wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:30 PM BST

PDB ID	:	3J7Y
EMDB ID:	:	EMD-2762
Title	:	Structure of the large ribosomal subunit from human mitochondria
Authors	:	Brown, A.; Amunts, A.; Bai, X.C.; Sugimoto, Y.; Edwards, P.C.; Murshudov, G.; Scheres, S.H.W.; Ramakrishnan, V.
Deposited on	:	2014-08-26
Resolution	:	3.40 Å(reported)

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

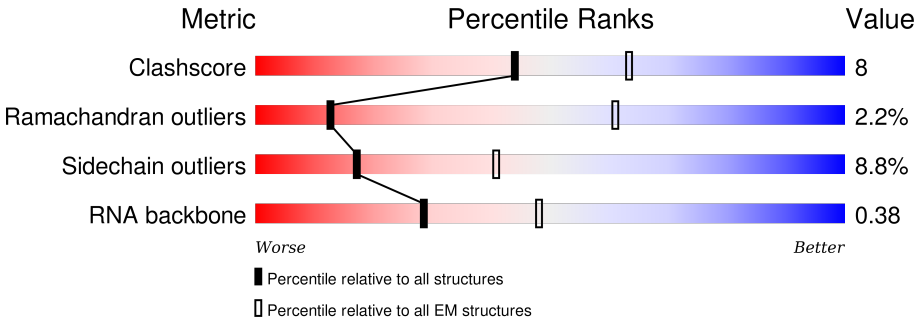
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 3.40 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	A	1559	36% 43% 14% • 6%
2	B	73	38% 29% 11% 22%
3	D	305	65% 11% • 23%
4	E	348	67% 18% • 14%
5	F	311	61% 19% • 20%
6	H	267	28% 7% 64%
7	I	261	44% 13% • 39%
8	J	192	56% 14% • 27%

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Mol	Chain	Length	Quality of chain
9	K	178	78% 19%
10	L	145	64% 15% 21%
11	M	296	77% 17%
12	N	251	69% 11% 18%
13	O	175	59% 22% 5% 13%
14	P	179	52% 20% 26%
15	Q	292	52% 15% 30%
16	R	149	77% 17% 6%
17	S	205	62% 12% 24%
18	T	212	59% 17% 22%
19	U	153	54% 18% 27%
20	V	216	73% 14% 13%
21	W	148	51% 19% 28%
22	X	256	76% 15% 5%
23	Y	250	54% 15% 30%
24	Z	161	59% 16% 25%
25	0	188	35% 15% 48%
26	1	65	60% 17% 20%
27	2	92	38% 8% 53%
28	3	188	42% 7% 49%
29	4	103	23% 10% 65%
30	5	423	65% 21% 11%
31	6	380	67% 16% 14%
32	7	338	67% 12% 21%
33	8	206	25% 72%

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Mol	Chain	Length	Quality of chain
34	9	137	64% 15% 20%
35	a	142	25% 73%
36	b	155	85% 10% 5%
37	c	332	76% 7% 17%
38	d	306	50% 47%
39	e	279	41% 6% 52%
40	f	211	41% 55%
41	g	166	69% 8% 22%
42	h	158	54% 9% 37%
43	i	128	64% 10% 25%
44	j	123	63% 6% 31%
45	k	112	64% 10% 25%
46	o	102	80% 11% 8%
47	p	206	35% 5% 60%
48	q	222	55% 42%
49	r	196	66% 9% 26%
50	s	439	76% 8% 16%
51	t	127	97%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	ZN	0	200	-	-	X	-

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 94121 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1472	31261	14025	5642	10122	1472	0	0

- Molecule 2 is a RNA chain called mt-tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	57	1211	543	217	394	57	0	0

- Molecule 3 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	236	1842	1145	373	315	9	0	0

- Molecule 4 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	300	2365	1523	410	422	10	0	0

- Molecule 5 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	250	2013	1294	365	348	6	0	0

- Molecule 6 is a protein called bL9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	H	95	784	498	152	134	0	0

- Molecule 7 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 8 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	140	Total	C	N	O	S	0	0
			1061	680	192	187	2		

- Molecule 9 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 10 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 11 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 12 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	205	Total	C	N	O	S	0	0
			1654	1056	308	280	10		

- Molecule 13 is a protein called bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 14 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	133	Total	C	N	O	S	0	0
			1080	677	209	189	5		

- Molecule 15 is a protein called bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	204	Total	C	N	O	S	0	0
			1704	1094	303	299	8		

- Molecule 16 is a protein called bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 17 is a protein called bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	156	Total	C	N	O	S	0	0
			1251	806	222	219	4		

- Molecule 18 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 19 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	111	Total	C	N	O	S	0	0
			922	591	176	153	2		

- Molecule 20 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	189	Total	C	N	O	S	0	0
			1551	987	278	278	8		

- Molecule 21 is a protein called bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	107	Total	C	N	O	S	0	0
			842	542	158	139	3		

- Molecule 22 is a protein called bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	243	Total	C	N	O	S	0	0
			2027	1310	350	362	5		

- Molecule 23 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 24 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 25 is a protein called bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	98	Total	C	N	O	S	0	0
			803	501	159	137	6		

- Molecule 26 is a protein called bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 27 is a protein called bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	43	Total	C	N	O	S	0	0
			351	218	76	56	1		

- Molecule 28 is a protein called bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 29 is a protein called bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	36	Total	C	N	O	S	0	0
			322	203	70	46	3		

- Molecule 30 is a protein called mL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	376	Total	C	N	O	S	0	0
			3064	1987	529	538	10		

- Molecule 31 is a protein called mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	325	Total	C	N	O	S	0	0
			2636	1692	465	470	9		

- Molecule 32 is a protein called mL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7	266	Total	C	N	O	S	0	0
			2158	1383	371	388	16		

- Molecule 33 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	8	57	Total	C	N	O	S	0	0
			482	302	86	92	2		

- Molecule 34 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	9	109	Total	C	N	O	S	0	0
			873	565	152	154	2		

- Molecule 35 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	39	Total	C	N	O	S	0	0
			343	217	68	55	3		

- Molecule 36 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 37 is a protein called mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 38 is a protein called mL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	162	Total	C	N	O	S	0	0
			1347	870	234	235	8		

- Molecule 39 is a protein called mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	134	Total	C	N	O	S	0	0
			1082	690	193	196	3		

- Molecule 40 is a protein called mL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	95	Total	C	N	O	S	0	0
			703	448	119	133	3		

- Molecule 41 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	129	Total	C	N	O	S	0	0
			1067	690	185	190	2		

- Molecule 42 is a protein called mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	100	Total	C	N	O	S	0	0
			827	524	146	155	2		

- Molecule 43 is a protein called mL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	96	Total	C	N	O	S	0	0
			816	526	161	125	4		

- Molecule 44 is a protein called mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	85	Total	C	N	O	S	0	0
			684	423	133	126	2		

- Molecule 45 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	84	Total	C	N	O	S	0	0
			655	407	122	121	5		

- Molecule 46 is a protein called mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	94	Total	C	N	O	S	0	0
			797	501	165	128	3		

- Molecule 47 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	83	Total	C	N	O	S	0	0
			674	421	125	125	3		

- Molecule 48 is a protein called CRIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 49 is a protein called bS18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

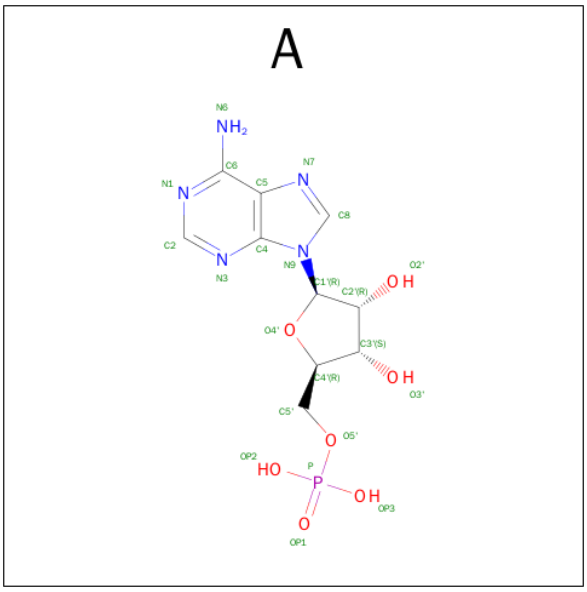
- Molecule 50 is a protein called mS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 51 is a protein called unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	t	123	Total	C	N	O	0	0
			615	369	123	123		

- Molecule 52 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					AltConf
52	A	1	Total	C	N	O	P	0
			22	10	5	6	1	

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	A	65	Total	Mg	0
			65	65	

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Mol	Chain	Residues	Atoms	AltConf
53	E	1	Total Mg 1 1	0

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

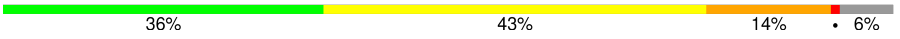
Mol	Chain	Residues	Atoms	AltConf
54	0	1	Total Zn 1 1	0
54	r	1	Total Zn 1 1	0
54	4	1	Total Zn 1 1	0

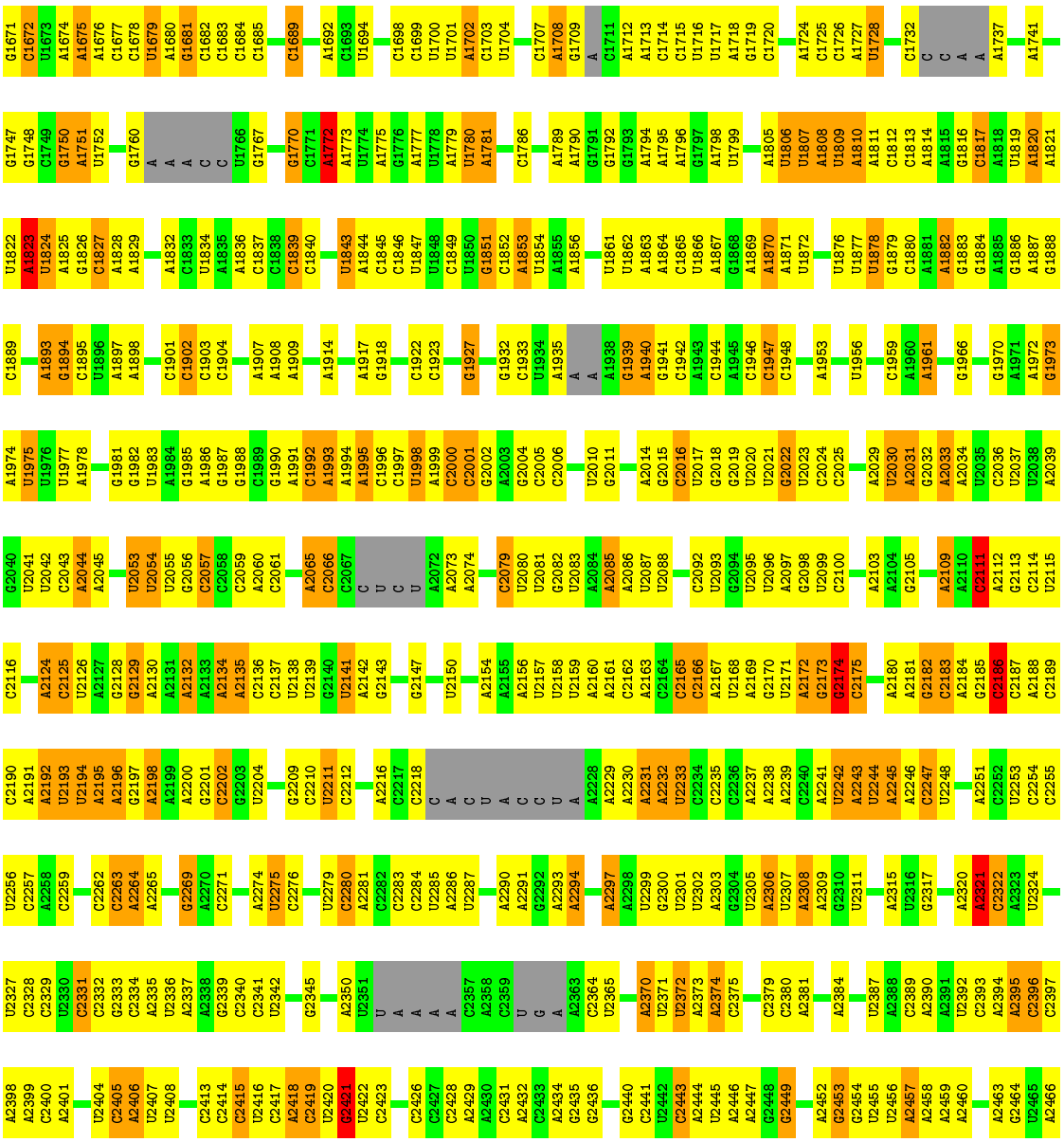
3 Residue-property plots (i)

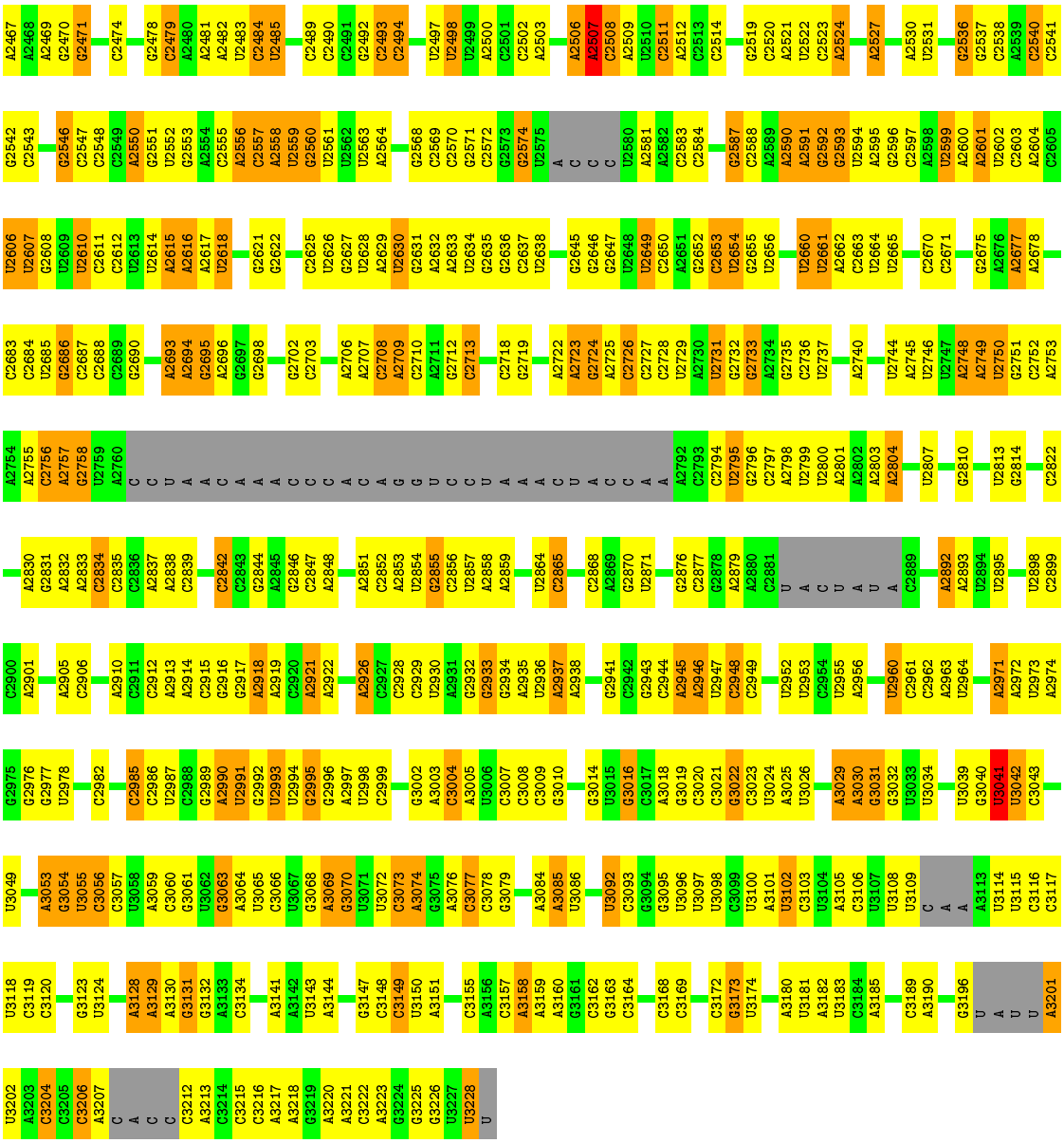
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

