2	1.95	0.48
1:2:1563:C:H2'	1:2:1564:U:O4'	2.13	0.48
15:X:6:PRO:C	15:X:8:GLY:N	2.67	0.48
1:2:19:A:H5'	15:X:109:ARG:HH21	1.78	0.48
25:Q:112:TYR:HB3	25:Q:114:ARG:NH2	2.29	0.48
1:2:1131:A:H2'	1:2:1132:A:H8	1.78	0.48
10:L:21:THR:HG22	10:L:32:LYS:H	1.79	0.48
28:T:22:LEU:HD22	28:T:28:LEU:HD12	1.96	0.48
1:2:1143:U:H2'	1:2:1144:U:C6	2.49	0.48
1:2:1510:G:H2'	1:2:1511:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:88:ILE:HG22	30:Z:89:ILE:HG13	1.96	0.48
12:O:61:MET:HG2	12:O:104:ALA:HB2	1.95	0.48
20:D:170:THR:HG22	20:D:187:LYS:HG2	1.96	0.48
10:L:15:LYS:HA	10:L:54:ILE:HG12	1.95	0.48
1:2:1664:U:H3	1:2:1733:U:H3	1.61	0.48
1:2:984:G:H1	1:2:1015:C:H5	1.60	0.48
10:L:101:GLU:OE2	15:X:13:ARG:N	2.47	0.48
1:2:1542:U:C4'	27:S:132:ARG:NH1	2.71	0.48
1:2:428:G:H2'	1:2:429:G:C8	2.48	0.48
21:F:189:ILE:HG21	30:Z:66:VAL:HG11	1.96	0.48
1:2:1482:G:C2	1:2:1483:C:C4	3.01	0.47
1:2:300:A:H5'	1:2:301:U:OP2	2.14	0.47
1:2:585:G:C6	1:2:586:C:C4	3.02	0.47
27:S:88:ARG:HG3	27:S:91:ASP:HA	1.96	0.47
1:2:1651:C:C2	1:2:1746:G:N2	2.82	0.47
10:L:124:THR:HB	10:L:141:LYS:HB3	1.96	0.47
5:E:248:ILE:HG13	5:E:248:ILE:H	1.57	0.47
1:2:1156:A:H3'	1:2:1159:A:H62	1.79	0.47
1:2:1253:U:H3	23:M:39:ARG:NH2	2.12	0.47
1:2:410:C:H2'	1:2:411:A:O4'	2.14	0.47
1:2:813:A:N6	1:2:856:U:C2	2.80	0.47
1:2:938:A:C6	1:2:939:A:C6	3.02	0.47
1:2:1774:A:H2'	1:2:1775:G:C8	2.49	0.47
1:2:38:C:H2'	1:2:39:A:O4'	2.14	0.47
1:2:1115:A:H2'	1:2:1116:U:C6	2.49	0.47
7:H:49:ILE:HG21	7:H:172:VAL:HA	1.97	0.47
14:W:11:LEU:HD13	14:W:72:CYS:HB3	1.97	0.47
1:2:248:U:H5	10:L:34:TRP:CD2	2.33	0.47
10:L:84:ILE:HD13	10:L:111:VAL:HG21	1.97	0.47
3:B:70:LEU:HD13	3:B:82:ARG:HD3	1.97	0.47
1:2:758:U:H5"	9:J:7:THR:HG21	1.96	0.47
6:G:25:ARG:HA	6:G:28:TYR:HD1	1.79	0.47
1:2:614:A:H5"	1:2:614:A:C8	2.50	0.47
1:2:142:G:H2'	1:2:143:G:C8	2.50	0.47
1:2:93:A:C6	1:2:397:G:C6	3.03	0.47
1:2:1768:U:H2'	1:2:1769:U:H6	1.77	0.47
7:H:173:TYR:CD1	7:H:181:ILE:CD1	2.97	0.47
2:A:62:ARG:NH1	13:V:37:ALA:O	2.47	0.47
1:2:996:G:H2'	1:2:997:A:O4'	2.14	0.47
29:U:41:ILE:HD11	29:U:107:THR:HB	1.96	0.47
4:C:183:ILE:HG21	4:C:190:LYS:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:459:A:H2'	1:2:460:G:H5'	1.97	0.47
1:2:1738:A:H2'	1:2:1739:U:C6	2.48	0.47
1:2:1299:A:H5"	4:C:91:VAL:HG11	1.96	0.47
1:2:484:A:N6	1:2:501:U:H3	2.13	0.47
1:2:1343:A:H2'	1:2:1344:A:C8	2.49	0.47
28:T:63:ARG:HD2	28:T:64:HIS:HD2	1.80	0.47
1:2:14:C:H2'	1:2:15:U:C6	2.49	0.47
1:2:1269:G:C6	1:2:1439:C:N3	2.83	0.47
1:2:623:G:C6	1:2:624:C:C4	3.02	0.47
26:R:5:ARG:HB2	26:R:10:LYS:HE3	1.97	0.47
5:E:139:VAL:HG12	5:E:147:ILE:HB	1.97	0.47
3:B:100:PHE:CG	3:B:185:THR:HG21	2.50	0.47
15:X:87:VAL:CG1	15:X:132:LEU:HD11	2.44	0.47
23:M:68:VAL:HG12	23:M:79:LEU:HD11	1.95	0.47
1:2:309:C:C2	1:2:356:G:C2	3.02	0.47
5:E:87:MET:CE	5:E:100:ARG:HD3	2.45	0.47
1:2:1330:A:H4'	26:R:46:LEU:HD23	1.97	0.47
1:2:1317:G:O5'	1:2:1317:G:H8	1.97	0.47
8:I:170:ILE:HA	8:I:182:GLY:HA3	1.96	0.47
5:E:9:LEU:HD12	5:E:30:ARG:HA	1.96	0.47
5:E:100:ARG:HH22	5:E:118:GLU:HG2	1.79	0.47
1:2:121:U:H2'	1:2:122:U:O4'	2.13	0.47
5:E:7:LYS:HE3	5:E:7:LYS:HA	1.96	0.47
1:2:1289:U:H2'	1:2:1290:G:C8	2.50	0.47
1:2:1032:C:N4	1:2:1033:C:N4	2.63	0.47
1:2:1161:C:H3'	1:2:1162:A:C8	2.50	0.47
5:E:86:PHE:CE2	5:E:87:MET:HG2	2.49	0.47
1:2:556:G:N2	1:2:558:C:C2	2.83	0.47
1:2:1571:A:H4'	1:2:1572:G:O5'	2.15	0.47
1:2:798:A:H5"	5:E:201:HIS:CE1	2.50	0.47
1:2:1333:U:H2'	1:2:1334:U:O4'	2.15	0.47
1:2:623:G:C2	1:2:624:C:C2	3.03	0.47
7:H:60:VAL:HG23	7:H:92:PHE:HA	1.97	0.47
1:2:756:A:H2'	1:2:757:A:C8	2.50	0.47
3:B:186:SER:O	3:B:190:PRO:HD3	2.14	0.47
1:2:512:U:O4'	1:2:512:U:O2	2.31	0.47
21:F:100:MET:SD	21:F:109:LYS:HG2	2.56	0.46
1:2:429:G:N2	1:2:430:C:C2	2.84	0.46
1:2:829:U:O2'	1:2:830:U:H6	1.96	0.46
9:J:146:PHE:HZ	9:J:149:ARG:CZ	2.28	0.46
1:2:242:G:H2'	1:2:243:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:D:8:LYS:HG3	20:D:9:ARG:H	1.79	0.46
12:O:16:VAL:O	12:O:30:VAL:HA	2.16	0.46
1:2:1653:A:N3	1:2:1653:A:H2'	2.30	0.46
1:2:813:A:H2'	1:2:815:G:H8	1.81	0.46
1:2:1583:U:C4	1:2:1609:A:N1	2.82	0.46
15:X:63:GLN:HB3	15:X:64:PRO:HD2	1.97	0.46
1:2:380:C:H2'	1:2:381:C:H6	1.79	0.46
23:M:20:ALA:HB1	23:M:124:ARG:HA	1.96	0.46
7:H:140:VAL:O	14:W:51:GLU:HA	2.15	0.46
1:2:349:U:H5"	1:2:351:A:O4'	2.15	0.46
1:2:1292:U:H2'	1:2:1293:G:O4'	2.14	0.46
1:2:854:A:C2	1:2:856:U:H1'	2.50	0.46
1:2:1562:U:H2'	1:2:1563:C:H6	1.77	0.46
7:H:98:ILE:CG1	7:H:121:VAL:HG21	2.45	0.46
9:J:146:PHE:CZ	9:J:149:ARG:CZ	2.98	0.46
1:2:184:U:H3	1:2:199:A:H61	1.63	0.46
5:E:103:TYR:CD1	5:E:189:LEU:HD21	2.50	0.46
1:2:935:G:C2	1:2:936:C:C2	3.04	0.46
1:2:531:U:H4'	16:Y:66:GLY:H	1.80	0.46
1:2:300:A:H5"	1:2:300:A:C8	2.51	0.46
25:Q:22:VAL:HG12	25:Q:65:ILE:CG1	2.45	0.46
1:2:1267:G:H1	1:2:1439:C:H42	1.64	0.46
1:2:990:G:H21	1:2:1012:A:H62	1.64	0.46
1:2:1482:G:N1	1:2:1483:C:C4	2.83	0.46
1:2:635:A:H5"	14:W:31:SER:HB3	1.97	0.46
1:2:100:A:H2'	1:2:101:U:O4'	2.16	0.46
1:2:1769:U:H3'	1:2:1770:C:H5"	1.98	0.46
4:C:178:PRO:HB3	14:W:97:ARG:HH12	1.81	0.46
2:A:120:LEU:HD11	2:A:144:ILE:HD12	1.98	0.46
20:D:192:PRO:HB3	20:D:201:ALA:HA	1.97	0.46
4:C:74:ILE:HG22	4:C:81:LEU:HD11	1.97	0.46
10:L:108:PRO:HB2	10:L:135:VAL:HG22	1.97	0.46
4:C:106:VAL:HG22	4:C:120:ILE:HD12	1.96	0.46
1:2:999:C:H5	1:2:1001:G:H3'	1.81	0.46
1:2:462:U:H2'	1:2:463:A:C8	2.51	0.46
9:J:112:GLN:HE22	9:J:115:LYS:HD2	1.81	0.46
16:Y:29:HIS:HE1	16:Y:69:SER:HB2	1.80	0.46
26:R:28:PHE:HA	26:R:55:THR:HG21	1.98	0.46
1:2:1140:G:C6	1:2:1141:A:C6	3.04	0.46
1:2:999:C:H5	1:2:1002:A:OP2	1.98	0.46
3:B:79:HIS:C	3:B:81:PHE:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:639:U:H2'	1:2:640:G:O4'	2.16	0.46
7:H:137:GLY:H	7:H:153:LEU:HB2	1.81	0.46
1:2:48:G:H2'	1:2:49:C:O4'	2.15	0.46
5:E:79:ASP:HB2	5:E:82:PHE:HB2	1.98	0.46
21:F:115:ILE:O	21:F:119:THR:HG23	2.16	0.46
2:A:79:ARG:HH12	2:A:170:ILE:HD12	1.81	0.46
1:2:1562:U:H5"	28:T:38:LYS:HG3	1.97	0.46
11:N:61:THR:H	11:N:66:ILE:HD11	1.80	0.46
28:T:84:LYS:HE3	28:T:94:VAL:H	1.80	0.46
1:2:486:G:H1	1:2:499:C:H42	1.63	0.46
1:2:1759:U:H1'	1:2:1760:A:N7	2.31	0.46
2:A:98:ILE:HD11	2:A:116:LYS:HG3	1.98	0.46
1:2:1174:U:C2'	1:2:1175:G:H8	2.27	0.46
9:J:30:LEU:HD13	9:J:34:TYR:HE2	1.81	0.46
1:2:168:A:N7	1:2:170:A:C5	2.84	0.46
7:H:152:ILE:HD13	7:H:181:ILE:HG23	1.97	0.46
21:F:102:ASN:HD21	21:F:182:ARG:HD3	1.81	0.46
24:P:17:TYR:HB2	24:P:25:LEU:HD21	1.98	0.46
1:2:1582:G:C8	25:Q:122:ARG:HB2	2.51	0.45
1:2:958:U:H6	11:N:61:THR:HB	1.81	0.45
11:N:18:TYR:HB2	14:W:56:HIS:CD2	2.51	0.45
6:G:48:TYR:HB3	6:G:113:ILE:HD11	1.98	0.45
1:2:144:A:N6	6:G:137:ARG:HH12	2.08	0.45
1:2:1476:G:H3'	1:2:1477:A:H8	1.81	0.45
4:C:50:VAL:HG21	4:C:73:ILE:HG23	1.98	0.45
29:U:21:LYS:HA	29:U:93:LEU:O	2.17	0.45
1:2:66:U:C2	6:G:173:PRO:HG3	2.51	0.45
1:2:1482:G:C6	1:2:1483:C:N4	2.84	0.45
2:A:155:TYR:HD1	13:V:60:ARG:HD3	1.82	0.45
25:Q:75:VAL:O	25:Q:79:TYR:HD1	1.99	0.45
1:2:1108:G:H1	1:2:1135:U:H3	1.63	0.45
1:2:878:G:C6	1:2:879:C:N4	2.84	0.45
20:D:32:GLU:HB3	20:D:58:VAL:HG22	1.96	0.45
1:2:1478:G:OP1	28:T:60:SER:HB2	2.16	0.45
1:2:1501:A:H61	27:S:84:TRP:HB2	1.78	0.45
16:Y:88:ALA:HA	16:Y:91:LEU:HD12	1.98	0.45
1:2:1378:U:H2'	1:2:1379:U:O4'	2.16	0.45
5:E:26:CYS:HA	9:J:3:ARG:HA	1.99	0.45
1:2:1016:U:H2'	1:2:1017:U:C6	2.51	0.45
1:2:1412:U:H5'	26:R:3:ARG:HG2	1.99	0.45
15:X:5:LYS:HA	15:X:6:PRO:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1133:C:O2	1:2:1133:C:H2'	2.16	0.45
1:2:1765:G:H3'	1:2:1765:G:P	2.56	0.45
29:U:58:LEU:HD12	29:U:88:LYS:HD3	1.98	0.45
9:J:11:THR:HB	9:J:12:TYR:CE1	2.52	0.45
25:Q:82:ARG:HH12	25:Q:114:ARG:HB2	1.81	0.45
1:2:1585:A:H2'	1:2:1586:G:O4'	2.17	0.45
3:B:138:PHE:HD1	3:B:138:PHE:N	2.13	0.45
1:2:1645:U:H2'	1:2:1646:A:O4'	2.16	0.45
14:W:7:LEU:HD23	14:W:33:VAL:HG12	1.99	0.45
1:2:602:U:H2'	1:2:603:A:H8	1.81	0.45
13:V:11:LEU:HD12	13:V:11:LEU:H	1.82	0.45
1:2:614:A:H5"	1:2:614:A:H8	1.81	0.45
1:2:121:U:H2'	1:2:122:U:C6	2.52	0.45
1:2:1551:G:O6	24:P:43:ARG:HD3	2.16	0.45
5:E:65:LEU:HD13	5:E:80:THR:HA	1.99	0.45
1:2:864:A:C2	1:2:964:U:H5	2.34	0.45
1:2:299:A:H2'	1:2:300:A:H8	1.80	0.45
1:2:1528:C:H2'	1:2:1529:G:H8	1.81	0.45
1:2:84:A:H3'	1:2:85:A:H8	1.81	0.45
1:2:861:A:H4'	14:W:57:ARG:HG3	1.98	0.45
1:2:48:G:C2	1:2:49:C:C2	3.04	0.45
1:2:1110:G:H1	1:2:1133:C:H42	1.64	0.45
4:C:92:GLN:HA	4:C:100:ARG:O	2.16	0.45
24:P:90:ILE:HA	24:P:107:ILE:HG22	1.98	0.45
15:X:62:LYS:HB2	15:X:116:ASP:O	2.17	0.45
1:2:1617:C:H2'	1:2:1618:C:H6	1.80	0.45
1:2:1617:C:H2'	1:2:1618:C:C6	2.52	0.45
1:2:1589:C:H42	1:2:1603:G:H1	1.64	0.44
1:2:471:U:H2'	1:2:472:A:C8	2.52	0.44
1:2:999:C:C5	1:2:1002:A:OP2	2.70	0.44
1:2:556:G:C6	1:2:558:C:N4	2.85	0.44
1:2:1464:G:N2	1:2:1465:C:C2	2.85	0.44
1:2:1106:G:C6	1:2:1107:G:O6	2.70	0.44
1:2:253:A:H2'	1:2:254:U:C6	2.52	0.44
1:2:1175:G:C2	1:2:1176:C:C2	3.05	0.44
1:2:1620:G:C2	1:2:1621:C:C2	3.05	0.44
9:J:12:TYR:CD1	9:J:44:ARG:HA	2.52	0.44
1:2:973:A:C5	1:2:974:C:C5	3.05	0.44
2:A:185:ARG:HG3	13:V:45:ALA:HB3	1.99	0.44
8:I:67:TRP:CD1	8:I:109:PHE:HD2	2.35	0.44
11:N:88:LEU:HD22	11:N:92:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:F:173:SER:O	21:F:177:LEU:HG	2.16	0.44
1:2:476:A:C2	1:2:511:A:C2	3.05	0.44
21:F:123:ILE:HD11	21:F:200:LEU:HD13	1.99	0.44
1:2:866:G:N1	1:2:961:C:C2	2.85	0.44
1:2:1473:A:H2'	1:2:1474:C:C6	2.52	0.44
1:2:1782:C:H2'	1:2:1783:U:H6	1.81	0.44
1:2:778:G:H22	16:Y:10:ARG:HE	1.65	0.44
1:2:1487:U:P	20:D:9:ARG:HH22	2.40	0.44
21:F:197:ALA:HA	21:F:200:LEU:HD12	1.98	0.44
8:I:84:HIS:HA	8:I:85:PRO:HD2	1.76	0.44
4:C:107:VAL:HG11	4:C:134:ILE:HA	1.98	0.44
1:2:964:U:H4'	11:N:128:TYR:CD2	2.52	0.44
1:2:1560:G:C5	1:2:1561:C:N4	2.86	0.44
1:2:1501:A:H62	27:S:84:TRP:HB2	1.82	0.44
1:2:1164:G:O2'	1:2:1165:A:H5'	2.18	0.44
1:2:88:U:H2'	1:2:89:G:O4'	2.17	0.44
24:P:22:LEU:HA	24:P:25:LEU:HB2	1.99	0.44
20:D:12:VAL:O	20:D:16:VAL:HG23	2.17	0.44
1:2:30:G:H2'	1:2:31:C:O4'	2.17	0.44
5:E:197:HIS:HB2	5:E:209:HIS:HD2	1.82	0.44
4:C:108:VAL:HB	4:C:195:LEU:HD12	2.00	0.44
20:D:8:LYS:HG3	20:D:9:ARG:N	2.32	0.44
6:G:58:LYS:O	6:G:59:GLN:HB2	2.17	0.44
1:2:1225:A:H4'	1:2:1226:A:H8	1.82	0.44
1:2:332:A:C6	1:2:333:G:C6	3.05	0.44
1:2:1291:G:C6	1:2:1292:U:C4	3.06	0.44
1:2:403:G:C6	1:2:404:C:N4	2.85	0.44
9:J:105:LEU:HD23	9:J:108:ARG:HD2	2.00	0.44
1:2:756:A:H2'	1:2:757:A:H8	1.82	0.44
12:O:14:PHE:HA	12:O:78:ALA:O	2.18	0.44
1:2:1171:G:C2	1:2:1172:C:C2	3.05	0.44
8:I:68:ALA:HB2	8:I:183:TYR:HE1	1.82	0.44
1:2:862:A:H4'	14:W:57:ARG:HD3	1.99	0.44
8:I:42:ARG:CZ	8:I:59:ARG:HH22	2.30	0.44
2:A:23:HIS:NE2	2:A:50:VAL:HG13	2.32	0.44
2:A:23:HIS:CG	2:A:50:VAL:HG22	2.52	0.44
1:2:459:A:H2'	1:2:460:G:C5'	2.48	0.44
4:C:205:SER:HB3	4:C:209:THR:HG21	1.99	0.44
1:2:1322:C:H2'	1:2:1323:G:C8	2.53	0.44
1:2:1175:G:C6	1:2:1176:C:C4	3.06	0.44
21:F:73:ALA:HB3	21:F:113:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1769:U:H2'	1:2:1770:C:O4'	2.18	0.44
2:A:122:ILE:HG23	2:A:144:ILE:HG22	2.00	0.44
1:2:1785:C:H2'	1:2:1786:G:H8	1.80	0.44
1:2:1467:A:H2'	1:2:1468:C:C6	2.53	0.44
1:2:1171:G:C6	1:2:1172:C:C4	3.06	0.44
1:2:472:A:OP1	9:J:44:ARG:NE	2.51	0.44
1:2:382:G:H5"	1:2:382:G:H8	1.83	0.44
1:2:69:G:C2	1:2:70:C:C2	3.06	0.44
1:2:69:G:C6	1:2:70:C:C4	3.05	0.44
7:H:77:LEU:HD22	7:H:92:PHE:HZ	1.83	0.44
26:R:31:ASN:HA	26:R:34:LEU:HD12	2.00	0.44
4:C:146:ARG:HA	4:C:158:SER:O	2.18	0.44
2:A:69:ASN:HB3	2:A:72:ASP:HB2	1.99	0.44
1:2:92:A:H5"	1:2:93:A:H5"	1.99	0.43
1:2:861:A:C2	1:2:962:A:C4	3.05	0.43
1:2:630:G:N2	1:2:1103:U:P	2.91	0.43
3:B:153:THR:HB	3:B:155:TYR:CE1	2.53	0.43
1:2:1365:C:H5'	25:Q:30:LYS:NZ	2.33	0.43
1:2:1710:A:H2'	1:2:1711:G:H4'	2.00	0.43
1:2:1455:C:H1'	27:S:137:HIS:CE1	2.53	0.43
1:2:1079:U:H3	1:2:1090:A:N6	2.15	0.43
1:2:1592:G:OP2	1:2:1594:C:N4	2.51	0.43
1:2:1620:G:N2	1:2:1621:C:C2	2.86	0.43
1:2:1464:G:C2	1:2:1465:C:C2	3.06	0.43
24:P:94:VAL:HG23	24:P:105:VAL:HB	2.00	0.43
1:2:991:A:N6	1:2:1011:U:H3	2.16	0.43
1:2:1038:A:C2	1:2:1039:G:C4	3.06	0.43
1:2:1609:A:C2	1:2:1610:U:C5	3.07	0.43
21:F:109:LYS:O	21:F:113:VAL:HG23	2.18	0.43
1:2:313:C:O2	1:2:353:C:N3	2.51	0.43
1:2:966:A:H2'	1:2:967:U:H6	1.84	0.43
1:2:444:A:H2'	1:2:445:A:H8	1.83	0.43
13:V:58:TYR:HB3	13:V:62:ARG:NH1	2.34	0.43
1:2:1279:C:H2'	1:2:1280:G:C8	2.52	0.43
1:2:556:G:H5"	5:E:57:ASN:HD22	68.11	0.43
1:2:48:G:C6	1:2:49:C:C4	3.06	0.43
5:E:191:ARG:HH22	5:E:216:ASN:HD22	1.66	0.43
10:L:57:LYS:HA	10:L:64:VAL:HG21	1.99	0.43
20:D:51:ARG:HB3	20:D:91:VAL:HG22	2.01	0.43
1:2:809:G:C6	7:H:111:LYS:HG3	2.54	0.43
1:2:258:U:H1'	8:I:179:ARG:HH21	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1306:U:O4'	1:2:1306:U:O2	2.34	0.43
1:2:1527:C:H2'	1:2:1528:C:C6	2.53	0.43
1:2:1031:G:C6	1:2:1032:C:C4	3.07	0.43
26:R:41:ILE:HD13	26:R:47:ARG:HB2	1.99	0.43
29:U:28:SER:HB3	29:U:112:VAL:HA	2.00	0.43
1:2:592:U:H4'	1:2:594:G:H4'	2.01	0.43
6:G:74:LYS:HA	6:G:96:SER:HA	2.01	0.43
9:J:108:ARG:HB2	9:J:110:GLN:HB2	2.00	0.43
1:2:1215:C:C2	1:2:1446:G:N2	2.87	0.43
1:2:338:C:H2'	1:2:339:U:H6	1.83	0.43
3:B:128:LYS:HG2	3:B:134:VAL:HG22	2.00	0.43
3:B:144:ARG:HH21	3:B:208:GLN:HA	1.84	0.43
8:I:154:GLU:O	8:I:156:ALA:N	2.52	0.43
9:J:76:LEU:HD21	9:J:96:VAL:HG11	2.00	0.43
1:2:1435:U:H4'	20:D:181:VAL:HG21	2.00	0.43
1:2:1541:A:H1'	1:2:1567:A:C2	2.54	0.43
1:2:870:G:C6	1:2:871:G:O6	2.72	0.43
1:2:1474:C:H2'	1:2:1475:G:H8	1.79	0.43
1:2:1670:G:H2'	1:2:1671:G:H8	1.81	0.43
1:2:1269:G:C2	1:2:1439:C:C2	3.06	0.43
1:2:827:U:H3	1:2:843:A:H61	1.67	0.43
2:A:130:ALA:HA	2:A:133:ILE:HD12	2.01	0.43
8:I:83:TYR:HD2	8:I:101:ILE:HD13	1.84	0.43
20:D:158:ILE:HD13	20:D:202:LEU:HD21	2.01	0.43
1:2:795:A:H2'	1:2:796:G:O4'	2.19	0.43
1:2:268:G:C6	1:2:269:C:N4	2.87	0.43
12:O:25:ASP:HA	12:O:54:GLU:HB3	1.99	0.43
1:2:1594:C:O4'	1:2:1594:C:O2	2.36	0.43
4:C:149:TRP:CB	4:C:178:PRO:HA	2.47	0.43
1:2:886:A:H1'	12:O:122:PRO:HB3	2.01	0.43
7:H:98:ILE:HG12	7:H:121:VAL:HG11	2.01	0.43
4:C:115:HIS:HA	4:C:142:ILE:O	2.18	0.43
1:2:968:C:H5'	1:2:1103:U:H1'	1.99	0.43
1:2:336:G:H3'	10:L:133:LYS:HB2	2.00	0.43
2:A:63:ILE:HG12	13:V:36:ILE:HG12	2.01	0.43
1:2:1355:U:H2'	1:2:1356:G:H8	1.83	0.43
9:J:110:GLN:O	9:J:126:ARG:NH2	2.52	0.43
1:2:399:A:H4'	1:2:400:A:H5"	1.99	0.43
1:2:325:G:C2	1:2:342:C:C2	3.07	0.43
1:2:1101:G:H2'	1:2:1102:U:O4'	2.18	0.43
8:I:100:ALA:O	8:I:169:ALA:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1136:A:H4'	1:2:1137:A:H4'	2.00	0.43
1:2:735:C:HO2'	1:2:736:C:H6	1.64	0.43
4:C:121:LYS:HG2	4:C:132:ALA:HB3	2.00	0.43
1:2:1034:G:H2'	1:2:1035:A:H8	1.83	0.43
11:N:37:ILE:HG23	11:N:50:ILE:HG21	2.01	0.43
2:A:109:ASN:C	2:A:109:ASN:HD22	2.22	0.43
3:B:194:ASN:ND2	3:B:211:HIS:HA	2.33	0.43
1:2:866:G:H2'	1:2:867:G:O4'	2.19	0.43
1:2:957:U:H2'	11:N:14:SER:HB2	2.01	0.43
1:2:860:U:H3'	1:2:861:A:C8	2.53	0.43
8:I:38:ILE:HA	8:I:60:ILE:O	2.19	0.43
8:I:113:TYR:HA	8:I:116:HIS:HB2	2.01	0.43
7:H:61:PHE:CE1	7:H:93:LEU:HD22	2.54	0.43
28:T:107:SER:HA	28:T:110:LYS:HD2	1.99	0.43
1:2:776:G:C2	1:2:777:C:C2	3.07	0.43
4:C:166:LYS:HA	4:C:170:VAL:O	2.18	0.43
1:2:1012:A:H2'	1:2:1013:G:O4'	2.18	0.42
3:B:140:ILE:HG13	3:B:213:ARG:HG3	2.01	0.42
1:2:1768:U:H5"	1:2:1768:U:H6	1.84	0.42
2:A:64:ILE:HG23	2:A:73:VAL:HG21	1.99	0.42
14:W:55:ASP:C	14:W:57:ARG:N	2.72	0.42
28:T:37:VAL:HG22	28:T:39:THR:H	1.83	0.42
15:X:127:VAL:O	15:X:130:VAL:HG22	2.19	0.42
1:2:372:G:H2'	1:2:372:G:N3	2.33	0.42
1:2:1791:G:H4'	1:2:1792:A:OP1	2.19	0.42
1:2:429:G:N1	1:2:430:C:C4	2.87	0.42
1:2:1161:C:C2	1:2:1614:G:C2	3.07	0.42
1:2:303:U:H2'	1:2:304:C:C6	2.54	0.42
1:2:521:U:H3	1:2:530:C:H42	1.66	0.42
1:2:1084:G:H2'	1:2:1085:A:H5"	2.01	0.42
3:B:176:VAL:C	3:B:178:ASN:H	2.23	0.42
1:2:700:C:N4	1:2:738:G:H1	2.18	0.42
1:2:1538:G:H1	1:2:1569:C:N4	2.17	0.42
1:2:1316:C:OP1	26:R:10:LYS:HD3	2.19	0.42
1:2:407:C:H2'	1:2:408:C:C6	2.54	0.42
3:B:137:ILE:HG13	3:B:215:VAL:HG22	2.02	0.42
4:C:230:LEU:HB3	4:C:235:TRP:HZ3	1.84	0.42
1:2:71:A:H61	6:G:169:TYR:HB2	1.82	0.42
15:X:66:SER:O	15:X:67:ALA:HB2	2.19	0.42
1:2:473:A:H8	1:2:473:A:OP2	2.02	0.42
1:2:1321:A:H2'	1:2:1322:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:507:U:O2	1:2:507:U:H2'	2.18	0.42
10:L:78:THR:HG22	10:L:84:ILE:HD11	2.00	0.42
2:A:23:HIS:CD2	2:A:50:VAL:HG22	2.54	0.42
16:Y:58:PHE:HB2	16:Y:90:ARG:HH21	1.84	0.42
16:Y:84:LYS:HG3	16:Y:85:PHE:HD1	1.83	0.42
1:2:385:G:H2'	1:2:386:A:C8	2.53	0.42
1:2:1517:U:H2'	1:2:1518:U:H5	1.85	0.42
20:D:182:LEU:HD13	20:D:184:ILE:HD11	2.00	0.42
29:U:108:ILE:HG12	29:U:114:VAL:HG21	2.01	0.42
1:2:144:A:H62	6:G:137:ARG:NH1	2.10	0.42
1:2:1213:U:H2'	1:2:1214:C:C6	2.54	0.42
5:E:159:THR:HG21	5:E:227:VAL:O	2.19	0.42
1:2:955:C:H2'	1:2:956:G:H8	1.84	0.42
1:2:797:C:H2'	1:2:798:A:H8	1.84	0.42
1:2:594:G:C2	1:2:595:C:C2	3.08	0.42
1:2:1479:C:H41	28:T:79:LEU:HD23	1.85	0.42
1:2:888:U:H2'	1:2:889:C:O4'	2.18	0.42
7:H:41:LEU:HB3	7:H:70:TYR:CZ	2.55	0.42
1:2:580:U:O2	1:2:580:U:H2'	2.19	0.42
1:2:939:A:H2'	1:2:940:A:C8	2.55	0.42
1:2:46:A:N6	1:2:432:C:H4'	2.35	0.42
12:O:121:VAL:HA	12:O:122:PRO:HD3	1.77	0.42
1:2:390:A:N6	1:2:405:U:H3	2.18	0.42
5:E:90:ILE:CD1	5:E:101:LEU:HG	2.50	0.42
23:M:34:LEU:HB3	23:M:36:ARG:HG3	2.02	0.42
1:2:1496:G:O6	1:2:1507:C:N4	2.52	0.42
10:L:55:ASP:OD1	10:L:55:ASP:N	2.52	0.42
1:2:1472:G:H1	1:2:1531:C:N4	2.17	0.42
1:2:1315:G:N2	1:2:1316:C:C2	2.87	0.42
1:2:568:C:H41	15:X:69:ARG:NH2	2.17	0.42
1:2:1082:G:H3'	1:2:1083:A:H5"	2.02	0.42
20:D:191:ASP:HA	20:D:192:PRO:HD2	1.84	0.42
1:2:36:C:H2'	1:2:36:C:O2	2.19	0.42
9:J:30:LEU:HD12	9:J:105:LEU:HD12	2.02	0.42
3:B:116:LYS:O	3:B:117:TRP:CB	2.66	0.42
2:A:156:VAL:CG1	2:A:159:ALA:HB2	2.47	0.42
1:2:883:A:C2	1:2:884:G:C4	3.08	0.42
1:2:958:U:C6	11:N:61:THR:HB	2.55	0.42
1:2:1131:A:H2'	1:2:1132:A:C8	2.55	0.42
1:2:808:G:H2'	1:2:809:G:C8	2.54	0.42
25:Q:11:GLY:O	25:Q:17:THR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:135:ALA:HA	9:J:140:ILE:HA	2.01	0.42