- Molecule 1: 16S rRNA

Chain A:

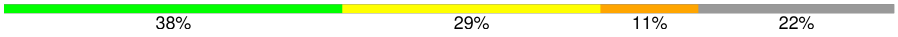


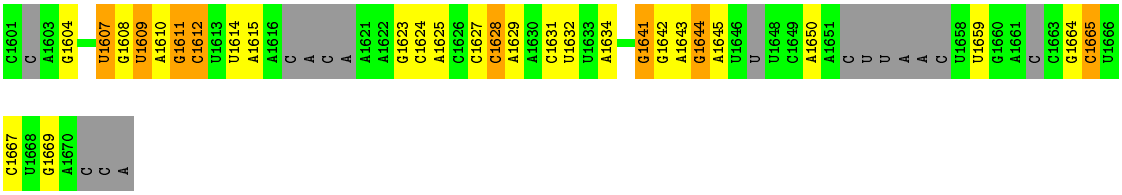




- Molecule 2: mt-tRNAVal

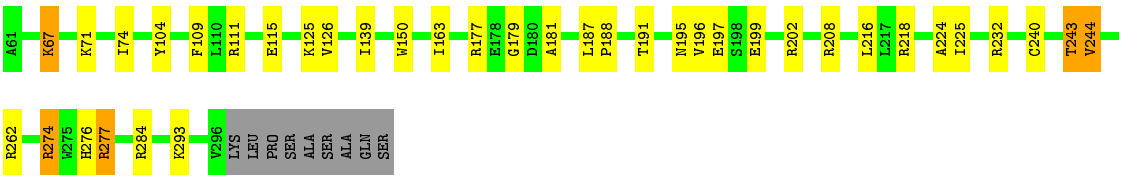
Chain B:





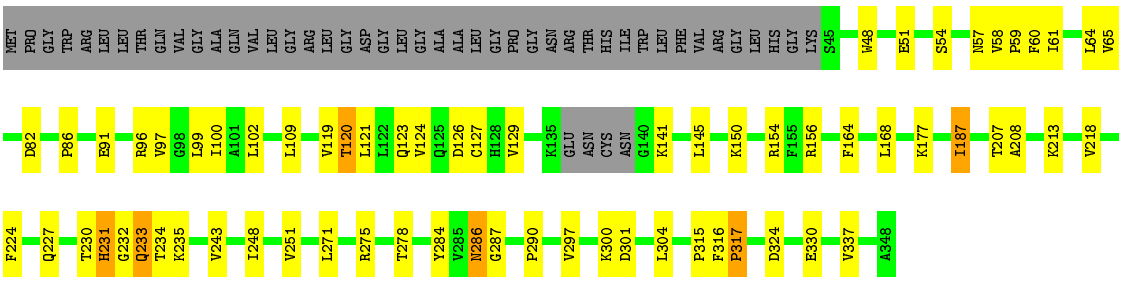
- Molecule 3: uL2

Chain D:



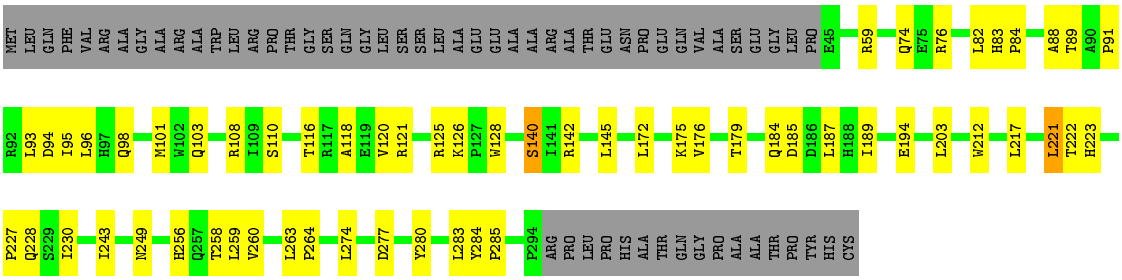
- Molecule 4: uL3

Chain E:



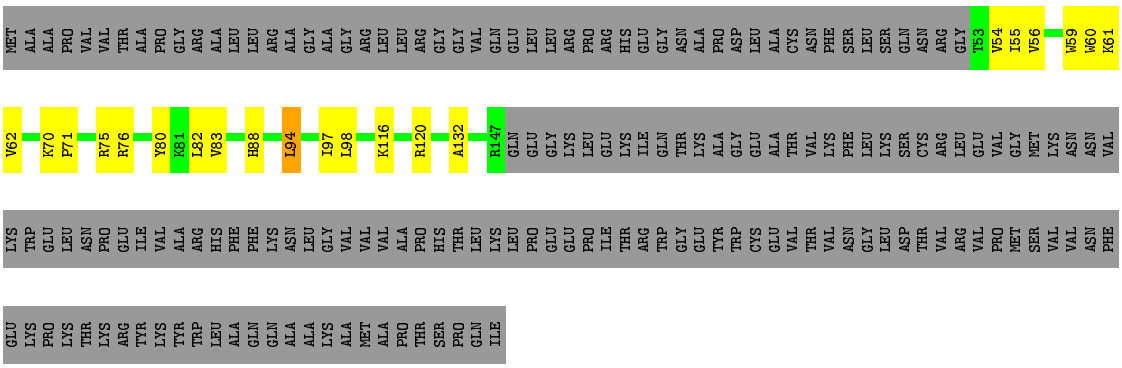
- Molecule 5: uL4

Chain F:



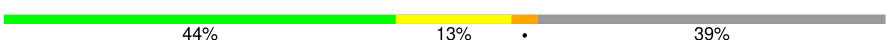
- Molecule 6: bL9

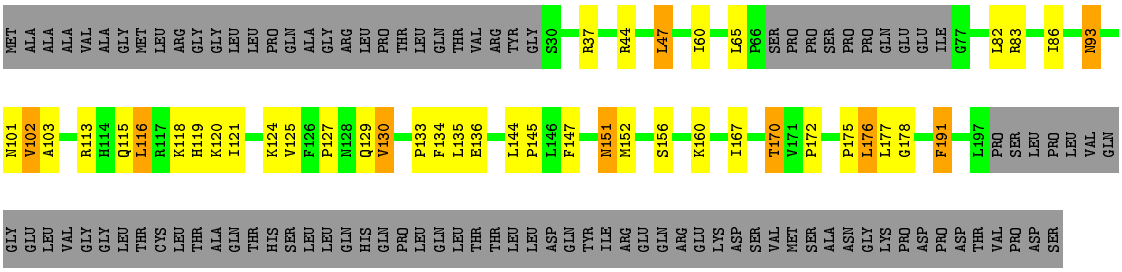
Chain H:



- Molecule 7: uL10

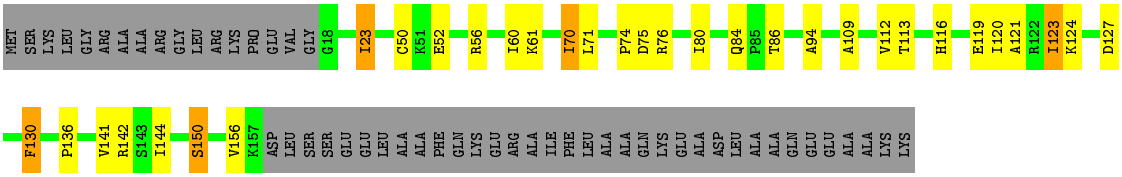
Chain I:





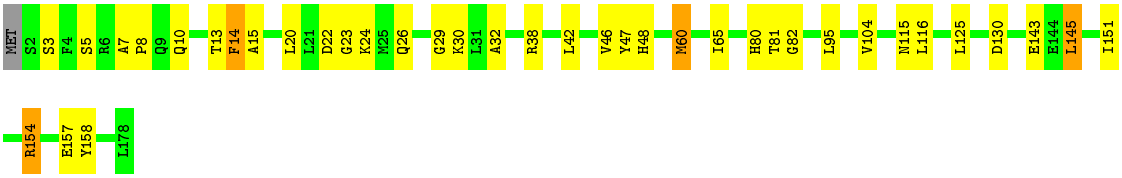
- Molecule 8: uL11

Chain J:



- Molecule 9: uL13

Chain K:

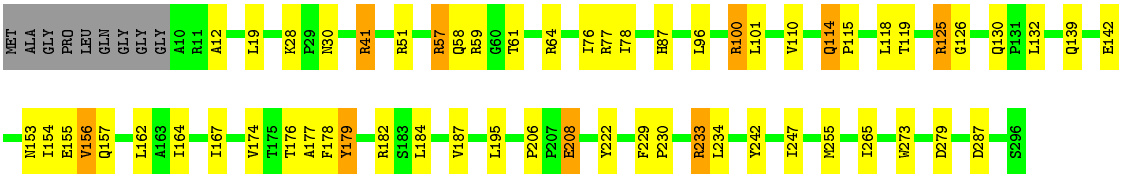


- Molecule 10: uL14

Chain L:

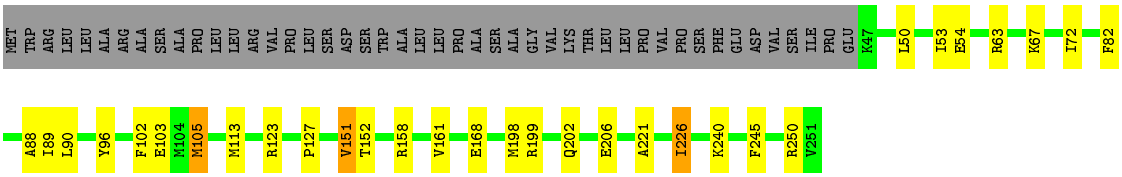
- Molecule 11: uL15

Chain M:



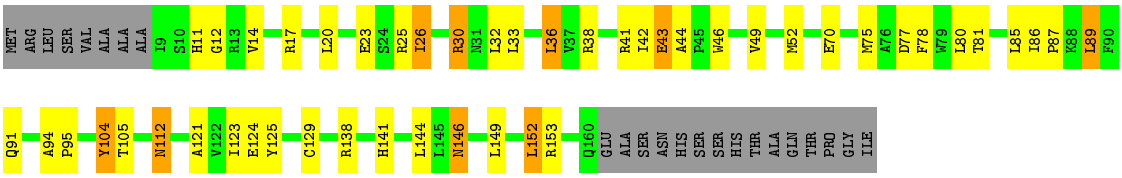
- Molecule 12: uL16

Chain N:



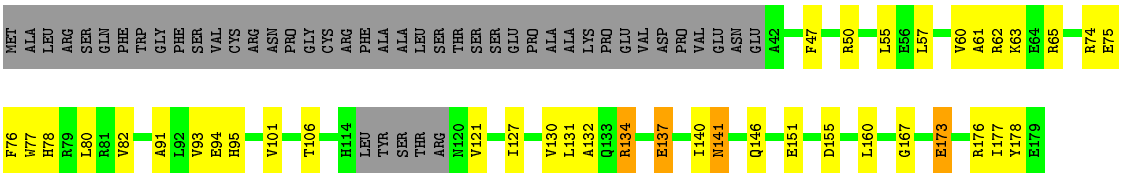
- Molecule 13: bL17

Chain O:



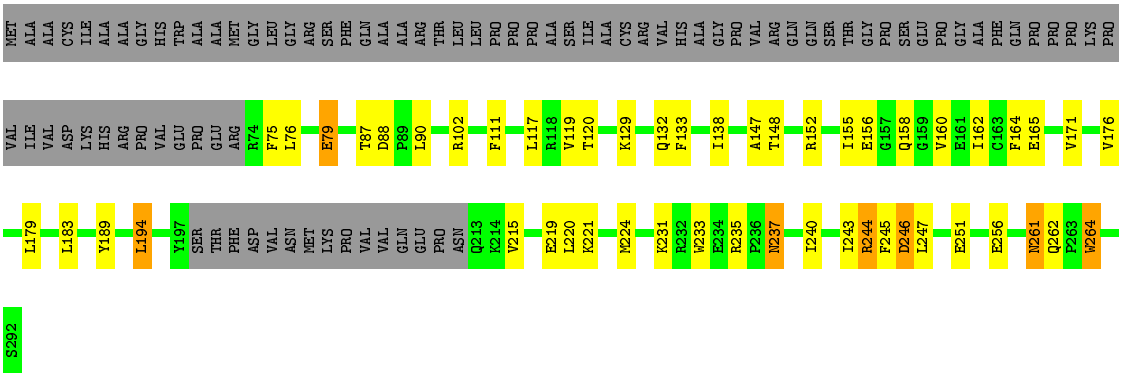
- Molecule 14: uL18

Chain P:



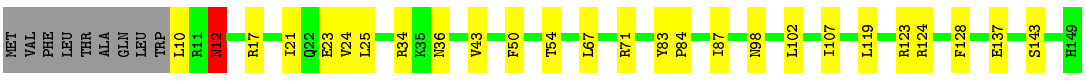
- Molecule 15: bL19

Chain Q:



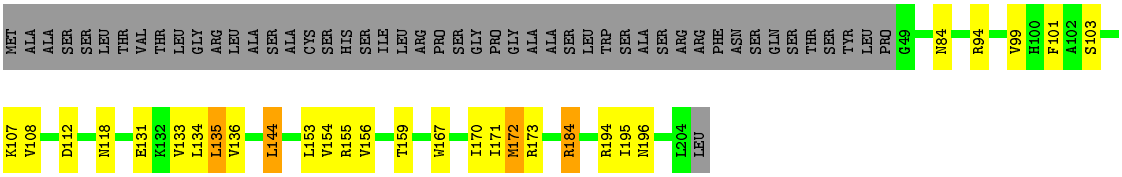
- Molecule 16: bL20

Chain R:



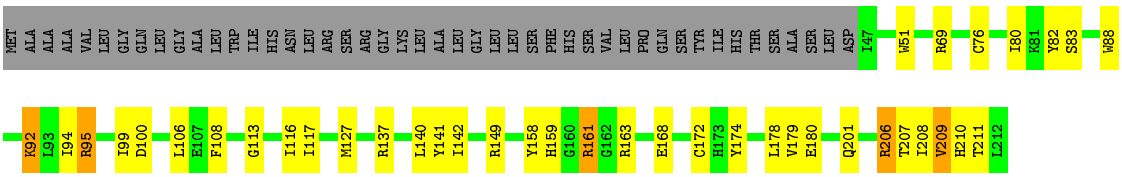
- Molecule 17: bL21

Chain S:



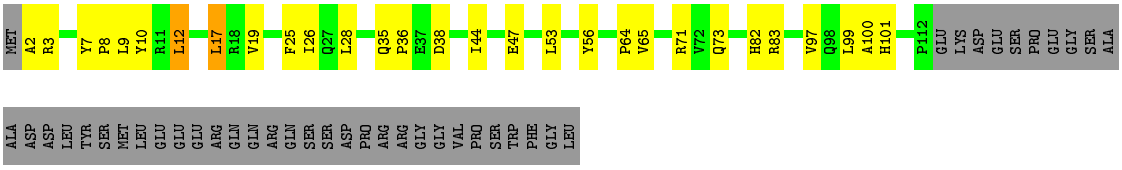
- Molecule 18: uL22

Chain T:



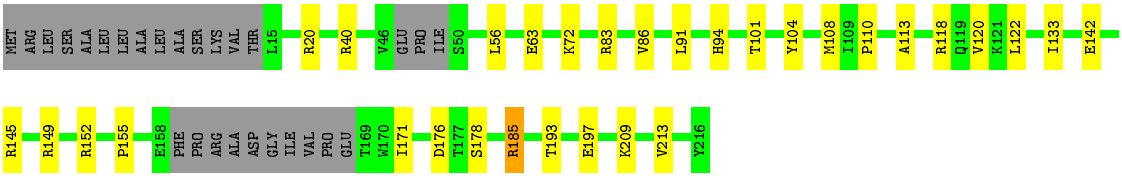
- Molecule 19: uL23

Chain U:



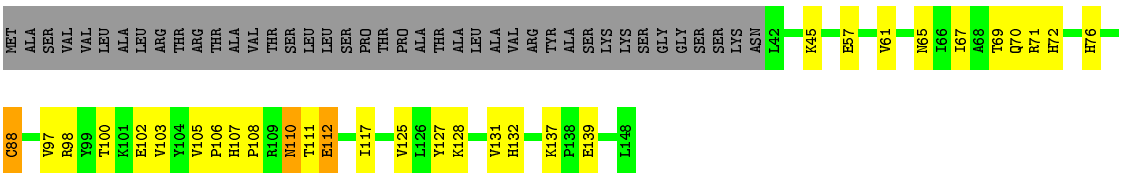
- Molecule 20: uL24

Chain V:



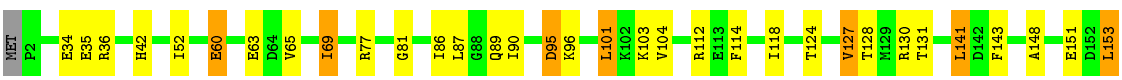
- Molecule 21: bL27

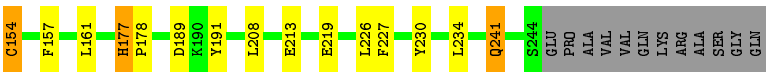
Chain W:



- Molecule 22: bL28

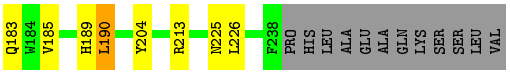
Chain X:





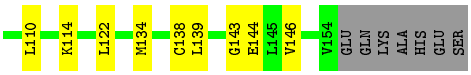
- Molecule 23: uL29

Chain Y:



- Molecule 24: uL30

Chain Z:



- Molecule 25: bL32

Chain 0:

- Molecule 26: bL33

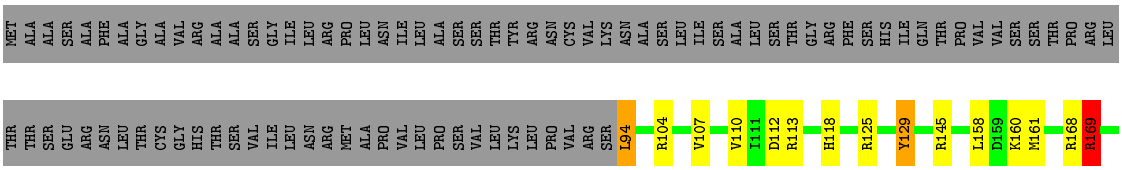
Chain 1:

- Molecule 27: bL34

Chain 2:

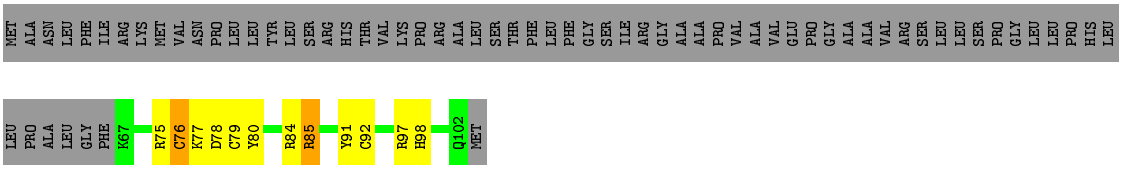
- Molecule 28: bL35

Chain 3:



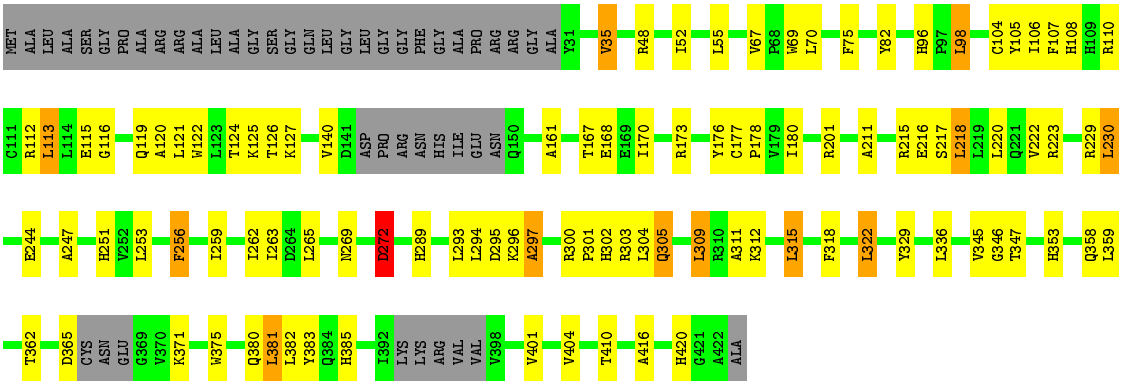
- Molecule 29: bL36

Chain 4:



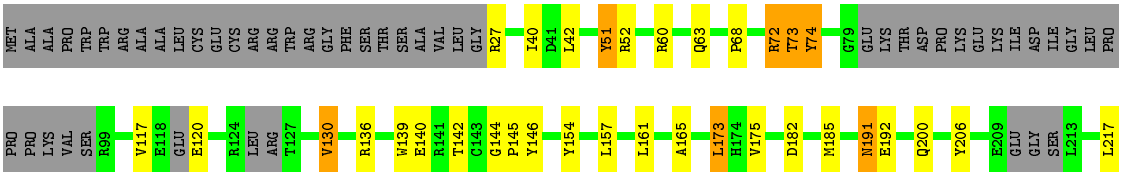
- Molecule 30: mL37

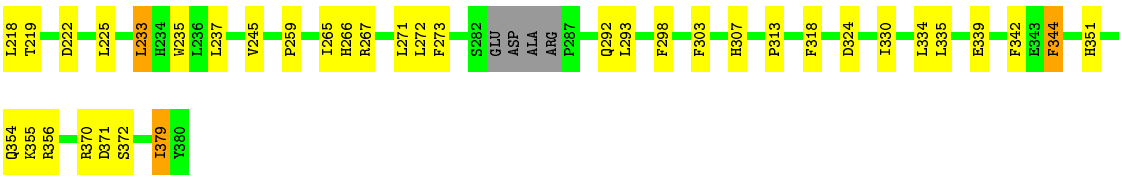
Chain 5:



- Molecule 31: mL38

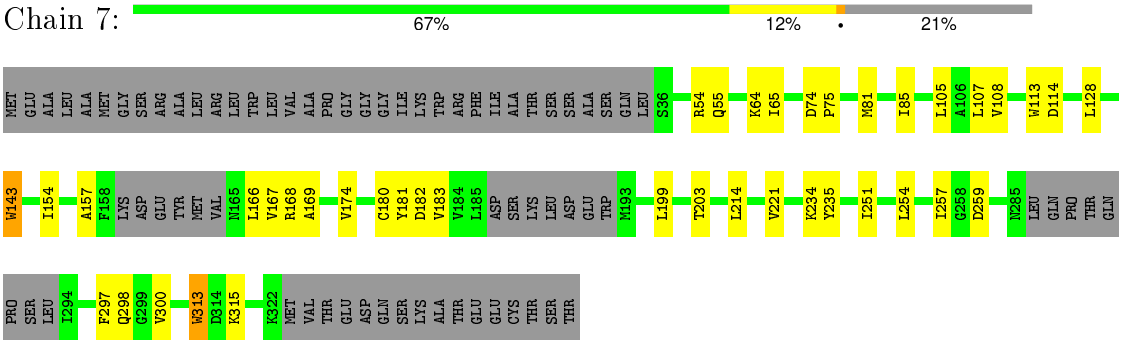
Chain 6:





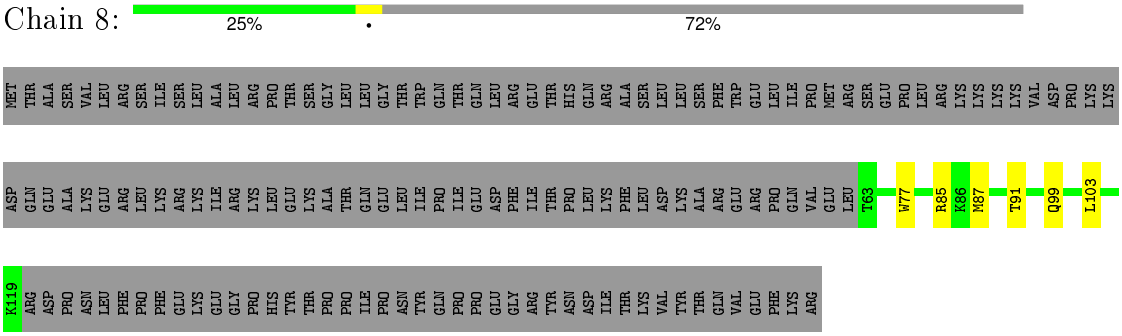
- Molecule 32: mL39

Chain 7:



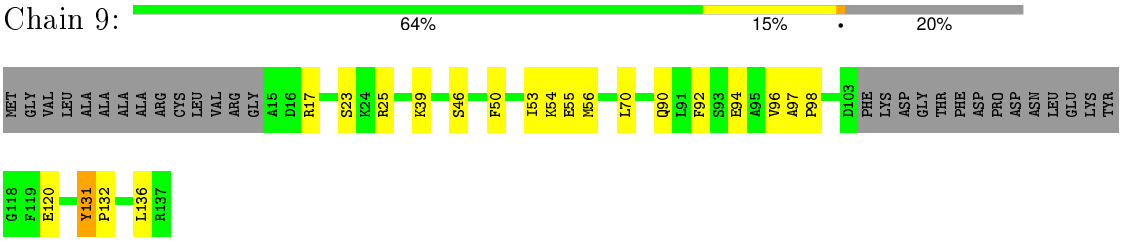
- Molecule 33: mL40

Chain 8:



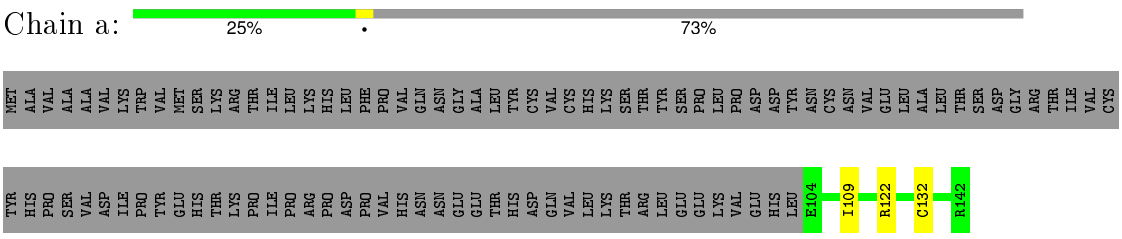
- Molecule 34: mL41

Chain 9:



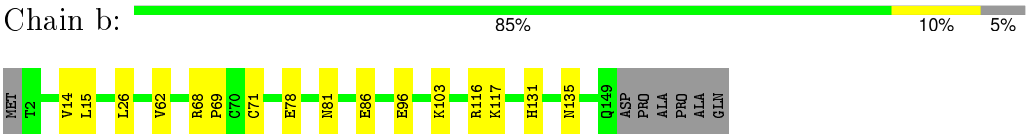
- Molecule 35: mL42

Chain a:



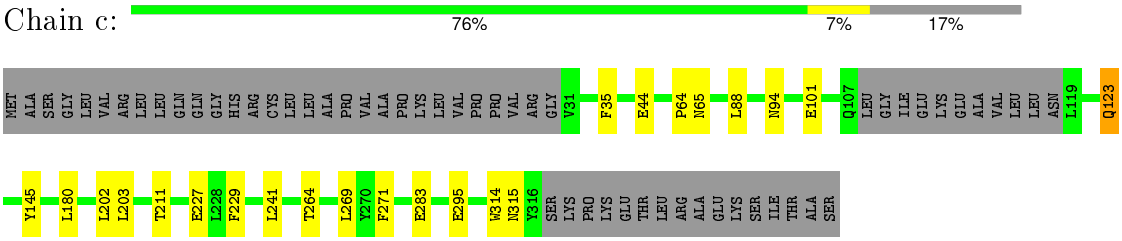
- Molecule 36: mL43

Chain b:



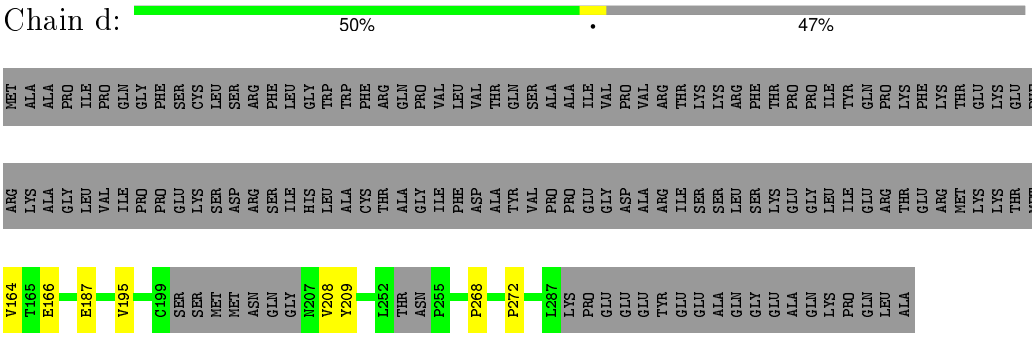
- Molecule 37: mL44

Chain c:



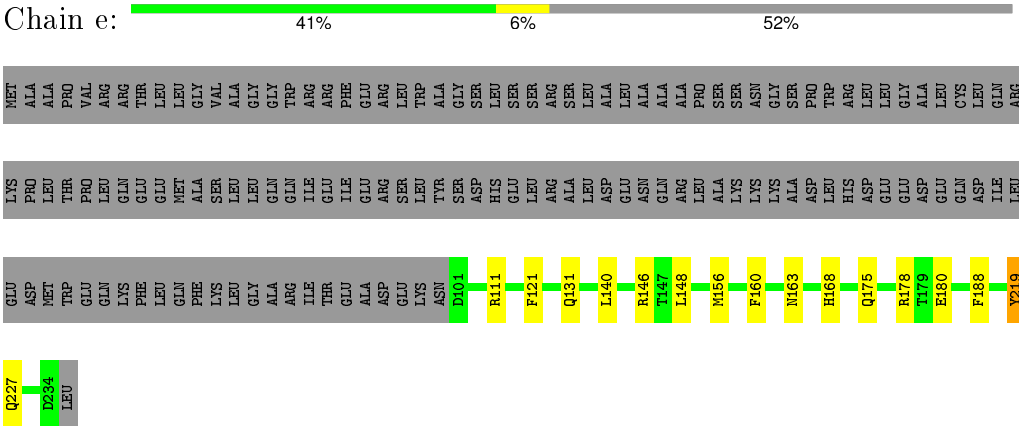
- Molecule 38: mL45

Chain d:



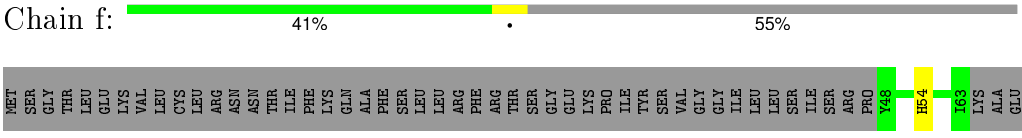
- Molecule 39: mL46

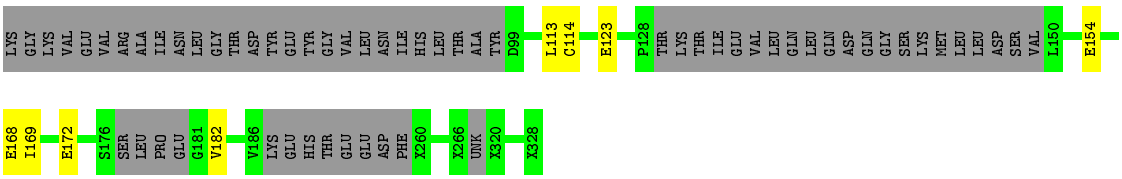
Chain e:



- Molecule 40: mL48

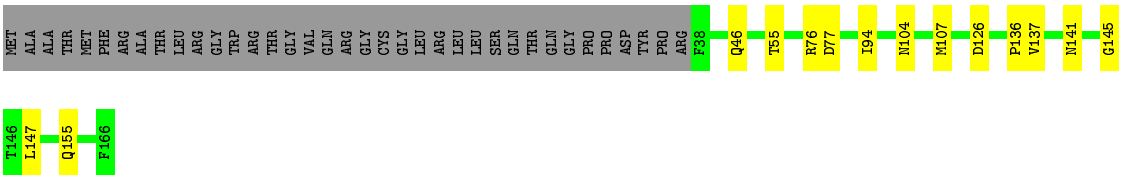
Chain f:





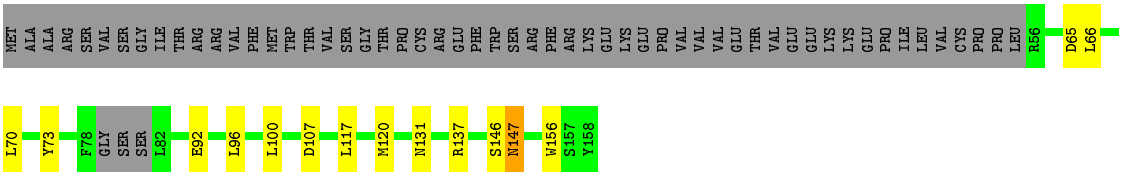
- Molecule 41: mL49

Chain g:



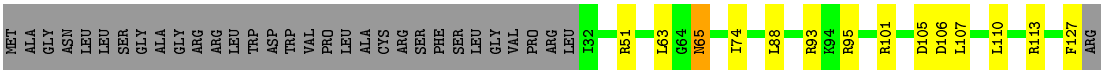
- Molecule 42: mL50

Chain h:



- Molecule 43: mL51

Chain i:



- Molecule 44: mL52

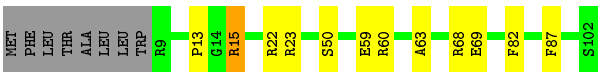
Chain j:

- Molecule 45: mL53

Chain k:

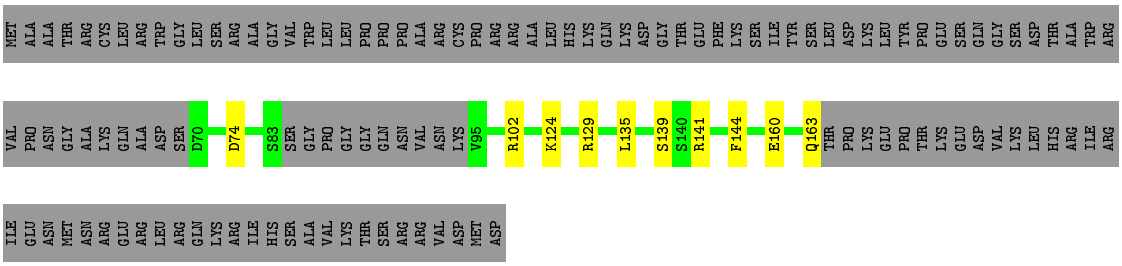
- Molecule 46: mL63

Chain o:



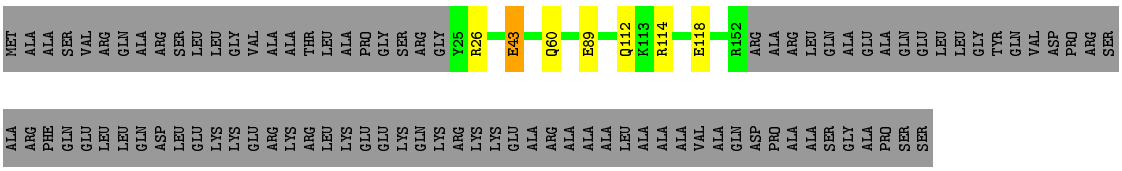
• Molecule 47: ICT1

Chain p:



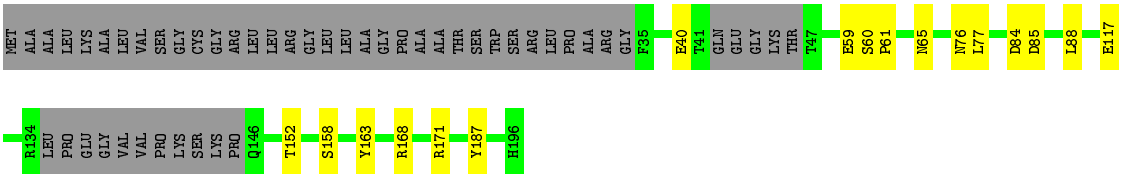
• Molecule 48: CRIF1

Chain q:



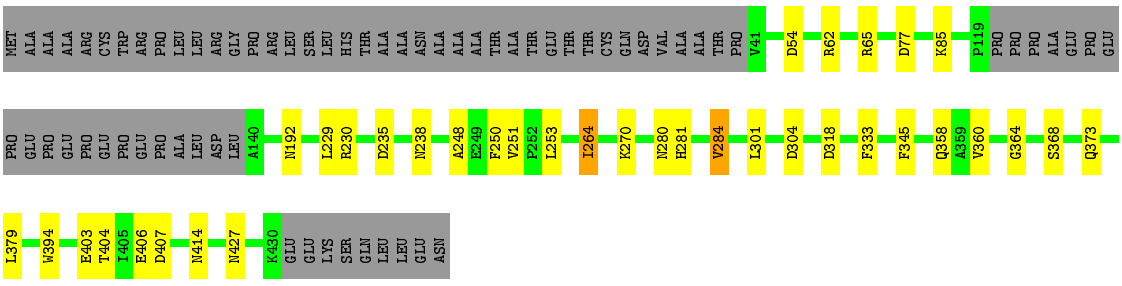
• Molecule 49: bS18a

Chain r:



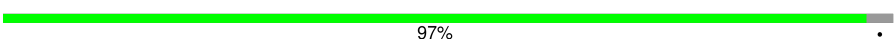
• Molecule 50: mS30

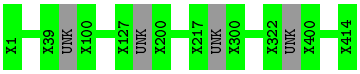
Chain s:



• Molecule 51: unknown protein

Chain t:




X1
X39
UNK
X100
X127
UNK
X200
X217
UNK
X300
X322
UNK
X400
X414

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	107679	Depositor
Resolution determination method	FSC 0.143 gold-standard	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	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	A	0.29	0/34967	0.76	15/54407 (0.0%)
10	L	0.39	0/904	0.71	0/1218
11	M	0.44	2/2359 (0.1%)	0.79	0/3185
12	N	0.45	1/1697 (0.1%)	0.76	1/2281 (0.0%)
13	O	0.58	3/1269 (0.2%)	0.85	0/1708
14	P	0.80	2/1103 (0.2%)	0.73	0/1491
15	Q	0.55	3/1741 (0.2%)	0.73	1/2340 (0.0%)
16	R	0.77	2/1174 (0.2%)	0.85	0/1572
17	S	0.37	0/1276	0.72	0/1729
18	T	0.47	0/1402	0.78	0/1886
19	U	0.63	2/946 (0.2%)	0.77	0/1283
2	B	0.23	0/1349	0.71	2/2086 (0.1%)
20	V	0.44	1/1590 (0.1%)	0.71	0/2151
21	W	0.47	0/864	0.76	0/1166
22	X	0.48	2/2081 (0.1%)	0.72	0/2812
23	Y	0.50	1/1552 (0.1%)	0.83	1/2079 (0.0%)
24	Z	0.50	1/1003 (0.1%)	0.64	0/1354
25	0	0.57	2/816 (0.2%)	0.80	1/1093 (0.1%)
26	1	0.53	1/438 (0.2%)	0.81	0/583
27	2	0.46	0/357	0.92	0/475
28	3	0.42	0/852	0.81	1/1136 (0.1%)
29	4	0.33	0/329	0.68	0/435
3	D	0.47	1/1879 (0.1%)	0.76	1/2527 (0.0%)
30	5	0.44	0/3154	0.75	1/4295 (0.0%)
31	6	0.51	3/2722 (0.1%)	0.74	0/3709
32	7	0.49	1/2207 (0.0%)	0.71	0/2978
33	8	0.52	0/487	0.83	0/649
34	9	0.75	6/896 (0.7%)	0.72	0/1205
35	a	0.46	0/355	0.76	0/475
36	b	0.80	4/1202 (0.3%)	0.73	0/1626
37	c	0.54	3/2264 (0.1%)	0.78	2/3059 (0.1%)
38	d	0.43	0/1385	0.67	0/1877

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
39	e	0.67	1/1107 (0.1%)	0.72	0/1494
4	E	0.42	1/2433 (0.0%)	0.72	0/3299
40	f	0.97	3/632 (0.5%)	0.70	0/850
41	g	0.42	0/1102	0.72	1/1503 (0.1%)
42	h	0.45	0/847	0.73	0/1150
43	i	0.46	0/838	0.85	0/1121
44	j	0.61	3/698 (0.4%)	0.79	0/940
45	k	0.61	0/665	0.77	0/897
46	o	0.56	1/818 (0.1%)	0.97	1/1097 (0.1%)
47	p	0.48	1/682 (0.1%)	0.75	0/917
48	q	0.55	2/1107 (0.2%)	0.78	0/1498
49	r	0.39	0/1238	0.67	0/1676
5	F	0.41	0/2071	0.73	0/2817
50	s	0.55	4/3114 (0.1%)	0.77	2/4225 (0.0%)
6	H	0.46	0/798	0.78	1/1073 (0.1%)
7	I	0.45	0/1308	0.79	0/1761
8	J	0.46	0/1077	0.77	0/1452
9	K	0.48	1/1495 (0.1%)	0.76	1/2029 (0.0%)
All	All	0.45	58/98650 (0.1%)	0.76	32/140669 (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
31	6	0	1
45	k	0	1
46	o	0	1
5	F	0	1
9	K	0	1
All	All	0	5

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	R	23	GLU	CD-OE2	18.73	1.46	1.25
14	P	151	GLU	CD-OE2	18.14	1.45	1.25
39	e	180	GLU	CD-OE2	15.19	1.42	1.25
36	b	78	GLU	CD-OE2	14.77	1.41	1.25
40	f	123	GLU	CD-OE1	14.32	1.41	1.25
40	f	123	GLU	CD-OE2	14.31	1.41	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	151	GLU	CD-OE1	13.91	1.41	1.25
36	b	86	GLU	CD-OE1	13.62	1.40	1.25
19	U	47	GLU	CD-OE2	12.06	1.39	1.25
34	9	94	GLU	CD-OE1	11.41	1.38	1.25
3	D	199	GLU	CD-OE1	11.20	1.38	1.25
36	b	86	GLU	CD-OE2	10.04	1.36	1.25
15	Q	256	GLU	CG-CD	9.35	1.66	1.51
19	U	47	GLU	CD-OE1	8.95	1.35	1.25
31	6	191	ASN	CG-OD1	8.67	1.43	1.24
50	s	318	ASP	CG-OD2	8.62	1.45	1.25
16	R	23	GLU	CD-OE1	8.29	1.34	1.25
36	b	78	GLU	CD-OE1	8.08	1.34	1.25
37	c	44	GLU	CD-OE1	8.08	1.34	1.25
24	Z	51	GLU	CD-OE1	7.47	1.33	1.25
25	0	108	ASP	CG-OD2	7.45	1.42	1.25
13	O	43	GLU	CD-OE1	7.44	1.33	1.25
13	O	70	GLU	CD-OE2	7.39	1.33	1.25
23	Y	97	ASP	CG-OD2	7.24	1.42	1.25
34	9	90	GLN	CD-OE1	7.19	1.39	1.24
31	6	63	GLN	CD-NE2	7.16	1.50	1.32
50	s	403	GLU	CD-OE2	7.16	1.33	1.25
25	0	108	ASP	CG-OD1	7.10	1.41	1.25
46	o	15	ARG	CZ-NH1	6.88	1.42	1.33
40	f	168	GLU	CD-OE1	6.79	1.33	1.25
34	9	120	GLU	CD-OE1	6.75	1.33	1.25
48	q	118	GLU	CG-CD	6.70	1.62	1.51
50	s	318	ASP	CG-OD1	6.70	1.40	1.25
32	7	259	ASP	CG-OD2	6.65	1.40	1.25
34	9	94	GLU	CD-OE2	6.39	1.32	1.25
20	V	176	ASP	CG-OD1	6.39	1.40	1.25
31	6	140	GLU	CD-OE1	6.25	1.32	1.25
34	9	120	GLU	CD-OE2	6.21	1.32	1.25
37	c	295	GLU	CD-OE2	6.19	1.32	1.25
44	j	95	GLN	CD-OE1	5.76	1.36	1.24
44	j	69	GLU	CD-OE1	5.75	1.31	1.25
34	9	90	GLN	CD-NE2	5.66	1.47	1.32
50	s	406	GLU	CG-CD	5.61	1.60	1.51
15	Q	79	GLU	CD-OE1	5.61	1.31	1.25
4	E	91	GLU	CD-OE1	5.48	1.31	1.25
12	N	202	GLN	CD-NE2	5.39	1.46	1.32
22	X	60	GLU	CD-OE2	5.38	1.31	1.25
11	M	139	GLN	CD-OE1	5.36	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	p	74	ASP	CG-OD1	5.33	1.37	1.25
37	c	101	GLU	CD-OE1	5.23	1.31	1.25
11	M	139	GLN	CD-NE2	5.22	1.45	1.32
13	O	70	GLU	CD-OE1	5.20	1.31	1.25
26	1	39	GLU	CD-OE2	5.19	1.31	1.25
48	q	118	GLU	CD-OE2	5.14	1.31	1.25
9	K	130	ASP	CG-OD2	5.12	1.37	1.25
22	X	35	GLU	CD-OE1	5.07	1.31	1.25
15	Q	79	GLU	CD-OE2	5.06	1.31	1.25
44	j	101	GLU	CD-OE2	5.03	1.31	1.25