16:Y:42:GLU:HG2	16:Y:52:LYS:HE2	2.02	0.42
1:2:959:U:O2	1:2:959:U:C2'	2.67	0.42
29:U:64:LYS:HD3	29:U:83:GLU:HB3	2.01	0.42
7:H:133:THR:HG21	7:H:162:ILE:HD13	2.01	0.42
25:Q:19:VAL:HG23	25:Q:68:LYS:HB2	2.02	0.42
20:D:122:VAL:O	20:D:126:VAL:HG23	2.20	0.42
14:W:73:GLY:HA3	14:W:128:PHE:CZ	2.54	0.42
3:B:48:VAL:HG12	3:B:49:ASN:H	1.84	0.42
1:2:1794:C:O2	1:2:1794:C:O4'	2.35	0.42
1:2:1265:U:H2'	1:2:1266:G:H8	1.85	0.42
5:E:181:VAL:HG22	5:E:225:VAL:HG22	2.02	0.42
6:G:61:PHE:HA	6:G:62:PRO:HD3	1.80	0.42
12:O:90:ARG:HB3	12:O:91:SER:H	1.77	0.42
1:2:1681:U:HO2'	1:2:1682:U:H6	1.68	0.42
1:2:1478:G:H1	1:2:1525:C:H42	1.66	0.41
1:2:594:G:C6	1:2:595:C:N4	2.88	0.41
1:2:566:A:H5'	1:2:567:G:OP2	2.20	0.41
1:2:873:C:H2'	1:2:874:G:C8	2.55	0.41
1:2:1607:U:H3'	1:2:1608:G:C8	2.55	0.41
13:V:60:ARG:HA	13:V:65:ALA:HB2	2.00	0.41
6:G:63:MET:SD	6:G:98:ARG:HG3	2.61	0.41
4:C:225:ASN:O	4:C:226:THR:C	2.57	0.41
21:F:71:TYR:CZ	25:Q:53:LEU:HD11	2.55	0.41
3:B:194:ASN:HA	3:B:197:ILE:HD12	2.03	0.41
6:G:190:GLN:HA	6:G:193:LEU:HD12	2.02	0.41
11:N:35:GLU:O	11:N:38:ILE:HG13	2.20	0.41
6:G:32:ILE:HA	6:G:52:ILE:HG23	2.01	0.41
1:2:1700:A:OP2	1:2:1701:C:H4'	2.19	0.41
1:2:541:A:H3'	1:2:542:C:H3'	2.01	0.41
1:2:406:A:C2	1:2:407:C:C2	3.09	0.41
16:Y:8:ARG:NH1	16:Y:9:THR:H	2.18	0.41
1:2:935:G:C6	1:2:936:C:C4	3.08	0.41
21:F:42:ILE:HB	21:F:44:LEU:HG	2.02	0.41
28:T:102:ARG:HH12	28:T:103:LYS:HE2	1.85	0.41
5:E:160:VAL:HG13	5:E:169:ILE:HG23	2.02	0.41
1:2:1598:A:C4'	1:2:1599:G:OP1	2.66	0.41
2:A:84:ARG:CZ	2:A:205:ARG:H	2.33	0.41
1:2:327:A:H2'	1:2:328:G:O4'	2.20	0.41
1:2:65:A:H2	1:2:84:A:H62	1.67	0.41
27:S:83:ALA:HB1	27:S:86:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1154:G:C2	1:2:1622:C:C2	3.07	0.41
16:Y:58:PHE:HB3	16:Y:90:ARG:HH21	1.85	0.41
9:J:45:ILE:HG22	9:J:101:VAL:HG12	2.02	0.41
2:A:23:HIS:HA	2:A:48:ILE:HD12	2.03	0.41
1:2:1573:G:H2'	1:2:1574:A:C8	2.55	0.41
1:2:1343:A:H4'	1:2:1344:A:OP1	2.20	0.41
2:A:109:ASN:HD22	2:A:111:ILE:H	1.68	0.41
4:C:61:ILE:HG23	4:C:66:LEU:HB2	2.03	0.41
1:2:1389:A:H2'	1:2:1390:U:C6	2.56	0.41
25:Q:105:LEU:HD23	25:Q:109:PHE:HE2	1.83	0.41
1:2:329:G:H2'	1:2:330:A:O4'	2.20	0.41
27:S:116:LEU:HA	27:S:119:ILE:HG12	2.03	0.41
3:B:32:ILE:HB	3:B:43:VAL:HB	2.02	0.41
15:X:97:ASP:HB3	15:X:98:GLU:H	1.69	0.41
9:J:30:LEU:HD12	9:J:105:LEU:CD1	2.50	0.41
6:G:102:VAL:HG13	6:G:106:LEU:HD13	2.03	0.41
20:D:40:ARG:NH2	29:U:68:ARG:HB2	37.35	0.41
1:2:914:A:N3	1:2:914:A:H2'	2.36	0.41
6:G:137:ARG:HD3	6:G:177:ARG:NH1	2.36	0.41
14:W:3:ARG:NH1	14:W:29:PRO:HG3	2.35	0.41
14:W:75:ILE:HD11	14:W:125:ILE:CG2	2.42	0.41
10:L:123:VAL:HG22	10:L:142:VAL:HG22	2.02	0.41
1:2:363:G:C2	1:2:380:C:N3	2.88	0.41
4:C:174:LEU:C	4:C:175:ILE:HG13	2.41	0.41
25:Q:54:LEU:HD11	25:Q:114:ARG:HH21	1.85	0.41
1:2:1034:G:H2'	1:2:1035:A:C8	2.56	0.41
10:L:8:GLN:NE2	10:L:14:GLN:H	2.19	0.41
5:E:180:LEU:HA	5:E:193:GLY:O	2.20	0.41
1:2:1387:C:H4'	26:R:49:LYS:HA	2.02	0.41
3:B:146:GLN:H	3:B:149:GLN:NE2	2.19	0.41
29:U:98:HIS:HA	29:U:101:LYS:HD2	2.03	0.41
15:X:19:ARG:HD3	15:X:19:ARG:HA	1.71	0.41
1:2:1793:U:HO2'	1:2:1795:A:H2	1.66	0.41
1:2:392:C:H42	1:2:403:G:H1	1.68	0.41
1:2:1584:A:H61	1:2:1608:G:H1'	1.85	0.41
5:E:45:ILE:HG23	5:E:49:ARG:HH21	1.86	0.41
5:E:125:LYS:HB2	5:E:226:PHE:CD2	2.54	0.41
1:2:339:U:H2'	1:2:340:A:C8	2.56	0.41
1:2:1651:C:N3	1:2:1746:G:C2	2.88	0.41
1:2:1344:A:H2'	1:2:1347:A:H62	1.86	0.41
4:C:121:LYS:HG2	4:C:132:ALA:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1208:C:C2	1:2:1453:G:N2	2.88	0.41
2:A:17:LEU:HD23	2:A:22:VAL:HG21	2.02	0.41
2:A:90:ALA:HA	2:A:95:ALA:HB3	2.03	0.41
1:2:938:A:N6	1:2:939:A:N6	2.69	0.41
8:I:107:THR:N	8:I:108:PRO:CD	2.84	0.41
7:H:64:VAL:C	7:H:66:SER:H	2.24	0.41
1:2:603:A:H2'	1:2:604:A:O4'	2.20	0.41
1:2:1464:G:C6	1:2:1465:C:C4	3.09	0.41
7:H:61:PHE:HE1	7:H:93:LEU:HD22	1.86	0.41
25:Q:78:VAL:HA	25:Q:81:ILE:HD12	2.02	0.41
1:2:320:C:O4'	1:2:320:C:O2	2.39	0.41
1:2:1767:U:O2	12:O:136:ARG:NE	2.54	0.41
4:C:64:HIS:HE1	4:C:241:THR:HB	1.86	0.41
6:G:4:ASN:HB3	6:G:110:ALA:HA	2.03	0.41
11:N:87:ASP:N	11:N:87:ASP:OD1	2.52	0.41
1:2:894:G:H4'	12:O:37:GLU:HG2	2.02	0.41
1:2:11:A:C2	1:2:1143:U:O2	2.74	0.41
4:C:235:TRP:CD2	14:W:68:ARG:HD3	2.56	0.41
1:2:1461:C:H41	27:S:140:THR:HG23	1.86	0.41
5:E:194:THR:O	5:E:195:ILE:HB	2.21	0.41
2:A:56:LYS:HE3	13:V:70:ASN:OD1	2.21	0.41
5:E:48:LEU:HA	5:E:52:LEU:HD12	2.03	0.41
1:2:1300:U:H5'	4:C:93:LYS:HE3	2.02	0.41
1:2:772:G:C6	1:2:773:C:N3	2.89	0.41
10:L:104:HIS:HB3	10:L:105:LYS:H	1.65	0.41
1:2:300:A:C2	1:2:301:U:C2	3.08	0.40
1:2:14:C:O2	1:2:1140:G:C2	2.74	0.40
1:2:630:G:H21	1:2:1103:U:P	2.44	0.40
7:H:62:VAL:HA	7:H:63:PRO:HD3	1.95	0.40
1:2:1137:A:H2'	1:2:1138:A:H8	1.85	0.40
1:2:797:C:H2'	1:2:798:A:C8	2.57	0.40
1:2:564:C:H5"	1:2:565:C:C6	2.56	0.40
12:O:19:ILE:HB	12:O:83:ILE:HA	2.03	0.40
1:2:489:C:H42	1:2:496:G:H1	1.69	0.40
5:E:12:LEU:C	5:E:14:ALA:N	2.74	0.40
9:J:36:LEU:HD23	9:J:110:GLN:OE1	2.21	0.40
1:2:1084:G:C2'	1:2:1085:A:H5"	2.51	0.40
10:L:123:VAL:HG11	10:L:139:VAL:HG22	2.04	0.40
1:2:1140:G:N1	1:2:1141:A:C6	2.89	0.40
9:J:11:THR:HB	9:J:12:TYR:CD1	2.56	0.40
1:2:425:G:N1	1:2:426:C:C4	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:524:A:H5”	16:Y:89:TYR:CD2	2.56	0.40
1:2:305:U:H2’	1:2:306:G:H8	1.84	0.40
25:Q:41:PRO:HG2	25:Q:78:VAL:HG21	2.03	0.40
14:W:32:LYS:O	14:W:36:LYS:HG2	2.21	0.40
9:J:153:GLU:C	9:J:155:HIS:H	2.24	0.40
21:F:72:VAL:HG21	25:Q:47:LYS:HG2	2.03	0.40
8:I:31:ARG:HH22	8:I:48:THR:HA	1.87	0.40
15:X:77:ILE:H	15:X:77:ILE:HG13	1.71	0.40
1:2:1774:A:C6	1:2:1784:G:C6	3.09	0.40
10:L:34:TRP:CH2	10:L:36:LYS:HB2	2.56	0.40
1:2:1656:G:H5’	1:2:1657:A:H5”	2.02	0.40
1:2:1656:G:N3	1:2:1656:G:C2’	2.82	0.40
1:2:381:C:H2’	1:2:382:G:C8	2.56	0.40
1:2:303:U:H2’	1:2:304:C:O4’	2.21	0.40
1:2:631:U:C4	1:2:632:U:C4	3.10	0.40
9:J:114:TYR:HD1	9:J:121:SER:H	1.69	0.40
1:2:1200:G:C2	1:2:1598:A:C2	3.10	0.40
1:2:939:A:H2’	1:2:940:A:H8	1.85	0.40
14:W:11:LEU:HA	14:W:11:LEU:HD23	1.86	0.40
1:2:979:G:H1	1:2:1020:C:H42	1.69	0.40
14:W:100:GLY:HA3	14:W:130:TYR:CG	2.56	0.40
1:2:1229:A:H2	1:2:1256:U:H5	1.70	0.40
1:2:828:A:H1’	1:2:829:U:O2	2.22	0.40
1:2:122:U:H2’	1:2:123:G:O4’	2.22	0.40
1:2:1467:A:H4’	1:2:1539:G:H5”	2.04	0.40
10:L:87:ARG:HG3	10:L:104:HIS:CE1	2.57	0.40
4:C:135:ILE:O	4:C:139:LEU:HG	2.22	0.40
1:2:954:A:OP1	11:N:3:ARG:HD2	2.22	0.40
1:2:131:C:H4’	1:2:132:U:OP1	2.22	0.40
10:L:76:VAL:HG12	10:L:77:SER:HB2	2.03	0.40
1:2:523:U:O2’	1:2:525:A:C8	2.75	0.40
1:2:1456:G:H5’	1:2:1456:G:C8	2.57	0.40
1:2:991:A:C2	1:2:1012:A:C6	3.10	0.40
1:2:403:G:C2	1:2:404:C:C2	3.10	0.40
1:2:1603:G:C2	1:2:1604:C:C2	3.10	0.40
1:2:452:U:O2	1:2:452:U:C2’	2.59	0.40
1:2:89:G:C2	1:2:90:C:C2	3.10	0.40
1:2:1786:G:H2’	1:2:1787:G:H8	1.87	0.40
4:C:116:VAL:HG22	4:C:144:ILE:HD11	2.03	0.40
1:2:21:U:H2’	1:2:22:A:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	204/254 (80%)	167 (82%)	24 (12%)	13 (6%)	2	26
3	B	212/255 (83%)	175 (82%)	25 (12%)	12 (6%)	2	28
4	C	215/259 (83%)	182 (85%)	23 (11%)	10 (5%)	3	33
5	E	258/261 (99%)	215 (83%)	36 (14%)	7 (3%)	6	48
6	G	224/236 (95%)	196 (88%)	24 (11%)	4 (2%)	11	56
7	H	182/190 (96%)	152 (84%)	15 (8%)	15 (8%)	1	18
8	I	184/201 (92%)	146 (79%)	26 (14%)	12 (6%)	1	26
9	J	180/188 (96%)	148 (82%)	20 (11%)	12 (7%)	1	25
10	L	153/156 (98%)	129 (84%)	18 (12%)	6 (4%)	4	38
11	N	148/151 (98%)	127 (86%)	17 (12%)	4 (3%)	6	48
12	O	125/137 (91%)	98 (78%)	20 (16%)	7 (6%)	2	29
13	V	85/87 (98%)	67 (79%)	11 (13%)	7 (8%)	1	18
14	W	127/130 (98%)	109 (86%)	13 (10%)	5 (4%)	4	38
15	X	142/145 (98%)	115 (81%)	13 (9%)	14 (10%)	1	13
16	Y	132/135 (98%)	114 (86%)	10 (8%)	8 (6%)	2	27
17	a	95/119 (80%)	64 (67%)	21 (22%)	10 (10%)	1	12
18	b	79/82 (96%)	62 (78%)	12 (15%)	5 (6%)	2	26
19	e	51/63 (81%)	47 (92%)	3 (6%)	1 (2%)	9	54
20	D	221/237 (93%)	197 (89%)	18 (8%)	6 (3%)	6	48
21	F	204/227 (90%)	169 (83%)	25 (12%)	10 (5%)	3	32
22	K	94/106 (89%)	81 (86%)	11 (12%)	2 (2%)	9	53
23	M	120/134 (90%)	96 (80%)	20 (17%)	4 (3%)	5	44
24	P	121/140 (86%)	99 (82%)	16 (13%)	6 (5%)	3	32
25	Q	139/143 (97%)	120 (86%)	15 (11%)	4 (3%)	6	46
26	R	116/136 (85%)	93 (80%)	18 (16%)	5 (4%)	3	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
27	S	143/146 (98%)	113 (79%)	23 (16%)	7 (5%)	3 32
28	T	141/144 (98%)	123 (87%)	15 (11%)	3 (2%)	9 53
29	U	104/117 (89%)	91 (88%)	5 (5%)	8 (8%)	1 20
30	Z	68/108 (63%)	53 (78%)	10 (15%)	5 (7%)	1 21
31	c	61/67 (91%)	55 (90%)	6 (10%)	0	100 100
32	d	51/56 (91%)	41 (80%)	9 (18%)	1 (2%)	9 54
33	f	67/150 (45%)	43 (64%)	17 (25%)	7 (10%)	1 12
34	g	312/326 (96%)	256 (82%)	48 (15%)	8 (3%)	7 48
35	h	23/25 (92%)	23 (100%)	0	0	100 100
36	i	94/153 (61%)	86 (92%)	8 (8%)	0	100 100
37	j	84/108 (78%)	75 (89%)	8 (10%)	1 (1%)	16 63
All	All	4959/5572 (89%)	4127 (83%)	603 (12%)	229 (5%)	5 34

All (229) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	26	ALA
2	A	95	ALA
3	B	100	PHE
3	B	117	TRP
4	C	141	VAL
4	C	153	LEU
5	E	201	HIS
6	G	122	GLU
7	H	13	PRO
7	H	31	SER
7	H	64	VAL
7	H	74	GLN
8	I	52	ASN
8	I	153	ILE
9	J	98	ALA
10	L	133	LYS
11	N	47	PRO
13	V	44	ARG
15	X	42	PRO
15	X	64	PRO
15	X	144	ARG
16	Y	30	PRO

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Mol	Chain	Res	Type
17	a	75	ILE
17	a	83	ILE
21	F	67	SER
22	K	83	PRO
22	K	88	PRO
23	M	74	GLU
24	P	29	PRO
26	R	85	VAL
26	R	88	VAL
28	T	11	ALA
37	j	72	PRO
2	A	49	ASN
2	A	81	TYR
3	B	158	SER
4	C	149	TRP
7	H	111	LYS
7	H	136	VAL
8	I	9	HIS
8	I	22	ARG
8	I	40	THR
8	I	58	LEU
8	I	147	ARG
9	J	118	LEU
10	L	30	LYS
10	L	105	LYS
12	O	124	ASP
14	W	29	PRO
14	W	83	ILE
14	W	98	GLN
15	X	67	ALA
15	X	115	GLY
16	Y	52	LYS
17	a	81	ALA
17	a	86	VAL
18	b	21	LEU
18	b	75	GLU
20	D	93	ASP
21	F	65	GLN
21	F	206	GLY
24	P	28	MET
24	P	121	ILE
27	S	28	VAL