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	o	15	ARG	NE-CZ-NH2	-7.78	116.41	120.30
25	0	108	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	A	1772	A	C2'-C3'-O3'	7.47	125.93	109.50
28	3	169	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	2174	G	C2'-C3'-O3'	7.26	125.47	109.50
1	A	2374	A	C2'-C3'-O3'	7.01	124.93	109.50
37	c	241	LEU	CA-CB-CG	6.51	130.28	115.30
1	A	2507	A	C2'-C3'-O3'	6.28	123.75	113.70
1	A	2421	G	C2'-C3'-O3'	6.08	123.42	113.70
1	A	2165	C	C2'-C3'-O3'	5.82	123.01	113.70
2	B	1628	C	C2'-C3'-O3'	5.64	122.72	113.70
23	Y	97	ASP	CB-CG-OD1	-5.56	113.30	118.30
6	H	70	LYS	C-N-CD	5.41	139.75	128.40
50	s	62	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	3041	U	C2'-C3'-O3'	5.34	122.24	113.70
1	A	2321	A	N9-C1'-C2'	5.34	120.94	114.00
9	K	145	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	1823	A	C2'-C3'-O3'	5.30	122.18	113.70
1	A	2649	U	C2'-C3'-O3'	5.25	122.11	113.70
1	A	2111	C	N1-C1'-C2'	5.25	120.83	114.00
41	g	77	ASP	CB-CG-OD2	5.24	123.01	118.30
12	N	199	ARG	NE-CZ-NH2	-5.22	117.69	120.30
50	s	54	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	2245	A	N9-C1'-C2'	5.20	120.76	114.00
1	A	2243	A	C2'-C3'-O3'	5.18	121.99	113.70
30	5	116	GLY	N-CA-C	-5.18	100.14	113.10
1	A	2186	C	C2'-C3'-O3'	5.13	121.91	113.70
2	B	1607	U	C2'-C3'-O3'	5.09	121.85	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Q	194	LEU	CA-CB-CG	5.06	126.94	115.30
37	c	241	LEU	CB-CA-C	-5.06	100.58	110.20
1	A	1806	U	C2'-C3'-O3'	5.06	121.80	113.70
3	D	277	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	6	191	ASN	Sidechain
5	F	140	SER	Peptide
9	K	82	GLY	Peptide
45	k	61	GLU	Peptide
46	o	63	ALA	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	A	31261	0	15879	642	0
2	B	1211	0	619	12	0
3	D	1842	0	1896	18	0
4	E	2365	0	2378	38	0
5	F	2013	0	2044	24	0
6	H	784	0	832	16	0
7	I	1283	0	1370	33	0
8	J	1061	0	1141	13	0
9	K	1451	0	1448	20	0
10	L	889	0	941	12	0
11	M	2305	0	2378	27	0
12	N	1654	0	1681	13	0
13	O	1245	0	1283	29	0
14	P	1080	0	1081	27	0
15	Q	1704	0	1744	35	0
16	R	1153	0	1214	13	0
17	S	1251	0	1322	11	0
18	T	1368	0	1410	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	U	922	0	935	17	0
20	V	1551	0	1558	5	0
21	W	842	0	869	25	0
22	X	2027	0	2040	35	0
23	Y	1517	0	1561	24	0
24	Z	978	0	1030	11	0
25	0	803	0	837	16	0
26	1	433	0	475	2	0
27	2	351	0	375	3	0
28	3	831	0	883	11	0
29	4	322	0	344	12	0
30	5	3064	0	3059	67	0
31	6	2636	0	2450	23	0
32	7	2158	0	2173	22	0
33	8	482	0	494	2	0
34	9	873	0	878	10	0
35	a	343	0	334	0	0
36	b	1178	0	1180	0	0
37	c	2217	0	2220	0	0
38	d	1347	0	1343	0	0
39	e	1082	0	1071	0	0
40	f	703	0	654	0	0
41	g	1067	0	1056	0	0
42	h	827	0	806	0	0
43	i	816	0	844	0	0
44	j	684	0	673	0	0
45	k	655	0	656	0	0
46	o	797	0	804	0	0
47	p	674	0	690	0	0
48	q	1076	0	1049	0	0
49	r	1203	0	1221	0	0
50	s	3036	0	3022	0	0
51	t	615	0	143	0	0
52	A	22	0	12	0	0
53	A	65	0	0	0	0
53	E	1	0	0	0	0
54	0	1	0	0	3	0
54	4	1	0	0	1	0
54	r	1	0	0	0	0
All	All	94121	0	78400	1181	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 8.