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Mol	Chain	Res	Type
27	S	51	ASP
29	U	49	LYS
29	U	106	ILE
29	U	118	ILE
30	Z	41	VAL
33	f	102	VAL
33	f	143	HIS
34	g	130	LYS
2	A	43	ASP
3	B	207	LEU
3	B	209	ASN
3	B	210	VAL
3	B	221	PRO
4	C	111	ASP
5	E	12	LEU
5	E	245	LYS
7	H	10	SER
7	H	159	VAL
8	I	148	ALA
8	I	155	HIS
10	L	55	ASP
10	L	104	HIS
11	N	3	ARG
11	N	24	ALA
12	O	40	ALA
12	O	114	ARG
13	V	4	ASP
13	V	30	SER
13	V	42	GLU
14	W	30	SER
15	X	3	LYS
15	X	7	ARG
15	X	63	GLN
15	X	89	ASN
15	X	90	ASP
15	X	128	SER
15	X	131	SER
16	Y	36	SER
16	Y	60	PHE
16	Y	61	ARG
17	a	60	ALA
17	a	64	LEU

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Mol	Chain	Res	Type
20	D	44	THR
20	D	143	ARG
20	D	217	VAL
21	F	155	GLY
24	P	12	PHE
27	S	61	LEU
28	T	50	SER
29	U	16	GLU
30	Z	54	ALA
30	Z	97	LYS
33	f	111	GLU
33	f	145	THR
34	g	106	GLY
34	g	168	ASP
34	g	278	ILE
34	g	301	TRP
2	A	35	PRO
2	A	82	GLY
2	A	158	VAL
2	A	193	GLN
2	A	197	ILE
3	B	54	LEU
3	B	206	PRO
4	C	41	VAL
4	C	155	GLN
5	E	120	SER
5	E	195	ILE
5	E	205	PHE
6	G	153	VAL
7	H	115	SER
7	H	132	PRO
9	J	65	LYS
9	J	120	LYS
9	J	121	SER
9	J	147	MET
12	O	24	ASN
12	O	42	VAL
13	V	10	GLU
15	X	5	LYS
16	Y	63	GLN
19	e	47	VAL
20	D	4	ILE

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Mol	Chain	Res	Type
20	D	219	GLU
21	F	66	ILE
23	M	82	VAL
23	M	98	ASP
24	P	69	GLU
24	P	101	VAL
25	Q	138	PHE
26	R	115	LEU
27	S	90	LYS
29	U	21	LYS
29	U	59	PRO
33	f	94	LYS
33	f	98	VAL
34	g	193	TYR
2	A	185	ARG
2	A	189	PRO
4	C	44	THR
4	C	228	GLY
5	E	77	ARG
7	H	134	GLU
8	I	10	LYS
8	I	41	LYS
8	I	59	ARG
9	J	18	PRO
9	J	67	PRO
9	J	134	ILE
9	J	171	ARG
10	L	4	GLU
11	N	27	LYS
13	V	7	GLN
13	V	12	TYR
14	W	57	ARG
16	Y	51	GLU
17	a	36	ILE
18	b	24	LEU
18	b	62	VAL
21	F	23	VAL
23	M	97	ILE
26	R	100	LEU
26	R	124	VAL
27	S	14	ILE
27	S	19	ASN

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Mol	Chain	Res	Type
28	T	29	GLU
29	U	119	ALA
30	Z	68	ARG
34	g	16	GLY
34	g	52	GLU
2	A	103	THR
3	B	22	ASP
3	B	148	ASN
4	C	253	THR
6	G	89	ASN
7	H	131	PHE
9	J	99	LEU
12	O	25	ASP
15	X	53	VAL
17	a	62	TYR
25	Q	14	LYS
25	Q	27	GLY
25	Q	115	THR
30	Z	88	ILE
3	B	190	PRO
12	O	88	GLY
21	F	53	VAL
7	H	8	ILE
7	H	53	GLY
18	b	39	GLY
21	F	24	PRO
21	F	152	GLY
27	S	9	GLY
32	d	11	PRO
33	f	87	THR
4	C	187	PRO
7	H	98	ILE
16	Y	5	ILE
29	U	17	VAL
6	G	69	LEU
9	J	166	GLY
21	F	77	GLY
17	a	84	VAL
17	a	97	PRO

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
2	A	174/211 (82%)	146 (84%)	28 (16%)	3 22
3	B	196/228 (86%)	176 (90%)	20 (10%)	9 43
4	C	176/203 (87%)	148 (84%)	28 (16%)	3 23
5	E	223/224 (100%)	189 (85%)	34 (15%)	3 25
6	G	192/200 (96%)	172 (90%)	20 (10%)	9 42
7	H	164/170 (96%)	140 (85%)	24 (15%)	4 27
8	I	148/159 (93%)	123 (83%)	25 (17%)	2 19
9	J	153/158 (97%)	129 (84%)	24 (16%)	3 24
10	L	136/137 (99%)	121 (89%)	15 (11%)	8 39
11	N	127/128 (99%)	114 (90%)	13 (10%)	9 43
12	O	96/104 (92%)	90 (94%)	6 (6%)	22 64
13	V	73/73 (100%)	59 (81%)	14 (19%)	2 13
14	W	110/111 (99%)	94 (86%)	16 (14%)	4 27
15	X	119/120 (99%)	104 (87%)	15 (13%)	5 32
16	Y	108/109 (99%)	88 (82%)	20 (18%)	2 15
17	a	82/100 (82%)	64 (78%)	18 (22%)	1 9
18	b	71/72 (99%)	60 (84%)	11 (16%)	3 24
19	e	47/55 (86%)	42 (89%)	5 (11%)	8 41
20	D	185/196 (94%)	161 (87%)	24 (13%)	5 32
21	F	174/194 (90%)	157 (90%)	17 (10%)	10 44
22	K	88/96 (92%)	79 (90%)	9 (10%)	9 43
23	M	97/109 (89%)	91 (94%)	6 (6%)	23 64
24	P	105/117 (90%)	92 (88%)	13 (12%)	6 33
25	Q	117/119 (98%)	102 (87%)	15 (13%)	5 32
26	R	109/124 (88%)	92 (84%)	17 (16%)	3 24
27	S	128/129 (99%)	110 (86%)	18 (14%)	4 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	T	117/118 (99%)	107 (92%)	10 (8%)	13 52
29	U	96/107 (90%)	82 (85%)	14 (15%)	4 27
30	Z	60/88 (68%)	57 (95%)	3 (5%)	30 70
31	c	55/59 (93%)	49 (89%)	6 (11%)	8 40
32	d	46/48 (96%)	39 (85%)	7 (15%)	3 25
33	f	58/133 (44%)	52 (90%)	6 (10%)	9 42
34	g	265/272 (97%)	251 (95%)	14 (5%)	28 69
35	h	23/23 (100%)	20 (87%)	3 (13%)	5 32
36	i	83/130 (64%)	76 (92%)	7 (8%)	14 53
37	j	77/96 (80%)	72 (94%)	5 (6%)	21 63
All	All	4278/4720 (91%)	3748 (88%)	530 (12%)	10 33

All (530) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	6	THR
2	A	8	ASP
2	A	9	LEU
2	A	13	ASP
2	A	24	LEU
2	A	33	GLN
2	A	37	VAL
2	A	43	ASP
2	A	47	VAL
2	A	56	LYS
2	A	57	ILE
2	A	59	LEU
2	A	79	ARG
2	A	81	TYR
2	A	84	ARG
2	A	93	THR
2	A	108	THR
2	A	109	ASN
2	A	134	LYS
2	A	135	GLU
2	A	137	SER
2	A	146	LEU
2	A	147	THR

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Mol	Chain	Res	Type
2	A	173	ILE
2	A	177	LEU
2	A	198	MET
2	A	200	ASP
2	A	206	ASN
3	B	22	ASP
3	B	28	GLU
3	B	32	ILE
3	B	47	LEU
3	B	48	VAL
3	B	68	VAL
3	B	70	LEU
3	B	84	VAL
3	B	96	LEU
3	B	99	ASN
3	B	100	PHE
3	B	118	GLN
3	B	127	VAL
3	B	138	PHE
3	B	181	LEU
3	B	184	LEU
3	B	191	GLU
3	B	212	ILE
3	B	214	LYS
3	B	228	LEU
4	C	49	LEU
4	C	50	VAL
4	C	58	ILE
4	C	59	GLU
4	C	71	PHE
4	C	83	ASP
4	C	89	LYS
4	C	91	VAL
4	C	93	LYS
4	C	95	THR
4	C	99	GLN
4	C	100	ARG
4	C	108	VAL
4	C	109	VAL
4	C	122	THR
4	C	142	ILE
4	C	149	TRP

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Mol	Chain	Res	Type
4	C	159	LEU
4	C	163	THR
4	C	174	LEU
4	C	179	ARG
4	C	195	LEU
4	C	208	SER
4	C	233	ASN
4	C	235	TRP
4	C	241	THR
4	C	246	ASP
4	C	250	ASP
5	E	3	ARG
5	E	7	LYS
5	E	9	LEU
5	E	10	LYS
5	E	18	TRP
5	E	19	MET
5	E	21	ASP
5	E	23	LEU
5	E	37	LYS
5	E	38	LEU
5	E	42	LEU
5	E	45	ILE
5	E	77	ARG
5	E	79	ASP
5	E	92	LEU
5	E	123	LEU
5	E	131	LEU
5	E	133	LYS
5	E	139	VAL
5	E	142	HIS
5	E	143	ASP
5	E	153	ASN
5	E	156	VAL
5	E	170	THR
5	E	187	ARG
5	E	192	VAL
5	E	206	ASP
5	E	208	VAL
5	E	223	ASN
5	E	225	VAL
5	E	227	VAL

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Mol	Chain	Res	Type
5	E	245	LYS
5	E	248	ILE
5	E	250	GLU
6	G	12	THR
6	G	13	GLN
6	G	52	ILE
6	G	56	ASN
6	G	75	LEU
6	G	77	LEU
6	G	95	LYS
6	G	97	VAL
6	G	112	ILE
6	G	136	LYS
6	G	141	ILE
6	G	151	ASP
6	G	159	ARG
6	G	164	LYS
6	G	178	LEU
6	G	180	THR
6	G	182	GLN
6	G	189	GLN
6	G	190	GLN
6	G	215	ARG
7	H	11	GLN
7	H	16	LEU
7	H	24	PHE
7	H	27	LEU
7	H	33	GLU
7	H	47	ARG
7	H	60	VAL
7	H	66	SER
7	H	71	HIS
7	H	80	GLU
7	H	81	LEU
7	H	93	LEU
7	H	99	LEU
7	H	112	ARG
7	H	114	ARG
7	H	122	HIS
7	H	126	LEU
7	H	130	VAL
7	H	133	THR

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Mol	Chain	Res	Type
7	H	139	ARG
7	H	142	TYR
7	H	153	LEU
7	H	162	ILE
7	H	174	ASN
8	I	6	ASP
8	I	8	ARG
8	I	17	LYS
8	I	21	PHE
8	I	22	ARG
8	I	24	LYS
8	I	29	LEU
8	I	36	THR
8	I	58	LEU
8	I	62	THR
8	I	66	SER
8	I	72	VAL
8	I	75	LYS
8	I	76	THR
8	I	77	ARG
8	I	86	SER
8	I	96	LEU
8	I	138	LYS
8	I	157	VAL
8	I	158	ASP
8	I	170	ILE
8	I	176	GLN
8	I	179	ARG
8	I	183	TYR
8	I	190	LEU
9	J	17	ARG
9	J	19	TYR
9	J	28	LEU
9	J	37	LYS
9	J	49	LEU
9	J	66	ASP
9	J	69	ARG
9	J	70	LEU
9	J	86	LEU
9	J	93	LEU
9	J	94	ASP
9	J	97	LEU

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Mol	Chain	Res	Type
9	J	100	LYS
9	J	109	LEU
9	J	116	LEU
9	J	122	VAL
9	J	126	ARG
9	J	127	VAL
9	J	142	ASN
9	J	149	ARG
9	J	150	LEU
9	J	151	GLU
9	J	174	ARG
9	J	175	LYS
10	L	10	GLU
10	L	32	LYS
10	L	55	ASP
10	L	67	ARG
10	L	71	LEU
10	L	80	MET
10	L	83	THR
10	L	84	ILE
10	L	87	ARG
10	L	92	HIS
10	L	94	VAL
10	L	102	LYS
10	L	116	ARG
10	L	128	CYS
10	L	136	ARG
11	N	3	ARG
11	N	49	GLN
11	N	64	LYS
11	N	72	LEU
11	N	75	LEU
11	N	88	LEU
11	N	89	TYR
11	N	99	ARG
11	N	105	ASN
11	N	121	ARG
11	N	125	LEU
11	N	139	TRP
11	N	142	GLU
12	O	61	MET
12	O	67	VAL

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Mol	Chain	Res	Type
12	O	81	ILE
12	O	83	ILE
12	O	86	THR
12	O	102	LEU
13	V	1	MET
13	V	4	ASP
13	V	8	LEU
13	V	12	TYR
13	V	24	ILE
13	V	28	ASP
13	V	32	VAL
13	V	34	ILE
13	V	40	ASP
13	V	59	ILE
13	V	60	ARG
13	V	64	GLU
13	V	66	ASP
13	V	69	LEU
14	W	3	ARG
14	W	7	LEU
14	W	14	ILE
14	W	19	LYS
14	W	23	ARG
14	W	24	GLN
14	W	25	VAL
14	W	28	ARG
14	W	35	ILE
14	W	55	ASP
14	W	63	VAL
14	W	66	ASN
14	W	70	ASN
14	W	81	VAL
14	W	83	ILE
14	W	130	TYR
15	X	5	LYS
15	X	17	VAL
15	X	19	ARG
15	X	22	ASN
15	X	23	ARG
15	X	55	GLU
15	X	63	GLN
15	X	77	ILE

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Mol	Chain	Res	Type
15	X	84	THR
15	X	100	ASP
15	X	107	PHE
15	X	109	ARG
15	X	117	ILE
15	X	132	LEU
15	X	142	LYS
16	Y	5	ILE
16	Y	6	THR
16	Y	8	ARG
16	Y	20	ARG
16	Y	35	VAL
16	Y	38	ASP
16	Y	46	GLU
16	Y	51	GLU
16	Y	53	ASP
16	Y	57	VAL
16	Y	62	THR
16	Y	64	TYR
16	Y	69	SER
16	Y	74	LEU
16	Y	81	ASP
16	Y	98	GLU
16	Y	110	GLN
16	Y	112	LYS
16	Y	121	THR
16	Y	125	ILE
17	a	4	LYS
17	a	5	ARG
17	a	7	SER
17	a	18	VAL
17	a	26	CYS
17	a	29	SER
17	a	30	VAL
17	a	33	ASP
17	a	34	LYS
17	a	37	LYS
17	a	44	ILE
17	a	45	VAL
17	a	58	VAL
17	a	70	LYS
17	a	79	ILE

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Mol	Chain	Res	Type
17	a	80	HIS
17	a	85	ARG
17	a	90	THR
18	b	7	LEU
18	b	8	LEU
18	b	9	HIS
18	b	21	LEU
18	b	34	ASP
18	b	35	VAL
18	b	43	ILE
18	b	44	THR
18	b	54	VAL
18	b	56	CYS
18	b	81	ARG
19	e	14	VAL
19	e	22	GLU
19	e	33	ARG
19	e	37	ARG
19	e	38	LEU
20	D	5	ILE
20	D	7	LYS
20	D	11	LEU
20	D	17	PHE
20	D	51	ARG
20	D	64	ARG
20	D	91	VAL
20	D	101	GLN
20	D	113	LEU
20	D	122	VAL
20	D	135	GLU
20	D	141	LYS
20	D	143	ARG
20	D	157	LEU
20	D	162	GLN
20	D	165	ASN
20	D	178	ARG
20	D	179	GLN
20	D	186	VAL
20	D	189	MET
20	D	202	LEU
20	D	208	ILE
20	D	212	LYS

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Mol	Chain	Res	Type
20	D	223	LYS
21	F	42	ILE
21	F	65	GLN
21	F	70	ILE
21	F	92	VAL
21	F	101	MET
21	F	109	LYS
21	F	114	ARG
21	F	116	VAL
21	F	150	ARG
21	F	158	ARG
21	F	162	VAL
21	F	187	ARG
21	F	188	ASN
21	F	192	ILE
21	F	196	LEU
21	F	220	GLU
21	F	221	ARG
22	K	20	VAL
22	K	21	LEU
22	K	35	ILE
22	K	40	LEU
22	K	46	LEU
22	K	76	LEU
22	K	80	LEU
22	K	86	ILE
22	K	90	THR
23	M	43	LYS
23	M	45	LEU
23	M	55	LEU
23	M	69	GLN
23	M	105	LYS
23	M	107	VAL
24	P	17	TYR
24	P	32	ASP
24	P	40	ARG
24	P	43	ARG
24	P	52	LYS
24	P	57	MET
24	P	79	HIS
24	P	84	ILE
24	P	86	VAL

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Mol	Chain	Res	Type
24	P	89	MET
24	P	106	GLU
24	P	121	ILE
24	P	127	ARG
25	Q	8	GLN
25	Q	13	LYS
25	Q	19	VAL
25	Q	52	LEU
25	Q	53	LEU
25	Q	66	ARG
25	Q	85	ILE
25	Q	98	ASP
25	Q	102	LYS
25	Q	105	LEU
25	Q	122	ARG
25	Q	125	GLU
25	Q	128	LYS
25	Q	132	ARG
25	Q	142	TYR
26	R	6	THR
26	R	7	LYS
26	R	16	LEU
26	R	17	ILE
26	R	32	LYS
26	R	36	ASP
26	R	38	ILE
26	R	46	LEU
26	R	47	ARG
26	R	54	THR
26	R	66	VAL
26	R	74	GLN
26	R	84	TYR
26	R	88	VAL
26	R	98	ASP
26	R	100	LEU
26	R	109	LEU
27	S	12	GLN
27	S	16	ARG
27	S	25	ASN
27	S	34	THR
27	S	41	ARG
27	S	45	LEU