All (1181) 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)
15:Q:244:ARG:HH11	15:Q:247:LEU:CD1	1.40	1.34
1:A:2556:A:C2	1:A:2559:U:O2	1.86	1.27
1:A:2556:A:H2	1:A:2559:U:O2	1.15	1.26
30:5:127:LYS:CD	30:5:251:HIS:CE1	2.20	1.25
1:A:2194:U:H2'	1:A:2195:A:C8	1.80	1.16
15:Q:244:ARG:NH1	15:Q:247:LEU:CD1	2.11	1.13
25:0:110:CYS:SG	25:0:112:GLU:O	2.05	1.13
9:K:154:ARG:NH1	9:K:157:GLU:OE2	1.86	1.09
9:K:154:ARG:HH12	9:K:157:GLU:CD	1.55	1.09
30:5:127:LYS:HG3	30:5:251:HIS:CE1	1.88	1.07
30:5:127:LYS:CG	30:5:251:HIS:CE1	2.40	1.04
30:5:127:LYS:CD	30:5:251:HIS:HE1	1.64	1.03
30:5:127:LYS:HD3	30:5:251:HIS:HE1	1.25	1.01
9:K:154:ARG:NH1	9:K:157:GLU:CD	2.14	0.99
30:5:125:LYS:HA	30:5:253:LEU:HD21	1.45	0.99
15:Q:244:ARG:NH1	15:Q:247:LEU:HD11	1.74	0.98
30:5:127:LYS:HD2	30:5:251:HIS:CE1	1.98	0.98
25:0:126:CYS:HG	54:0:200:ZN:ZN	0.69	0.97
15:Q:244:ARG:HH11	15:Q:247:LEU:HD11	1.26	0.97
29:4:76:CYS:SG	29:4:98:HIS:CD2	2.58	0.96
1:A:2194:U:C2	1:A:2195:A:C5	2.54	0.96
1:A:2194:U:N3	1:A:2195:A:C6	2.34	0.95
1:A:2193:U:H3'	1:A:2194:U:H5'	1.48	0.95
1:A:2559:U:O2'	1:A:2560:G:O4'	1.85	0.94
1:A:3131:G:C6	1:A:3132:G:C4	2.56	0.93
22:X:81:GLY:O	22:X:154:CYS:SG	2.28	0.92
30:5:127:LYS:HG3	30:5:251:HIS:NE2	1.85	0.91
1:A:2194:U:O2	1:A:2195:A:C4	2.26	0.88
1:A:3030:A:C2'	1:A:3031:G:H5'	2.04	0.86
15:Q:244:ARG:HH11	15:Q:247:LEU:HD13	1.40	0.86
29:4:76:CYS:SG	29:4:98:HIS:HD2	1.98	0.86
1:A:2550:A:C2	1:A:2551:G:C8	2.65	0.85
1:A:3131:G:N7	1:A:3132:G:N7	2.24	0.85
21:W:106:PRO:CD	21:W:117:ILE:CD1	2.54	0.85
21:W:106:PRO:HD2	21:W:117:ILE:CD1	2.06	0.85
1:A:3131:G:C5	1:A:3132:G:C5	2.64	0.85
1:A:2556:A:C3'	1:A:2557:C:H5'	2.06	0.84
1:A:2556:A:H2'	1:A:2557:C:H5'	1.58	0.83
1:A:3131:G:C8	1:A:3132:G:C8	2.67	0.83
1:A:3131:G:O2'	1:A:3132:G:H5'	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2556:A:C2'	1:A:2557:C:H5'	2.09	0.82
21:W:102:GLU:OE2	31:6:74:TYR:HB2	1.79	0.82
29:4:79:CYS:SG	54:4:200:ZN:ZN	1.69	0.82
30:5:127:LYS:HD3	30:5:251:HIS:CE1	2.02	0.82
1:A:2556:A:C2	1:A:2559:U:C2	2.69	0.80
1:A:2185:G:N1	1:A:2186:C:C4	2.50	0.80
1:A:2185:G:N2	1:A:2186:C:C2	2.50	0.79
22:X:148:ALA:HB3	22:X:153:LEU:HD23	1.64	0.79
6:H:56:VAL:CG1	6:H:80:TYR:HB3	2.12	0.79
1:A:3131:G:C5	1:A:3132:G:C8	2.71	0.79
21:W:106:PRO:CD	21:W:117:ILE:HD12	2.13	0.78
25:0:123:CYS:HB3	25:0:126:CYS:HB2	1.64	0.78
1:A:3131:G:C4	1:A:3132:G:C8	2.72	0.78
1:A:2731:U:O4	1:A:2918:A:N1	2.17	0.78
1:A:3131:G:C5	1:A:3132:G:C4	2.72	0.77
14:P:77:TRP:O	14:P:95:HIS:HD2	1.68	0.77
9:K:65:ILE:HD11	9:K:104:VAL:HG23	1.66	0.77
1:A:2799:U:H2'	1:A:2800:U:C6	2.21	0.76
4:E:231:HIS:N	4:E:232:GLY:HA2	1.99	0.76
1:A:2194:U:O2'	1:A:2195:A:O5'	2.03	0.75
28:3:104:ARG:NH1	28:3:160:LYS:O	2.20	0.75
32:7:154:ILE:HD13	32:7:183:VAL:HG21	1.66	0.75
15:Q:244:ARG:HD3	15:Q:247:LEU:HD13	1.68	0.75
1:A:3030:A:H2'	1:A:3031:G:H5'	1.67	0.75
1:A:2195:A:O2'	1:A:2196:A:H5'	1.86	0.75
16:R:107:ILE:HD13	18:T:211:THR:HG21	1.69	0.75
1:A:3016:G:N7	29:4:97:ARG:NH2	2.34	0.75
4:E:129:VAL:HG21	4:E:187:ILE:HD13	1.68	0.74
1:A:3131:G:C6	1:A:3132:G:C5	2.76	0.74
1:A:1789:A:H2'	1:A:1790:A:C8	2.22	0.74
1:A:2540:C:C5	1:A:2541:C:C6	2.77	0.73
1:A:2492:G:H1'	1:A:2506:A:H5'	1.69	0.73
14:P:74:ARG:HH21	14:P:74:ARG:HG3	1.53	0.72
31:6:161:LEU:HD21	31:6:271:LEU:HD21	1.72	0.72
1:A:3131:G:H2'	1:A:3132:G:O4'	1.89	0.72
1:A:1719:G:C2	1:A:1720:C:N3	2.57	0.72
15:Q:244:ARG:NH1	15:Q:247:LEU:HD12	2.03	0.72
22:X:36:ARG:N	22:X:151:GLU:OE2	2.21	0.72
8:J:113:THR:HA	8:J:156:VAL:HB	1.71	0.72
27:2:60:ARG:HD2	27:2:92:HIS:CE1	2.24	0.71
1:A:2085:A:H2'	1:A:2086:A:C8	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2194:U:N3	1:A:2195:A:C5	2.56	0.71
1:A:2756:C:H5"	1:A:2756:C:H6	1.54	0.71
14:P:106:THR:HG23	14:P:127:ILE:HD11	1.72	0.71
1:A:2033:A:N6	1:A:2041:U:O4	2.20	0.71
14:P:77:TRP:HB2	14:P:173:GLU:OE1	1.90	0.70
1:A:2194:U:C2'	1:A:2195:A:C8	2.67	0.70
1:A:2111:C:H2'	1:A:2112:A:C8	2.27	0.70
1:A:2294:A:OP2	11:M:41:ARG:NH1	2.24	0.70
1:A:2686:G:N2	1:A:2687:C:C2	2.60	0.70
1:A:2263:C:O2	1:A:2263:C:H2'	1.91	0.69
9:K:29:GLY:HA2	9:K:32:ALA:HB3	1.74	0.69
1:A:2590:A:O2'	1:A:2591:A:C8	2.40	0.69
9:K:48:HIS:NE2	18:T:209:VAL:HG11	2.07	0.69
30:5:122:TRP:O	30:5:215:ARG:NH1	2.24	0.69
1:A:3131:G:C8	1:A:3132:G:N7	2.61	0.69
2:B:1611:G:N2	2:B:1612:C:C2	2.61	0.69
15:Q:221:LYS:CB	15:Q:244:ARG:HG3	2.22	0.69
15:Q:138:ILE:HD11	15:Q:152:ARG:HB2	1.75	0.68
21:W:106:PRO:CD	21:W:117:ILE:HD11	2.22	0.68
21:W:107:HIS:ND1	21:W:108:PRO:HD2	2.08	0.68
15:Q:221:LYS:HB2	15:Q:244:ARG:HG3	1.74	0.68
25:0:110:CYS:SG	54:0:200:ZN:ZN	1.82	0.68
1:A:2041:U:H2'	1:A:2042:U:C6	2.30	0.67
12:N:96:TYR:HB3	12:N:151:VAL:HG11	1.75	0.67
1:A:2493:C:N4	1:A:2540:C:H1'	2.10	0.67
1:A:2756:C:H5"	1:A:2756:C:C6	2.29	0.67
30:5:124:THR:HG23	30:5:318:PHE:HD2	1.60	0.67
9:K:22:ASP:O	9:K:26:GLN:NE2	2.28	0.66
4:E:61:ILE:HD11	13:O:149:LEU:HD22	1.75	0.66
1:A:2193:U:H3'	1:A:2194:U:C5'	2.22	0.66
21:W:106:PRO:HD3	21:W:117:ILE:HD11	1.76	0.66
5:F:103:GLN:NE2	5:F:249:ASN:HD22	1.93	0.66
5:F:217:LEU:HD11	5:F:243:ILE:HD11	1.76	0.66
1:A:2541:C:N3	1:A:2542:G:N7	2.44	0.66
1:A:2803:A:H2'	1:A:2804:A:O4'	1.96	0.66
14:P:134:ARG:O	14:P:137:GLU:HG3	1.95	0.66
1:A:1876:U:H2'	1:A:1877:U:C6	2.30	0.66
17:S:99:VAL:HG22	17:S:133:VAL:HG12	1.77	0.66
1:A:2756:C:OP1	22:X:112:ARG:NH2	2.29	0.66
7:I:129:GLN:O	7:I:133:PRO:HD2	1.96	0.66
22:X:124:THR:O	30:5:48:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3131:G:C2'	1:A:3132:G:H5'	2.26	0.66
4:E:208:ALA:HB2	4:E:297:VAL:HG12	1.78	0.66
1:A:2493:C:C4	1:A:2540:C:H1'	2.31	0.65
18:T:99:ILE:HD11	18:T:178:LEU:HD13	1.78	0.65
12:N:72:ILE:HD11	12:N:96:TYR:CE2	2.31	0.65
1:A:2868:C:O2'	11:M:77:ARG:NH1	2.28	0.65
6:H:56:VAL:HG12	6:H:80:TYR:HB3	1.76	0.65
1:A:2540:C:C5	1:A:2541:C:C5	2.84	0.65
30:5:216:GLU:N	30:5:217:SER:HA	2.11	0.65
14:P:57:LEU:HD13	31:6:265:ILE:HD13	1.79	0.65
1:A:2428:C:C2	1:A:2436:G:C2	2.84	0.65
1:A:2194:U:C4	1:A:2195:A:C6	2.84	0.65
1:A:2194:U:H2'	1:A:2195:A:N7	2.12	0.65
1:A:2493:C:H2'	1:A:2494:C:C5'	2.27	0.65
1:A:1939:G:O2'	1:A:1973:G:H4'	1.97	0.65
3:D:111:ARG:HG2	3:D:181:ALA:HB2	1.78	0.64
1:A:1826:G:N2	1:A:2686:G:N7	2.46	0.64
1:A:2231:A:O2'	1:A:2232:A:O4'	2.15	0.64
1:A:2601:A:C2	1:A:3092:U:O2	2.51	0.63
1:A:2194:U:P	7:I:124:LYS:NZ	2.71	0.63
15:Q:120:THR:HG22	15:Q:132:GLN:HG2	1.80	0.63
4:E:123:GLN:HE22	15:Q:90:LEU:HD13	1.64	0.63
30:5:127:LYS:CG	30:5:251:HIS:HE1	1.95	0.63
1:A:2490:C:C2	1:A:2646:G:C2	2.86	0.63
6:H:55:ILE:HD12	6:H:55:ILE:N	2.13	0.63
1:A:2556:A:N1	1:A:2559:U:C2	2.67	0.63
5:F:217:LEU:HD13	5:F:256:HIS:CE1	2.34	0.63
3:D:111:ARG:NH2	3:D:179:GLY:O	2.32	0.63
22:X:153:LEU:O	22:X:153:LEU:HD13	1.98	0.63
21:W:102:GLU:HA	21:W:102:GLU:OE1	1.99	0.62
9:K:46:VAL:HG13	18:T:208:ILE:HG23	1.81	0.62
1:A:2995:G:HO2'	1:A:3041:U:HO2'	1.21	0.62
30:5:107:PHE:CE1	30:5:315:LEU:HD13	2.33	0.62
30:5:244:GLU:O	30:5:247:ALA:HB3	1.98	0.62
1:A:1807:U:O2'	1:A:1808:A:C8	2.44	0.62
18:T:94:ILE:CD1	18:T:117:ILE:HG21	2.29	0.62
31:6:237:LEU:HD13	31:6:245:VAL:HG13	1.82	0.62
1:A:2194:U:OP1	7:I:124:LYS:HE2	2.00	0.62
1:A:3131:G:C4	1:A:3132:G:N9	2.68	0.61
1:A:2660:U:N3	1:A:2661:U:C5	2.68	0.61
30:5:105:TYR:CD1	30:5:262:ILE:HD13	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:6:259:PRO:HB3	31:6:266:HIS:CD2	2.35	0.61
1:A:2800:U:C2	1:A:2801:A:C8	2.88	0.61
32:7:143:TRP:HE1	32:7:174:VAL:HA	1.63	0.61
1:A:1990:G:C2	1:A:1992:C:C5	2.89	0.61
1:A:2185:G:C2	1:A:2186:C:C4	2.88	0.61
7:I:130:VAL:HG13	7:I:134:PHE:CZ	2.35	0.61
7:I:86:ILE:HG21	7:I:134:PHE:CD2	2.36	0.61
21:W:100:THR:OG1	21:W:132:HIS:NE2	2.32	0.61
1:A:2601:A:H2	1:A:3092:U:O2	1.83	0.61
1:A:2467:A:N1	1:A:2660:U:O2	2.34	0.61
1:A:2370:A:N7	19:U:73:GLN:NE2	2.48	0.61
1:A:2748:A:H2'	1:A:2749:A:C8	2.35	0.61
18:T:117:ILE:HG23	18:T:174:TYR:CE2	2.36	0.61
29:4:79:CYS:SG	29:4:92:CYS:HB2	2.41	0.61
30:5:120:ALA:HB2	30:5:311:ALA:HB1	1.83	0.61
30:5:318:PHE:CE1	30:5:322:LEU:HD13	2.36	0.61
11:M:178:PHE:CE2	11:M:206:PRO:HA	2.35	0.61
14:P:130:VAL:HG12	14:P:134:ARG:HE	1.66	0.60
1:A:2194:U:C2	1:A:2195:A:C4	2.84	0.60
16:R:71:ARG:HD3	16:R:107:ILE:HD11	1.82	0.60
1:A:2053:U:H2'	1:A:2054:U:C6	2.35	0.60
1:A:1897:A:H2'	1:A:1898:A:C8	2.35	0.60
18:T:94:ILE:CG2	18:T:142:ILE:HD13	2.31	0.60
1:A:2194:U:O2	1:A:2195:A:N9	2.34	0.60
1:A:2731:U:O4	1:A:2918:A:C2	2.54	0.60
1:A:2194:U:O2	1:A:2195:A:C5	2.52	0.60
1:A:1819:U:H3'	1:A:1820:A:H5"	1.84	0.60
1:A:3131:G:N9	1:A:3132:G:C8	2.70	0.60
9:K:65:ILE:HD11	9:K:104:VAL:CG2	2.31	0.60
30:5:309:LEU:HD21	30:5:347:THR:CG2	2.32	0.60
1:A:2194:U:P	7:I:124:LYS:HZ3	2.25	0.60
1:A:2506:A:H4'	1:A:2507:A:OP1	2.02	0.60
1:A:2329:C:C2	1:A:2449:G:C2	2.90	0.60
1:A:2185:G:C2	1:A:2186:C:C5	2.90	0.59
1:A:2474:C:O2	4:E:231:HIS:HE1	1.84	0.59
1:A:1959:C:H2'	1:A:1959:C:O2	2.01	0.59
25:0:126:CYS:SG	54:0:200:ZN:ZN	1.83	0.59
1:A:3131:G:C2	1:A:3132:G:H1'	2.37	0.59
1:A:2065:A:H2'	1:A:2066:C:O4'	2.03	0.59
13:O:36:LEU:HD12	13:O:52:MET:CE	2.33	0.59
32:7:167:VAL:HG23	32:7:235:TYR:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3077:C:H2'	1:A:3077:C:O2	2.02	0.59
1:A:2686:G:N1	1:A:2687:C:C4	2.70	0.59
1:A:2081:U:H2'	1:A:2082:G:C8	2.37	0.59
1:A:2103:A:HO2'	24:Z:35:LYS:N	2.01	0.59
1:A:2596:G:N1	1:A:2597:C:C2	2.71	0.59
1:A:2467:A:C6	1:A:2655:G:C8	2.91	0.58
1:A:1953:A:O2'	1:A:2463:A:OP1	2.21	0.58
1:A:2129:G:N2	1:A:2137:C:C2	2.71	0.58
1:A:1671:G:N2	1:A:1672:C:C2	2.71	0.58
1:A:3131:G:N7	1:A:3132:G:C5	2.68	0.58
30:5:309:LEU:HD21	30:5:347:THR:HG23	1.85	0.58
1:A:2466:A:N1	1:A:2467:A:C6	2.72	0.58
1:A:2612:C:C2	1:A:2621:G:C2	2.91	0.58
1:A:3131:G:C5	1:A:3132:G:N7	2.67	0.58
1:A:1904:C:C2	1:A:2019:G:C2	2.91	0.58
1:A:1718:A:H2'	1:A:1719:G:C8	2.39	0.58
1:A:1851:G:H2'	1:A:2693:A:N7	2.18	0.58
1:A:2467:A:N6	1:A:2655:G:C8	2.72	0.58
11:M:119:THR:HG23	11:M:187:VAL:HG13	1.86	0.58
5:F:103:GLN:HE22	5:F:249:ASN:HD22	1.49	0.58
1:A:2466:A:C2	1:A:2661:U:N3	2.72	0.58
7:I:130:VAL:HG22	7:I:134:PHE:CE1	2.39	0.58
4:E:121:LEU:HD22	4:E:284:TYR:CD2	2.39	0.58
3:D:111:ARG:HG2	3:D:181:ALA:CB	2.34	0.58
1:A:3131:G:H2'	1:A:3132:G:C5'	2.34	0.58
4:E:102:LEU:HD21	4:E:150:LYS:HG3	1.86	0.57
1:A:3030:A:N3	1:A:3031:G:C8	2.73	0.57
1:A:2507:A:H5'	1:A:2507:A:H8	1.68	0.57
1:A:1904:C:C2	1:A:2019:G:N2	2.72	0.57
1:A:2556:A:H3'	1:A:2557:C:H5'	1.87	0.57
1:A:2467:A:N1	1:A:2660:U:C2	2.72	0.57
2:B:1611:G:C2	2:B:1612:C:C4	2.92	0.57
1:A:2750:U:C2	1:A:2751:G:C8	2.92	0.57
1:A:2317:G:H1'	1:A:2452:A:N6	2.19	0.57
1:A:3129:A:H2'	1:A:3130:A:C8	2.40	0.57
1:A:2947:U:H2'	1:A:2948:C:O5'	2.05	0.57
22:X:128:THR:O	22:X:131:THR:OG1	2.22	0.57
30:5:336:LEU:HD21	30:5:362:THR:HG23	1.86	0.57
1:A:2615:A:H2'	1:A:2616:A:C8	2.40	0.57
1:A:2065:A:C2'	1:A:2066:C:O4'	2.53	0.56
1:A:1719:G:C6	1:A:1720:C:N4	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2086:A:H2'	1:A:2087:U:C6	2.41	0.56
5:F:217:LEU:HD11	5:F:243:ILE:CD1	2.35	0.56
8:J:76:ARG:NH2	24:Z:99:VAL:O	118.96	0.56
15:Q:240:ILE:HG21	15:Q:243:ILE:HG13	1.87	0.56
19:U:99:LEU:HD21	23:Y:64:LEU:HD11	1.87	0.56
1:A:2235:C:O4'	1:A:2235:C:O2	2.23	0.56
1:A:2497:U:H6	1:A:2497:U:O5'	1.89	0.56
1:A:3131:G:N7	1:A:3132:G:C8	2.72	0.56
22:X:230:TYR:HB3	34:9:92:PHE:CD2	2.40	0.56
21:W:106:PRO:HD3	21:W:117:ILE:CD1	2.31	0.56
18:T:88:TRP:CZ2	18:T:92:LYS:HG3	2.41	0.56
5:F:95:ILE:HD13	5:F:172:LEU:HD22	1.87	0.56
1:A:3030:A:C4	1:A:3031:G:C8	2.94	0.56
22:X:148:ALA:HB3	22:X:153:LEU:CD2	2.34	0.56
1:A:2043:C:C2	1:A:2044:A:C8	2.94	0.56
1:A:2466:A:C2	1:A:2467:A:C5	2.94	0.56
1:A:1827:C:C5	1:A:2698:G:C2	2.94	0.56
9:K:154:ARG:NH1	9:K:157:GLU:CG	2.68	0.56
1:A:2600:A:O2'	1:A:2601:A:P	2.64	0.56
28:3:183:ARG:NH1	31:6:355:LYS:O	2.38	0.56
25:0:156:THR:HG22	25:0:173:ARG:HD3	1.88	0.56
2:B:1627:C:C2	2:B:1642:G:C2	2.94	0.56
1:A:1807:U:O2'	1:A:1808:A:O5'	2.23	0.55
1:A:2726:C:O2	1:A:2937:A:N1	2.39	0.55
4:E:100:ILE:HD11	4:E:177:LYS:HB2	1.88	0.55
1:A:2537:G:C6	1:A:2538:C:C4	2.94	0.55
1:A:1816:G:H2'	1:A:1817:C:O4'	2.04	0.55
5:F:84:PRO:O	5:F:88:ALA:N	2.38	0.55
23:Y:112:LEU:HD13	23:Y:132:LEU:HA	1.87	0.55
1:A:2194:U:O2	1:A:2195:A:C8	2.60	0.55
14:P:141:ASN:N	14:P:141:ASN:OD1	2.38	0.55
15:Q:240:ILE:HG21	15:Q:243:ILE:CD1	2.37	0.55
14:P:60:VAL:HG11	31:6:344:PHE:CZ	2.42	0.55
13:O:43:GLU:HG2	25:0:127:TYR:OH	2.07	0.55
1:A:1977:U:H2'	1:A:1978:A:C8	2.42	0.55
21:W:111:THR:HG23	21:W:112:GLU:N	2.21	0.55
23:Y:189:HIS:HB2	30:5:75:PHE:CE2	2.41	0.55
1:A:2670:C:N3	1:A:2671:C:C5	2.74	0.55
1:A:2061:C:O2	1:A:2061:C:O4'	2.24	0.55
1:A:2995:G:O2'	1:A:3041:U:O2'	2.03	0.55
12:N:221:ALA:O	24:Z:114:LYS:NZ	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:75:LEU:HD23	10:L:77:ILE:HD11	1.89	0.55
22:X:114:PHE:HB3	22:X:141:LEU:HD13	1.88	0.55
31:6:72:ARG:HA	31:6:73:THR:HG22	1.88	0.55
18:T:113:GLY:HA2	18:T:116:ILE:HD12	1.89	0.55
14:P:74:ARG:NH2	14:P:74:ARG:HG3	2.19	0.55
1:A:1882:A:N6	1:A:1893:A:O4'	2.40	0.55
1:A:2484:C:H2'	1:A:2485:U:C6	2.41	0.55
1:A:3084:A:H2'	1:A:3085:A:C8	2.43	0.54
30:5:161:ALA:CB	30:5:180:ILE:HG13	2.38	0.54
11:M:115:PRO:HA	11:M:153:ASN:HD21	1.71	0.54
1:A:2256:U:O4'	17:S:103:SER:OG	2.23	0.54
1:A:2756:C:H5'	1:A:2757:A:OP2	2.06	0.54
14:P:63:LYS:HB3	14:P:75:GLU:HG3	1.89	0.54
30:5:385:HIS:O	30:5:404:VAL:HG12	2.06	0.54
1:A:3131:G:C5	1:A:3132:G:N9	2.74	0.54
6:H:116:LYS:HB3	6:H:120:ARG:NH2	2.22	0.54
1:A:1961:A:H5'	18:T:161:ARG:HA	1.88	0.54
14:P:78:HIS:HA	14:P:94:GLU:O	2.07	0.54
4:E:230:THR:O	4:E:231:HIS:HB2	2.07	0.54
2:B:1611:G:N1	2:B:1612:C:C4	2.75	0.54
1:A:2242:U:OP2	9:K:30:LYS:NZ	2.39	0.54
1:A:2194:U:O2'	1:A:2195:A:O4'	2.23	0.54
1:A:3030:A:C2	1:A:3031:G:C8	2.95	0.54
1:A:2944:C:H2'	1:A:2945:A:O4'	2.08	0.54
30:5:67:VAL:HG11	30:5:69:TRP:NE1	2.23	0.54
1:A:1837:C:O2	1:A:1837:C:O4'	2.23	0.54
1:A:2755:A:C5'	1:A:2756:C:OP2	2.55	0.54
1:A:2174:G:C6	1:A:2175:C:C4	2.95	0.54
1:A:1863:A:H2'	1:A:1864:A:C8	2.43	0.54
1:A:1689:C:O4'	1:A:1689:C:O2	2.25	0.54
1:A:3020:C:O2'	1:A:3132:G:H5"	2.08	0.54
1:A:3173:G:H2'	1:A:3174:U:O4'	2.08	0.54
5:F:221:LEU:HG	5:F:222:THR:HG23	1.90	0.54
22:X:95:ASP:OD1	22:X:95:ASP:N	2.41	0.54
1:A:2141:U:O2	1:A:2141:U:C2'	2.56	0.54
21:W:103:VAL:HG13	21:W:125:VAL:CG1	2.37	0.54
1:A:1737:A:N6	1:A:1760:G:O2'	2.40	0.54
29:4:78:ASP:HB2	29:4:92:CYS:SG	2.48	0.53
1:A:1719:G:H2'	1:A:1720:C:C6	2.43	0.53
30:5:161:ALA:HB1	30:5:180:ILE:HG13	1.90	0.53
1:A:2733:G:C2	1:A:2929:C:C2	2.96	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:107:HIS:CE1	21:W:108:PRO:HD2	2.43	0.53
1:A:2511:C:O4'	1:A:2511:C:O2	2.26	0.53
1:A:2467:A:C6	1:A:2655:G:N7	2.77	0.53
1:A:2484:C:O4'	1:A:2484:C:O2	2.24	0.53
1:A:2636:G:C6	1:A:2637:C:C4	2.96	0.53
8:J:52:GLU:HB3	8:J:80:ILE:HD12	1.90	0.53
23:Y:102:TRP:HE3	23:Y:142:LEU:HD22	1.73	0.53
1:A:2194:U:OP1	7:I:113:ARG:NH2	2.38	0.53
1:A:3131:G:C2'	1:A:3132:G:C5'	2.87	0.53
1:A:2440:G:C6	1:A:2441:C:C4	2.96	0.53
32:7:107:LEU:HG	32:7:128:LEU:HD11	1.90	0.53
1:A:2837:A:H2'	1:A:2838:A:C8	2.44	0.53
1:A:1823:A:O2'	1:A:1824:U:OP2	2.22	0.53
1:A:2322:C:O2	1:A:2322:C:O4'	2.26	0.53
1:A:2129:G:C2	1:A:2137:C:C2	2.96	0.53
18:T:88:TRP:CH2	25:0:95:ARG:HG3	2.44	0.53
1:A:2079:C:O4'	1:A:2079:C:O2	2.24	0.53
1:A:2712:G:C6	1:A:2713:C:C4	2.97	0.53
14:P:55:LEU:HB3	14:P:61:ALA:HB2	1.91	0.53
1:A:2574:G:N2	1:A:2584:C:C2	2.76	0.53
21:W:106:PRO:CG	21:W:117:ILE:HD12	2.38	0.53
1:A:1917:A:C8	1:A:1983:U:C4	2.97	0.53
31:6:225:LEU:HD12	31:6:293:LEU:HD21	1.89	0.53
14:P:176:ARG:HD3	14:P:178:TYR:CE1	2.44	0.53
1:A:3134:C:O4'	1:A:3134:C:O2	2.25	0.53
1:A:2552:U:C2	1:A:2553:G:C8	2.97	0.53
32:7:143:TRP:HA	32:7:143:TRP:CE3	2.44	0.53
11:M:233:ARG:NH2	11:M:247:ILE:HD11	2.24	0.53
1:A:2479:C:H2'	1:A:2479:C:O2	2.08	0.53
1:A:2542:G:N2	1:A:2543:C:C2	2.77	0.52
3:D:188:PRO:O	3:D:191:THR:HG23	2.10	0.52
4:E:233:GLN:OE1	4:E:233:GLN:N	2.42	0.52
1:A:3212:C:O4'	1:A:3212:C:O2	2.24	0.52
30:5:309:LEU:HD11	30:5:347:THR:OG1	2.09	0.52
1:A:3066:C:O2'	4:E:233:GLN:HA	2.09	0.52
13:O:77:ASP:HA	13:O:86:ILE:HD11	1.90	0.52
1:A:2042:U:N3	1:A:2043:C:C5	2.76	0.52
1:A:2686:G:C2	1:A:2687:C:C4	2.98	0.52
1:A:2428:C:C2	1:A:2436:G:N2	2.78	0.52
1:A:2596:G:C2	1:A:2597:C:C2	2.97	0.52
22:X:177:HIS:HB3	22:X:178:PRO:CD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2524:A:H2'	1:A:2524:A:N3	2.25	0.52
29:4:79:CYS:SG	29:4:92:CYS:SG	3.02	0.52
1:A:2493:C:N3	1:A:2540:C:H1'	2.24	0.52
1:A:2263:C:O2	1:A:2263:C:C2'	2.57	0.52
6:H:94:LEU:HD22	6:H:116:LYS:HA	1.91	0.52
2:B:1623:G:C6	2:B:1624:C:C4	2.98	0.52
6:H:55:ILE:CD1	6:H:55:ILE:N	2.73	0.52
30:5:329:TYR:CE2	30:5:336:LEU:HD22	2.45	0.52
1:A:1683:C:C2	1:A:1770:G:C2	2.98	0.52
1:A:2254:C:N3	1:A:2255:C:C5	2.77	0.52
1:A:2086:A:H2'	1:A:2087:U:H6	1.74	0.52
1:A:2724:G:H1'	1:A:2990:A:C5	2.44	0.52
1:A:2735:G:C6	1:A:2736:C:C4	2.98	0.52
1:A:3206:C:O2	1:A:3206:C:O4'	2.25	0.52
1:A:1822:U:O2	1:A:2707:A:O2'	2.27	0.52
1:A:3019:G:C6	1:A:3020:C:C4	2.97	0.52
1:A:3022:G:C6	1:A:3023:C:C4	2.98	0.52
1:A:2660:U:C4	1:A:2661:U:C5	2.97	0.52
1:A:2660:U:N3	1:A:2661:U:C4	2.78	0.52
1:A:2661:U:C2	1:A:2662:A:C8	2.97	0.52
1:A:2141:U:O2	1:A:2141:U:H2'	2.07	0.52
30:5:140:VAL:CG2	30:5:416:ALA:HB2	2.40	0.52
5:F:82:LEU:HD21	5:F:189:ILE:CD1	2.40	0.52
9:K:14:PHE:CE2	18:T:206:ARG:HG3	2.45	0.52
3:D:139:ILE:HD12	3:D:150:TRP:CE3	2.45	0.52
1:A:2688:C:C2	1:A:2702:G:C2	2.98	0.52
1:A:3009:C:O4'	1:A:3009:C:O2	2.24	0.52
1:A:2960:U:O2	1:A:2960:U:H2'	2.10	0.52
1:A:2333:G:N2	1:A:2334:C:C2	2.78	0.52
1:A:1894:G:C6	1:A:1895:C:C4	2.98	0.52
13:O:26:ILE:HD12	15:Q:264:TRP:HE3	1.75	0.52
1:A:2661:U:N3	1:A:2662:A:N7	2.58	0.52
1:A:2004:G:C6	1:A:2005:C:C4	2.98	0.52
13:O:146:ASN:H	13:O:146:ASN:HD22	1.58	0.52
1:A:3024:U:C2	1:A:3025:A:C8	2.98	0.51
1:A:2493:C:N4	1:A:2540:C:O2	2.43	0.51
1:A:2022:G:H1'	1:A:2294:A:C2	2.45	0.51
1:A:2615:A:C5	10:L:58:ILE:HG23	2.44	0.51
1:A:2030:U:O4	1:A:2124:A:N1	2.43	0.51
1:A:2865:C:O2	1:A:2865:C:H2'	2.10	0.51
1:A:1975:U:H6	1:A:1975:U:O5'	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2192:A:H2'	1:A:2193:U:C6	2.45	0.51
1:A:2011:G:O6	7:I:113:ARG:NH2	138.93	0.51
1:A:2043:C:C4	1:A:2044:A:N7	2.79	0.51
33:8:99:GLN:HE22	33:8:103:LEU:HD21	1.75	0.51
23:Y:90:LEU:HB3	23:Y:145:VAL:HG21	1.92	0.51
1:A:3204:C:O2	1:A:3204:C:O4'	2.26	0.51
26:1:41:LEU:HD22	26:1:43:LEU:HG	1.93	0.51
22:X:148:ALA:CB	22:X:153:LEU:HD23	2.39	0.51
1:A:2004:G:C2	1:A:2005:C:C2	2.98	0.51
28:3:107:VAL:HB	28:3:161:MET:HG2	1.92	0.51
1:A:1809:U:O2	1:A:1809:U:H2'	2.10	0.51
1:A:2194:U:C4	1:A:2195:A:N6	2.79	0.51
7:I:116:LEU:HG	7:I:121:ILE:HG23	1.91	0.51
1:A:2331:C:O2	1:A:2331:C:C2'	2.59	0.51
19:U:12:LEU:HB2	30:5:82:TYR:CE2	2.46	0.51
21:W:107:HIS:ND1	21:W:108:PRO:CD	2.74	0.51
11:M:157:GLN:HG3	11:M:177:ALA:O	2.09	0.51
1:A:2822:C:O2'	1:A:2915:C:OP2	2.27	0.51
1:A:2489:C:C2	1:A:2647:G:C2	2.98	0.51
1:A:1922:C:C4	1:A:1923:C:C5	2.99	0.51
1:A:1946:C:H2'	1:A:1946:C:O2	2.11	0.51
1:A:2022:G:C2	1:A:2023:U:C6	2.98	0.51
1:A:2702:G:C6	1:A:2703:C:C4	2.99	0.51
1:A:2587:G:C6	1:A:2588:C:C4	2.99	0.51
1:A:2987:U:O2	1:A:2991:U:H5	1.93	0.51
9:K:48:HIS:CD2	18:T:209:VAL:HG11	2.45	0.51
1:A:2193:U:H5"	1:A:2193:U:H6	1.76	0.51
30:5:124:THR:HG23	30:5:318:PHE:CD2	2.42	0.51
4:E:119:VAL:HG11	4:E:284:TYR:HB3	1.93	0.51
13:O:30:ARG:NH1	13:O:78:PHE:O	2.44	0.51
1:A:2275:U:H1'	16:R:12:ASN:HB3	1.93	0.51
1:A:3143:U:C2	1:A:3144:A:C8	2.98	0.51
1:A:2694:A:C6	1:A:2985:C:H1'	2.46	0.51
1:A:2610:U:C2	1:A:2611:C:C5	2.98	0.51
1:A:2185:G:C2	1:A:2186:C:C6	2.98	0.51
1:A:2493:C:H2'	1:A:2494:C:O5'	2.11	0.51
18:T:94:ILE:HG23	18:T:142:ILE:HD13	1.92	0.51
1:A:2542:G:C6	1:A:2543:C:C4	2.99	0.50
13:O:43:GLU:OE2	25:0:127:TYR:OH	2.24	0.50
1:A:2080:U:O4'	1:A:2080:U:O2	2.27	0.50
1:A:2574:G:C2	1:A:2584:C:C2	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:56:LEU:HD13	20:V:86:VAL:HG21	1.92	0.50
1:A:3030:A:C3'	1:A:3031:G:H5'	2.40	0.50
1:A:2600:A:HO2'	1:A:2601:A:P	2.32	0.50
1:A:3055:U:H2'	1:A:3056:C:O4'	2.11	0.50
19:U:19:VAL:HG22	34:9:136:LEU:HD13	1.92	0.50
1:A:3022:G:N2	1:A:3023:C:C2	2.79	0.50
32:7:105:LEU:HB2	32:7:128:LEU:HD12	1.92	0.50
1:A:2712:G:C6	1:A:2713:C:N4	2.79	0.50
1:A:2796:G:C6	1:A:2797:C:C4	2.99	0.50
1:A:2607:U:C2	1:A:2618:U:O2	2.65	0.50
1:A:2087:U:C2	1:A:2088:U:C6	3.00	0.50
3:D:126:VAL:CG2	3:D:163:ILE:HD11	2.42	0.50
1:A:1671:G:C2	1:A:1672:C:C2	3.00	0.50
1:A:1671:G:N1	1:A:1672:C:C4	2.79	0.50
1:A:2652:G:C2	1:A:2653:C:C2	3.00	0.50
1:A:1907:A:N3	1:A:2930:U:O2'	2.39	0.50
1:A:2161:A:C2	1:A:3182:A:C2	2.99	0.50
30:5:318:PHE:C	30:5:318:PHE:CD1	2.84	0.50
1:A:2921:A:H2'	1:A:2921:A:N3	2.26	0.50
5:F:120:VAL:HG11	5:F:142:ARG:HB3	1.94	0.50
1:A:1940:A:C2	1:A:1941:G:C8	2.99	0.50
19:U:64:PRO:HB2	19:U:100:ALA:HB3	1.93	0.50
1:A:2596:G:C6	1:A:2597:C:C4	2.99	0.50
5:F:175:LYS:O	5:F:179:THR:HG23	2.12	0.50
1:A:3102:U:O2	1:A:3102:U:H2'	2.11	0.50
1:A:2415:C:O4'	1:A:2415:C:O2	2.27	0.50
1:A:2731:U:C4	1:A:2918:A:N1	2.79	0.50
23:Y:167:ALA:HB3	23:Y:169:ARG:NH1	2.27	0.50
13:O:94:ALA:HB3	13:O:95:PRO:HD3	1.93	0.50
3:D:216:LEU:HD11	3:D:224:ALA:HB1	1.94	0.50
1:A:1747:G:N2	1:A:1750:G:O2'	2.45	0.50
1:A:1894:G:C2	1:A:1895:C:C2	3.00	0.49
1:A:2568:G:C6	1:A:2569:C:C4	3.00	0.49
1:A:2571:G:N2	1:A:2572:C:C2	2.80	0.49
30:5:112:ARG:HD3	30:5:304:LEU:HD13	1.93	0.49
1:A:2926:A:H5"	1:A:2926:A:C8	2.46	0.49
1:A:3131:G:HO2'	1:A:3132:G:H5'	1.77	0.49
1:A:2493:C:H3'	1:A:2493:C:O2	2.12	0.49
1:A:2751:G:C6	1:A:2752:C:C4	3.00	0.49
1:A:2595:A:H2'	1:A:2596:G:O4'	2.12	0.49
1:A:2440:G:C2	1:A:2441:C:C2	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2065:A:O2'	1:A:2066:C:O4'	2.31	0.49
1:A:2587:G:C2	1:A:2588:C:C2	3.01	0.49
1:A:3003:A:H2'	1:A:3004:C:O4'	2.13	0.49
21:W:69:THR:HG22	21:W:88:CYS:HB2	1.93	0.49
15:Q:237:ASN:N	15:Q:237:ASN:OD1	2.43	0.49
4:E:231:HIS:N	4:E:232:GLY:CA	2.72	0.49
23:Y:90:LEU:HD21	23:Y:142:LEU:HG	1.93	0.49
6:H:62:VAL:HG11	22:X:65:VAL:HG21	1.93	0.49
1:A:3131:G:C6	1:A:3132:G:N3	2.80	0.49
22:X:36:ARG:NH1	22:X:151:GLU:HG3	2.26	0.49
1:A:2466:A:C2	1:A:2467:A:C6	3.00	0.49
13:O:36:LEU:N	13:O:42:ILE:HD11	2.27	0.49
14:P:65:ARG:HA	14:P:75:GLU:OE2	2.13	0.49
15:Q:261:ASN:HD22	15:Q:262:GLN:N	2.10	0.49
1:A:2540:C:C6	1:A:2541:C:C6	3.01	0.49
17:S:108:VAL:HG11	17:S:195:ILE:HG12	1.95	0.49
7:I:83:ARG:HA	7:I:134:PHE:CE1	2.47	0.49
1:A:2395:A:OP1	30:5:173:ARG:NH2	2.44	0.49
7:I:47:LEU:HD12	12:N:226:ILE:HG12	1.94	0.49
21:W:67:ILE:HG21	21:W:131:VAL:HG11	1.94	0.49
1:A:2976:G:H2'	1:A:2977:G:O4'	2.12	0.49
21:W:102:GLU:OE2	31:6:74:TYR:CB	2.56	0.49
1:A:2748:A:H2'	1:A:2749:A:C1'	2.43	0.49
1:A:2395:A:H1'	30:5:385:HIS:HB2	1.95	0.49
1:A:2420:U:C2'	1:A:2421:G:H5'	2.43	0.49
11:M:156:VAL:O	11:M:176:THR:HA	2.13	0.49
1:A:3215:C:C2	1:A:3226:G:C2	3.00	0.49
10:L:123:ILE:HD12	10:L:141:ALA:CB	2.43	0.49
1:A:3030:A:C2	1:A:3031:G:N9	2.80	0.49
2:B:1623:G:C2	2:B:1624:C:C2	3.00	0.49
23:Y:173:PHE:CZ	27:2:79:ILE:HG21	2.48	0.49
1:A:2630:U:H2'	1:A:2631:G:C8	2.46	0.49
1:A:2000:C:H2'	1:A:2000:C:O2	2.13	0.49
6:H:56:VAL:CG1	6:H:80:TYR:CB	2.86	0.49
1:A:1824:U:C5	9:K:116:LEU:HD13	2.48	0.49
17:S:136:VAL:HG21	17:S:154:VAL:HG11	1.93	0.49
2:B:1643:A:H2'	2:B:1644:G:O4'	2.13	0.49
25:0:125:TYR:C	25:0:125:TYR:CD2	2.85	0.49
1:A:2611:C:C2	1:A:2622:G:C2	3.01	0.49
1:A:1993:A:C6	1:A:1995:A:C8	3.00	0.49
20:V:122:LEU:HD12	20:V:133:ILE:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:119:VAL:HG11	15:Q:164:PHE:CD2	2.48	0.49
1:A:2405:C:O4'	1:A:2405:C:O2	2.31	0.49
1:A:2541:C:C4	1:A:2542:G:N7	2.81	0.48
14:P:55:LEU:CB	14:P:61:ALA:HB2	2.43	0.48
31:6:144:GLY:N	31:6:145:PRO:HD2	2.27	0.48
23:Y:164:ARG:NH1	23:Y:181:PHE:O	2.46	0.48
4:E:234:THR:OG1	4:E:235:LYS:N	2.46	0.48
10:L:84:ALA:HB1	10:L:105:VAL:CG1	2.43	0.48
1:A:1728:U:O2'	22:X:96:LYS:O	2.26	0.48
1:A:2558:A:H4'	1:A:2559:U:OP2	2.10	0.48
30:5:127:LYS:HD2	30:5:251:HIS:ND1	2.25	0.48
8:J:127:ASP:HB3	8:J:130:PHE:HB2	1.94	0.48
29:4:75:ARG:HB2	29:4:98:HIS:CD2	2.49	0.48
1:A:3020:C:C5	1:A:3021:C:C5	3.02	0.48
1:A:2129:G:C2	1:A:2137:C:N3	2.81	0.48
1:A:1845:C:O2'	1:A:2297:A:N1	2.38	0.48
7:I:125:VAL:HG22	7:I:151:ASN:O	2.13	0.48
14:P:132:ALA:HB1	14:P:167:GLY:HA3	1.94	0.48
13:O:38:ARG:HG2	13:O:85:LEU:HD11	1.96	0.48
1:A:2973:U:C2	1:A:2974:A:C8	3.01	0.48
1:A:2339:G:C6	1:A:2340:C:C4	3.02	0.48
1:A:2507:A:C8	1:A:2507:A:H5'	2.47	0.48
1:A:2466:A:H2'	1:A:2467:A:C8	2.47	0.48
1:A:2987:U:O2	1:A:2991:U:C5	2.66	0.48
1:A:1941:G:C6	1:A:1942:C:C4	3.01	0.48
31:6:117:VAL:CB	31:6:120:GLU:N	2.76	0.48
19:U:8:PRO:HA	23:Y:183:GLN:HE22	1.77	0.48
5:F:280:TYR:CD1	11:M:125:ARG:HD2	2.49	0.48
24:Z:67:HIS:CD2	24:Z:102:ASN:HB2	2.49	0.48
7:I:121:ILE:HD12	7:I:156:SER:HB2	1.96	0.48
1:A:1750:G:OP2	28:3:113:ARG:NH2	2.47	0.48
1:A:2132:A:H2	1:A:2690:G:N3	2.11	0.48
1:A:3021:C:C4	1:A:3022:G:C8	3.02	0.48
32:7:180:CYS:SG	32:7:298:GLN:NE2	2.86	0.48
32:7:169:ALA:HB2	32:7:181:TYR:CE1	2.49	0.48
1:A:2892:A:O2'	1:A:2893:A:C8	2.60	0.48
31:6:173:LEU:HD22	31:6:175:VAL:HG23	1.96	0.48
1:A:2130:A:O2'	13:O:25:ARG:NH1	81.92	0.48
1:A:2327:U:H2'	1:A:2328:C:O4'	2.14	0.48
25:0:119:LYS:O	25:0:120:HIS:CG	2.67	0.48
1:A:2546:G:N1	1:A:2547:C:C4	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:2:ALA:N	19:U:7:TYR:HH	2.11	0.48
1:A:2493:C:C4	1:A:2540:C:C2	3.01	0.48
1:A:2996:G:C2	1:A:2997:A:C8	3.02	0.48
1:A:1981:G:C2	1:A:1982:G:C8	3.01	0.48
1:A:1707:C:C5	23:Y:185:VAL:HG11	2.48	0.48
1:A:2256:U:C4	1:A:2257:C:C5	3.02	0.48
1:A:1946:C:C6	1:A:1946:C:H5"	2.49	0.48
1:A:2194:U:C2	1:A:2195:A:N7	2.82	0.47
12:N:72:ILE:HD11	12:N:96:TYR:CZ	2.49	0.47
1:A:2467:A:C2	1:A:2660:U:O2	2.67	0.47
19:U:9:LEU:HB3	20:V:213:VAL:HG11	1.96	0.47
7:I:135:LEU:HD11	7:I:147:PHE:CD2	2.48	0.47
24:Z:66:LEU:HD12	24:Z:122:LEU:HD23	1.96	0.47
1:A:2193:U:C6	1:A:2193:U:H5"	2.49	0.47
32:7:154:ILE:HD11	32:7:297:PHE:CG	2.49	0.47
4:E:99:LEU:HD13	4:E:124:VAL:HG21	1.96	0.47
1:A:2056:G:C6	1:A:2057:C:C4	3.02	0.47
4:E:230:THR:C	4:E:232:GLY:HA2	2.34	0.47
15:Q:189:TYR:CD1	15:Q:243:ILE:HG12	2.49	0.47
1:A:3066:C:O2'	4:E:233:GLN:HG3	2.14	0.47
1:A:2173:G:N2	8:J:150:SER:O	2.44	0.47
1:A:2685:U:O2	1:A:3103:C:O2'	2.32	0.47
10:L:95:ARG:HA	10:L:95:ARG:NE	2.29	0.47
30:5:105:TYR:CG	30:5:262:ILE:HD13	2.50	0.47
13:O:36:LEU:HD13	13:O:125:TYR:CZ	2.49	0.47
1:A:2943:G:C6	1:A:2944:C:C4	3.02	0.47
16:R:21:ILE:HG22	16:R:25:LEU:HD12	1.95	0.47
1:A:1681:G:C6	1:A:1682:C:C4	3.03	0.47
1:A:2087:U:N3	1:A:2088:U:C5	2.83	0.47
9:K:22:ASP:HA	9:K:60:MET:HG3	1.97	0.47
7:I:127:PRO:O	7:I:130:VAL:HG12	2.14	0.47
1:A:1671:G:C4	1:A:1672:C:C5	3.02	0.47
19:U:17:LEU:HD21	34:9:136:LEU:HD12	1.96	0.47
1:A:2949:C:C2	1:A:2976:G:C2	3.03	0.47
10:L:123:ILE:CG2	10:L:127:LEU:HD12	2.44	0.47
1:A:1914:A:O3'	27:2:74:ALA:HB1	2.15	0.47
14:P:77:TRP:O	14:P:95:HIS:CD2	2.59	0.47
1:A:2600:A:O2'	1:A:2601:A:O5'	2.22	0.47
1:A:2707:A:H2'	1:A:2708:C:O4'	2.14	0.47
1:A:2031:A:C2	1:A:2865:C:C2	3.02	0.47
25:0:120:HIS:CD2	25:0:121:VAL:HG23	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:161:LEU:HD23	30:5:52:ILE:HD12	1.97	0.47
31:6:217:LEU:HD21	31:6:219:THR:HG23	1.96	0.47
1:A:2932:G:C2'	1:A:2933:G:H5'	2.45	0.47
1:A:2184:A:C2	1:A:2185:G:C8	3.03	0.47
4:E:129:VAL:HG21	4:E:187:ILE:CD1	2.40	0.47
1:A:2512:A:O2'	1:A:2541:C:OP1	2.21	0.47
1:A:2109:A:N6	1:A:2946:A:C8	2.83	0.47
30:5:218:LEU:HD23	30:5:262:ILE:HD11	1.96	0.47
1:A:2797:C:C2	1:A:2798:A:C8	3.03	0.47
1:A:2406:A:N1	30:5:112:ARG:NH2	2.62	0.47
30:5:113:LEU:HD23	30:5:265:LEU:HD21	1.96	0.47
3:D:196:VAL:HG12	3:D:197:GLU:O	2.14	0.47
1:A:1879:G:C6	1:A:1880:C:C4	3.03	0.47
5:F:91:PRO:HG2	11:M:12:ALA:HB1	1.95	0.47
5:F:83:HIS:CE1	5:F:274:LEU:HD21	2.50	0.47
1:A:2212:C:H5'	29:4:77:LYS:NZ	2.30	0.47
1:A:3228:U:O4'	1:A:3228:U:O2	2.30	0.47
32:7:251:ILE:HG23	32:7:251:ILE:O	2.14	0.47
1:A:2428:C:C4	1:A:2436:G:N1	2.83	0.47
7:I:60:ILE:HG21	7:I:65:LEU:HD21	1.95	0.47
9:K:80:HIS:ND1	9:K:81:THR:O	2.45	0.47
1:A:3022:G:C2	1:A:3023:C:C2	3.03	0.47
1:A:2733:G:N2	1:A:2929:C:C2	2.83	0.47
1:A:2056:G:C2	1:A:2057:C:C2	3.03	0.47
1:A:3221:A:H2'	1:A:3222:C:O4'	2.15	0.47
1:A:2025:C:C2	1:A:2269:G:N2	2.83	0.47
1:A:3158:A:C8	1:A:3159:A:C8	3.03	0.47
1:A:2428:C:N3	1:A:2436:G:C2	2.82	0.47
1:A:2395:A:C2	1:A:2396:C:C6	3.04	0.47
1:A:2198:A:N3	1:A:2198:A:H2'	2.29	0.47
8:J:119:GLU:O	8:J:123:ILE:HG23	2.15	0.47
20:V:72:LYS:HD2	20:V:91:LEU:HD22	1.97	0.47
1:A:2855:G:C6	1:A:2856:C:C4	3.03	0.47
1:A:2311:U:C5	1:A:2675:G:N2	2.83	0.47
1:A:2096:U:O4	11:M:57:ARG:NH1	2.47	0.47
24:Z:75:THR:HB	24:Z:83:LYS:HG2	1.97	0.47
1:A:3149:C:N3	1:A:3163:G:C2	2.83	0.47
3:D:187:LEU:HD21	3:D:244:VAL:HG12	1.97	0.47
1:A:1780:U:HO2'	1:A:1781:A:P	2.37	0.47
32:7:166:LEU:HD22	32:7:183:VAL:HG22	1.97	0.46
1:A:2542:G:N1	1:A:2543:C:C4	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2042:U:C2	1:A:2043:C:C6	3.03	0.46
11:M:115:PRO:HA	11:M:153:ASN:ND2	2.30	0.46
1:A:2952:U:N3	1:A:2953:U:C5	2.83	0.46
1:A:2560:G:H8	1:A:2560:G:H5"	1.80	0.46
1:A:2551:G:C6	1:A:2552:U:C4	3.04	0.46
1:A:2494:C:O2	1:A:2494:C:H2'	2.13	0.46
30:5:211:ALA:HB1	30:5:322:LEU:HD22	1.96	0.46
1:A:2596:G:C6	1:A:2597:C:N3	2.83	0.46
1:A:2596:G:H2'	1:A:2597:C:O4'	2.16	0.46
15:Q:240:ILE:CG2	15:Q:243:ILE:HG13	2.45	0.46
22:X:157:PHE:CZ	22:X:161:LEU:HD11	2.51	0.46
14:P:62:ARG:NH1	21:W:137:LYS:O	2.48	0.46
1:A:1684:C:H41	23:Y:225:ASN:HD21	1.63	0.46
4:E:97:VAL:HG22	4:E:145:LEU:CD1	2.44	0.46
1:A:2752:C:C2	1:A:2753:A:C8	3.03	0.46
1:A:1977:U:H2'	1:A:1978:A:H8	1.77	0.46
1:A:2593:G:N2	1:A:2631:G:H2'	2.31	0.46
2:B:1664:G:C6	2:B:1665:C:C4	3.04	0.46
1:A:2794:C:N3	1:A:2795:U:C5	2.83	0.46
1:A:2443:C:O2	1:A:2443:C:O4'	2.30	0.46
13:O:146:ASN:N	13:O:146:ASN:HD22	2.14	0.46
1:A:2757:A:H5'	1:A:2758:G:OP2	2.15	0.46
1:A:3158:A:O2'	13:O:11:HIS:O	2.33	0.46
1:A:2938:A:C2	1:A:2993:U:O4	2.68	0.46
11:M:100:ARG:NH1	11:M:126:GLY:O	2.48	0.46
22:X:241:GLN:HA	22:X:241:GLN:HE21	1.79	0.46
1:A:2556:A:C3'	1:A:2557:C:C5'	2.86	0.46
1:A:2551:G:C5	1:A:2552:U:C5	3.04	0.46
11:M:155:GLU:OE1	11:M:177:ALA:CB	2.64	0.46
1:A:2606:U:N3	1:A:2608:G:O4'	2.49	0.46
24:Z:100:HIS:HB3	24:Z:106:VAL:HG11	1.98	0.46
1:A:2550:A:N1	1:A:2551:G:N7	2.64	0.46
1:A:2043:C:N3	1:A:2044:A:C8	2.83	0.46
1:A:2173:G:C6	1:A:2188:A:C2	3.04	0.46
2:B:1664:G:C2	2:B:1665:C:C2	3.03	0.46
5:F:93:LEU:HD12	13:O:91:GLN:HG2	131.74	0.46
1:A:2182:G:N1	1:A:2183:C:C4	2.84	0.46
19:U:82:HIS:CE1	19:U:83:ARG:HG3	2.51	0.46
1:A:2469:A:H2'	1:A:2470:G:O4'	2.15	0.46
1:A:3073:C:C5	1:A:3095:G:N2	2.83	0.46
1:A:2139:U:C4	24:Z:76:ARG:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1927:G:H5"	1:A:1927:G:H8	1.80	0.46
18:T:99:ILE:HD12	18:T:140:LEU:HB2	1.97	0.46
1:A:2568:G:C2	1:A:2569:C:C2	3.04	0.46
1:A:3116:C:C2	1:A:3117:C:C6	3.04	0.46
30:5:346:GLY:N	30:5:353:HIS:O	2.49	0.46
30:5:297:ALA:HB1	30:5:302:HIS:HB2	1.98	0.46
1:A:2503:A:C2	1:A:3074:A:C5	3.04	0.46
1:A:1675:A:N3	1:A:1813:C:N4	2.63	0.46
1:A:2185:G:N3	1:A:2186:C:C6	2.84	0.46
1:A:2686:G:C6	1:A:2687:C:N4	2.84	0.46
1:A:1750:G:O2'	1:A:1751:A:OP2	2.32	0.46
7:I:119:HIS:HB3	7:I:160:LYS:HD2	1.97	0.46
32:7:221:VAL:HG21	32:7:254:LEU:HD12	1.98	0.46
22:X:101:LEU:N	22:X:101:LEU:HD23	2.31	0.46
18:T:209:VAL:HG12	18:T:210:HIS:CD2	2.50	0.46
1:A:2750:U:N3	1:A:2751:G:N7	2.63	0.46
11:M:154:ILE:HD12	11:M:167:ILE:HD13	1.98	0.46
22:X:118:ILE:HD11	22:X:191:TYR:CD2	2.51	0.46
15:Q:231:LYS:HB3	15:Q:233:TRP:CZ2	2.51	0.46
1:A:1932:G:C6	1:A:1933:C:C4	3.04	0.46
1:A:2852:C:O2	1:A:2852:C:O4'	2.31	0.46
1:A:2194:U:OP1	7:I:124:LYS:CE	2.64	0.45
15:Q:240:ILE:HG21	15:Q:243:ILE:CG1	2.47	0.45
28:3:94:LEU:HD13	28:3:161:MET:HA	1.98	0.45
12:N:89:