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Mol	Chain	Res	Type
27	S	49	LYS
27	S	52	VAL
27	S	62	THR
27	S	74	GLN
27	S	85	PHE
27	S	88	ARG
27	S	91	ASP
27	S	126	ARG
27	S	128	PHE
27	S	131	LEU
27	S	137	HIS
27	S	144	ARG
28	T	7	ARG
28	T	36	ILE
28	T	44	GLU
28	T	57	ARG
28	T	63	ARG
28	T	79	LEU
28	T	86	ARG
28	T	122	ARG
28	T	124	ILE
28	T	129	LEU
29	U	25	ASN
29	U	31	VAL
29	U	43	LYS
29	U	52	LYS
29	U	77	LYS
29	U	80	ASP
29	U	84	MET
29	U	85	ARG
29	U	86	ILE
29	U	92	ASP
29	U	94	GLU
29	U	103	ILE
29	U	114	VAL
29	U	118	ILE
30	Z	41	VAL
30	Z	60	VAL
30	Z	97	LYS
31	c	11	LYS
31	c	16	LEU
31	c	19	THR

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Mol	Chain	Res	Type
31	c	25	VAL
31	c	53	ILE
31	c	56	LEU
32	d	19	ARG
32	d	20	GLN
32	d	21	CYS
32	d	36	LEU
32	d	37	ASN
32	d	40	ARG
32	d	50	ILE
33	f	82	LYS
33	f	103	LEU
33	f	105	TYR
33	f	113	LYS
33	f	120	GLU
33	f	136	ARG
34	g	22	THR
34	g	26	THR
34	g	35	VAL
34	g	40	ASP
34	g	52	GLU
34	g	60	ARG
34	g	143	TYR
34	g	188	LEU
34	g	195	ILE
34	g	203	ASN
34	g	271	ASP
34	g	293	ASP
34	g	299	LEU
34	g	316	VAL
35	h	8	LYS
35	h	10	THR
35	h	12	ARG
36	i	31	GLU
36	i	39	THR
36	i	46	ARG
36	i	62	ARG
36	i	70	TRP
36	i	75	ASP
36	i	97	LEU
37	j	24	ASN
37	j	40	THR

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Mol	Chain	Res	Type
37	j	53	ARG
37	j	71	ASP
37	j	87	LYS

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

Mol	Chain	Res	Type
2	A	30	GLN
2	A	33	GLN
2	A	92	HIS
2	A	109	ASN
3	B	124	ASN
3	B	149	GLN
3	B	183	GLN
4	C	64	HIS
5	E	50	ASN
5	E	57	ASN
5	E	142	HIS
5	E	216	ASN
5	E	224	ASN
6	G	4	ASN
6	G	81	HIS
6	G	139	ASN
7	H	108	GLN
8	I	116	HIS
8	I	160	GLN
9	J	112	GLN
10	L	8	GLN
10	L	14	GLN
10	L	104	HIS
11	N	49	GLN
11	N	62	GLN
12	O	99	GLN
13	V	74	GLN
14	W	15	ASN
14	W	24	GLN
15	X	22	ASN
15	X	79	ASN
16	Y	15	ASN
16	Y	29	HIS
19	e	57	ASN
20	D	159	HIS

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Mol	Chain	Res	Type
21	F	102	ASN
21	F	106	ASN
21	F	188	ASN
24	P	114	HIS
25	Q	74	HIS
25	Q	83	GLN
25	Q	94	GLN
27	S	27	ASN
27	S	99	HIS
27	S	136	GLN
28	T	70	GLN
30	Z	95	HIS
32	d	10	HIS
34	g	226	GLN
36	i	112	ASN
37	j	43	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1799 (98%)	836 (47%)	132 (7%)

All (836) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	5	U
1	2	11	A
1	2	16	G
1	2	17	C
1	2	22	A
1	2	25	C
1	2	26	A
1	2	31	C
1	2	32	U
1	2	34	G
1	2	36	C
1	2	40	A
1	2	42	G

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Mol	Chain	Res	Type
1	2	45	U
1	2	46	A
1	2	47	A
1	2	48	G
1	2	50	C
1	2	51	A
1	2	55	A
1	2	56	U
1	2	57	G
1	2	58	U
1	2	59	C
1	2	60	U
1	2	61	A
1	2	62	A
1	2	63	G
1	2	67	A
1	2	68	A
1	2	69	G
1	2	71	A
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	76	A
1	2	77	U
1	2	78	A
1	2	79	C
1	2	80	A
1	2	81	G
1	2	84	A
1	2	86	A
1	2	90	C
1	2	93	A
1	2	104	A
1	2	105	A
1	2	109	G
1	2	111	U
1	2	114	C
1	2	115	G
1	2	123	G
1	2	124	A
1	2	125	U

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Mol	Chain	Res	Type
1	2	126	A
1	2	127	G
1	2	129	U
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	139	C
1	2	140	A
1	2	141	U
1	2	142	G
1	2	143	G
1	2	144	A
1	2	145	U
1	2	146	A
1	2	147	U
1	2	148	C
1	2	150	G
1	2	154	U
1	2	157	U
1	2	158	U
1	2	159	C
1	2	160	U
1	2	161	A
1	2	167	A
1	2	168	A
1	2	169	U
1	2	173	U
1	2	178	A
1	2	187	A
1	2	189	C
1	2	190	C
1	2	191	U
1	2	194	G
1	2	195	G
1	2	199	A
1	2	200	G
1	2	203	G
1	2	209	A

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Mol	Chain	Res	Type
1	2	210	U
1	2	217	A
1	2	218	A
1	2	220	A
1	2	225	A
1	2	226	U
1	2	228	U
1	2	230	U
1	2	231	U
1	2	232	C
1	2	233	G
1	2	234	G
1	2	237	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	245	G
1	2	248	U
1	2	249	C
1	2	251	U
1	2	256	A
1	2	258	U
1	2	260	U
1	2	264	A
1	2	265	A
1	2	266	U
1	2	270	A
1	2	272	G
1	2	273	G
1	2	275	C
1	2	276	U
1	2	278	G
1	2	279	U
1	2	280	G
1	2	282	U
1	2	287	A
1	2	288	U
1	2	289	G
1	2	292	U
1	2	294	A
1	2	298	A
1	2	300	A

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Mol	Chain	Res	Type
1	2	301	U
1	2	308	C
1	2	311	A
1	2	313	C
1	2	314	A
1	2	315	A
1	2	318	U
1	2	319	U
1	2	320	C
1	2	321	G
1	2	322	A
1	2	328	G
1	2	332	A
1	2	336	G
1	2	337	C
1	2	345	G
1	2	347	U
1	2	349	U
1	2	351	A
1	2	358	A
1	2	359	A
1	2	360	C
1	2	362	G
1	2	368	A
1	2	369	A
1	2	371	G
1	2	372	G
1	2	373	U
1	2	374	U
1	2	377	A
1	2	378	U
1	2	380	C
1	2	382	G
1	2	384	A
1	2	385	G
1	2	386	A
1	2	387	G
1	2	389	G
1	2	390	A
1	2	392	C
1	2	399	A
1	2	400	A

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Mol	Chain	Res	Type
1	2	401	C
1	2	403	G
1	2	411	A
1	2	412	U
1	2	415	A
1	2	416	A
1	2	417	G
1	2	421	G
1	2	422	G
1	2	423	C
1	2	424	A
1	2	425	G
1	2	427	A
1	2	433	G
1	2	434	C
1	2	438	U
1	2	439	U
1	2	440	A
1	2	442	C
1	2	443	C
1	2	444	A
1	2	447	C
1	2	448	C
1	2	452	U
1	2	453	U
1	2	456	G
1	2	458	G
1	2	459	A
1	2	460	G
1	2	467	A
1	2	468	C
1	2	469	A
1	2	473	A
1	2	474	A
1	2	476	A
1	2	477	A
1	2	478	C
1	2	479	G
1	2	480	A
1	2	481	U
1	2	483	C
1	2	489	C

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Mol	Chain	Res	Type
1	2	491	A
1	2	492	U
1	2	493	U
1	2	495	G
1	2	496	G
1	2	499	C
1	2	502	G
1	2	504	A
1	2	505	A
1	2	506	U
1	2	507	U
1	2	508	G
1	2	512	U
1	2	513	G
1	2	514	A
1	2	515	G
1	2	516	U
1	2	517	A
1	2	518	C
1	2	521	U
1	2	522	G
1	2	523	U
1	2	524	A
1	2	525	A
1	2	526	A
1	2	532	U
1	2	533	A
1	2	534	A
1	2	536	G
1	2	537	A
1	2	538	G
1	2	539	G
1	2	540	A
1	2	541	A
1	2	542	C
1	2	543	A
1	2	544	A
1	2	545	C
1	2	547	G
1	2	554	A
1	2	557	U
1	2	558	C

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Mol	Chain	Res	Type
1	2	563	G
1	2	564	C
1	2	565	C
1	2	566	A
1	2	567	G
1	2	568	C
1	2	571	C
1	2	573	G
1	2	577	U
1	2	578	A
1	2	580	U
1	2	581	U
1	2	584	A
1	2	587	U
1	2	593	A
1	2	594	G
1	2	600	A
1	2	605	A
1	2	607	U
1	2	608	U
1	2	609	G
1	2	610	U
1	2	614	A
1	2	618	A
1	2	619	A
1	2	622	A
1	2	623	G
1	2	628	U
1	2	634	A
1	2	635	A
1	2	637	U
1	2	638	U
1	2	640	G
1	2	641	G
1	2	642	G
1	2	646	G
1	2	648	U
1	2	649	U
1	2	651	U
1	2	653	C
1	2	654	G
1	2	655	G

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Mol	Chain	Res	Type
1	2	656	U
1	2	657	C
1	2	684	A
1	2	687	C
1	2	691	U
1	2	692	C
1	2	693	U
1	2	694	U
1	2	695	U
1	2	696	C
1	2	697	C
1	2	698	U
1	2	701	U
1	2	702	G
1	2	704	C
1	2	705	U
1	2	706	A
1	2	707	A
1	2	709	C
1	2	710	U
1	2	712	U
1	2	714	C
1	2	715	U
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	724	G
1	2	725	U
1	2	727	C
1	2	728	A
1	2	732	G
1	2	734	A
1	2	735	C
1	2	736	C
1	2	738	G
1	2	741	C
1	2	742	U
1	2	743	U

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Mol	Chain	Res	Type
1	2	747	C
1	2	753	A
1	2	754	A
1	2	765	G
1	2	766	U
1	2	767	U
1	2	768	C
1	2	771	A
1	2	774	A
1	2	778	G
1	2	780	A
1	2	781	A
1	2	782	G
1	2	783	C
1	2	785	C
1	2	786	G
1	2	787	A
1	2	788	A
1	2	789	U
1	2	791	U
1	2	793	U
1	2	794	U
1	2	795	A
1	2	796	G
1	2	802	A
1	2	811	A
1	2	812	U
1	2	813	A
1	2	814	G
1	2	817	C
1	2	818	G
1	2	819	U
1	2	820	U
1	2	821	U
1	2	822	G
1	2	825	U
1	2	827	U
1	2	828	A
1	2	829	U
1	2	830	U
1	2	831	U
1	2	832	U

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Mol	Chain	Res	Type
1	2	837	G
1	2	839	U
1	2	840	U
1	2	843	A
1	2	845	G
1	2	853	U
1	2	855	A
1	2	857	G
1	2	860	U
1	2	861	A
1	2	862	A
1	2	863	U
1	2	872	U
1	2	875	G
1	2	876	G
1	2	881	U
1	2	889	C
1	2	895	U
1	2	896	C
1	2	897	A
1	2	904	A
1	2	905	A
1	2	907	U
1	2	908	U
1	2	910	U
1	2	912	G
1	2	913	G
1	2	915	U
1	2	919	U
1	2	920	U
1	2	927	U
1	2	931	U
1	2	932	A
1	2	933	C
1	2	934	U
1	2	939	A
1	2	941	G
1	2	943	A
1	2	944	U
1	2	945	U
1	2	946	U
1	2	947	G

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Mol	Chain	Res	Type
1	2	948	C
1	2	950	A
1	2	953	G
1	2	958	U
1	2	959	U
1	2	965	A
1	2	969	A
1	2	970	A
1	2	972	A
1	2	974	C
1	2	978	A
1	2	981	U
1	2	982	A
1	2	983	G
1	2	984	G
1	2	985	G
1	2	986	G
1	2	987	A
1	2	989	C
1	2	991	A
1	2	993	G
1	2	994	A
1	2	997	A
1	2	1002	A
1	2	1003	U
1	2	1011	U
1	2	1015	C
1	2	1018	A
1	2	1019	A
1	2	1020	C
1	2	1022	A
1	2	1023	U
1	2	1024	A
1	2	1025	A
1	2	1026	A
1	2	1027	C
1	2	1028	U
1	2	1029	A
1	2	1030	U
1	2	1031	G
1	2	1033	C
1	2	1034	G

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Mol	Chain	Res	Type
1	2	1038	A
1	2	1039	G
1	2	1041	G
1	2	1042	A
1	2	1048	U
1	2	1050	G
1	2	1051	U
1	2	1052	G
1	2	1057	U
1	2	1058	C
1	2	1059	U
1	2	1060	U
1	2	1062	U
1	2	1065	C
1	2	1071	C
1	2	1074	C
1	2	1075	A
1	2	1079	U
1	2	1080	A
1	2	1081	C
1	2	1082	G
1	2	1083	A
1	2	1085	A
1	2	1086	A
1	2	1090	A
1	2	1091	A
1	2	1092	A
1	2	1095	C
1	2	1096	U
1	2	1097	U
1	2	1099	G
1	2	1100	G
1	2	1103	U
1	2	1108	G
1	2	1113	G
1	2	1115	A
1	2	1118	G
1	2	1119	U
1	2	1121	G
1	2	1125	G
1	2	1130	A
1	2	1133	C

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Mol	Chain	Res	Type
1	2	1137	A
1	2	1141	A
1	2	1142	A
1	2	1145	G
1	2	1146	A
1	2	1149	G
1	2	1150	A
1	2	1152	G
1	2	1153	G
1	2	1157	C
1	2	1158	C
1	2	1161	C
1	2	1162	A
1	2	1165	A
1	2	1166	G
1	2	1167	U
1	2	1173	C
1	2	1174	U
1	2	1179	C
1	2	1181	U
1	2	1182	A
1	2	1184	U
1	2	1188	A
1	2	1189	C
1	2	1193	A
1	2	1194	C
1	2	1195	A
1	2	1196	C
1	2	1198	G
1	2	1199	G
1	2	1201	A
1	2	1202	A
1	2	1203	A
1	2	1204	C
1	2	1205	U
1	2	1206	C
1	2	1207	A
1	2	1211	G
1	2	1212	G
1	2	1215	C
1	2	1216	A
1	2	1217	G

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Mol	Chain	Res	Type
1	2	1218	A
1	2	1222	A
1	2	1223	A
1	2	1224	U
1	2	1225	A
1	2	1226	A
1	2	1227	G
1	2	1228	G
1	2	1229	A
1	2	1232	G
1	2	1234	C
1	2	1236	G
1	2	1237	A
1	2	1240	G
1	2	1241	A
1	2	1242	G
1	2	1243	A
1	2	1244	G
1	2	1249	U
1	2	1250	U
1	2	1254	G
1	2	1255	A
1	2	1256	U
1	2	1259	U
1	2	1263	G
1	2	1265	U
1	2	1268	U
1	2	1269	G
1	2	1272	G
1	2	1274	A
1	2	1275	U
1	2	1282	U
1	2	1284	U
1	2	1287	G
1	2	1293	G
1	2	1294	G
1	2	1296	G
1	2	1305	C
1	2	1306	U
1	2	1311	A
1	2	1313	U
1	2	1314	U

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Mol	Chain	Res	Type
1	2	1316	C
1	2	1317	G
1	2	1320	A
1	2	1321	A
1	2	1324	A
1	2	1336	A
1	2	1337	C
1	2	1339	U
1	2	1343	A
1	2	1344	A
1	2	1345	A
1	2	1346	U
1	2	1347	A
1	2	1348	G
1	2	1350	G
1	2	1351	U
1	2	1353	G
1	2	1355	U
1	2	1359	A
1	2	1360	C
1	2	1361	U
1	2	1362	U
1	2	1363	G
1	2	1364	C
1	2	1366	G
1	2	1369	U
1	2	1370	G
1	2	1371	A
1	2	1380	A
1	2	1381	G
1	2	1383	G
1	2	1386	A
1	2	1387	C
1	2	1388	U
1	2	1391	C
1	2	1393	G
1	2	1396	U
1	2	1397	C
1	2	1398	A
1	2	1400	G
1	2	1410	G
1	2	1411	U

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Mol	Chain	Res	Type
1	2	1412	U
1	2	1413	U
1	2	1416	G
1	2	1422	A
1	2	1425	A
1	2	1426	G
1	2	1428	U
1	2	1429	C
1	2	1430	U
1	2	1431	G
1	2	1432	U
1	2	1433	G
1	2	1434	A
1	2	1441	U
1	2	1442	A
1	2	1443	G
1	2	1444	A
1	2	1446	G
1	2	1449	C
1	2	1450	U
1	2	1455	C
1	2	1456	G
1	2	1457	C
1	2	1458	A
1	2	1460	G
1	2	1461	C
1	2	1463	C
1	2	1464	G
1	2	1467	A
1	2	1469	A
1	2	1470	C
1	2	1471	U
1	2	1475	G
1	2	1476	G
1	2	1477	A
1	2	1484	G
1	2	1485	A
1	2	1487	U
1	2	1488	A
1	2	1489	C
1	2	1490	A
1	2	1491	A

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Mol	Chain	Res	Type
1	2	1492	C
1	2	1494	U
1	2	1495	U
1	2	1498	C
1	2	1499	C
1	2	1502	G
1	2	1503	A
1	2	1504	G
1	2	1509	G
1	2	1510	G
1	2	1512	U
1	2	1513	A
1	2	1514	A
1	2	1515	U
1	2	1519	G
1	2	1521	G
1	2	1522	A
1	2	1527	C
1	2	1531	C
1	2	1534	G
1	2	1535	C
1	2	1536	U
1	2	1537	G
1	2	1539	G
1	2	1543	A
1	2	1544	G
1	2	1548	A
1	2	1552	U
1	2	1554	A
1	2	1555	U
1	2	1557	A
1	2	1563	C
1	2	1566	C
1	2	1570	G
1	2	1571	A
1	2	1572	G
1	2	1573	G
1	2	1579	C
1	2	1580	U
1	2	1581	A
1	2	1582	G
1	2	1583	U

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Mol	Chain	Res	Type
1	2	1588	G
1	2	1593	U
1	2	1594	C
1	2	1595	A
1	2	1597	C
1	2	1598	A
1	2	1599	G
1	2	1600	C
1	2	1602	U
1	2	1603	G
1	2	1605	G
1	2	1607	U
1	2	1612	A
1	2	1614	G
1	2	1617	C
1	2	1626	U
1	2	1633	A
1	2	1634	C
1	2	1636	G
1	2	1637	C
1	2	1638	C
1	2	1641	U
1	2	1646	A
1	2	1648	U
1	2	1650	C
1	2	1654	U
1	2	1655	U
1	2	1656	G
1	2	1657	A
1	2	1658	A
1	2	1660	G
1	2	1662	C
1	2	1667	U
1	2	1674	U
1	2	1678	G
1	2	1679	A
1	2	1680	U
1	2	1682	U
1	2	1685	U
1	2	1686	U
1	2	1687	A
1	2	1688	G

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Mol	Chain	Res	Type
1	2	1689	A
1	2	1692	A
1	2	1693	G
1	2	1694	G
1	2	1695	G
1	2	1696	G
1	2	1697	G
1	2	1698	C
1	2	1699	A
1	2	1700	A
1	2	1701	C
1	2	1702	U
1	2	1703	C
1	2	1704	C
1	2	1705	A
1	2	1706	U
1	2	1707	C
1	2	1709	C
1	2	1710	A
1	2	1711	G
1	2	1712	A
1	2	1724	G
1	2	1725	G
1	2	1728	A
1	2	1729	A
1	2	1730	A
1	2	1733	U
1	2	1734	G
1	2	1737	C
1	2	1738	A
1	2	1740	U
1	2	1742	A
1	2	1743	G
1	2	1744	A
1	2	1747	A
1	2	1750	U
1	2	1753	A
1	2	1754	A
1	2	1755	G
1	2	1758	G
1	2	1759	U
1	2	1760	A

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Mol	Chain	Res	Type
1	2	1763	A
1	2	1764	A
1	2	1765	G
1	2	1766	G
1	2	1767	U
1	2	1769	U
1	2	1770	C
1	2	1771	C
1	2	1778	G
1	2	1780	A
1	2	1781	C
1	2	1784	G
1	2	1787	G
1	2	1788	A
1	2	1789	A
1	2	1790	G
1	2	1791	G
1	2	1792	A
1	2	1793	U
1	2	1794	C
1	2	1796	U
1	2	1797	U

All (132) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	25	C
1	2	44	U
1	2	45	U
1	2	66	U
1	2	68	A
1	2	72	A
1	2	73	U
1	2	80	A
1	2	103	A
1	2	129	U
1	2	130	C
1	2	131	C
1	2	135	A
1	2	139	C
1	2	140	A

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Mol	Chain	Res	Type
1	2	141	U
1	2	145	U
1	2	146	A
1	2	157	U
1	2	186	G
1	2	190	C
1	2	209	A
1	2	216	A
1	2	217	A
1	2	230	U
1	2	231	U
1	2	232	C
1	2	239	C
1	2	266	U
1	2	275	C
1	2	277	U
1	2	279	U
1	2	300	A
1	2	318	U
1	2	320	C
1	2	321	G
1	2	398	A
1	2	422	G
1	2	437	A
1	2	451	A
1	2	452	U
1	2	453	U
1	2	497	G
1	2	538	G
1	2	542	C
1	2	564	C
1	2	566	A
1	2	577	U
1	2	593	A
1	2	695	U
1	2	700	C
1	2	704	C
1	2	720	G
1	2	721	U
1	2	724	G
1	2	737	A
1	2	740	A

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Mol	Chain	Res	Type
1	2	742	U
1	2	747	C
1	2	809	G
1	2	812	U
1	2	818	G
1	2	827	U
1	2	828	A
1	2	839	U
1	2	854	A
1	2	896	C
1	2	907	U
1	2	912	G
1	2	1015	C
1	2	1025	A
1	2	1051	U
1	2	1056	U
1	2	1080	A
1	2	1081	C
1	2	1095	C
1	2	1099	G
1	2	1107	G
1	2	1149	G
1	2	1157	C
1	2	1161	C
1	2	1173	C
1	2	1195	A
1	2	1203	A
1	2	1206	C
1	2	1216	A
1	2	1226	A
1	2	1241	A
1	2	1243	A
1	2	1244	G
1	2	1252	U
1	2	1255	A
1	2	1273	C
1	2	1315	G
1	2	1320	A
1	2	1343	A
1	2	1346	U
1	2	1380	A
1	2	1412	U

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Mol	Chain	Res	Type
1	2	1424	C
1	2	1432	U
1	2	1445	C
1	2	1460	G
1	2	1469	A
1	2	1470	C
1	2	1491	A
1	2	1501	A
1	2	1515	U
1	2	1519	G
1	2	1521	G
1	2	1534	G
1	2	1535	C
1	2	1555	U
1	2	1556	U
1	2	1570	G
1	2	1571	A
1	2	1580	U
1	2	1598	A
1	2	1613	C
1	2	1632	C
1	2	1655	U
1	2	1678	G
1	2	1711	G
1	2	1725	G
1	2	1743	G
1	2	1759	U
1	2	1765	G
1	2	1770	C
1	2	1778	G
1	2	1788	A
1	2	1792	A

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

Of 70 ligands modelled in this entry, 70 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.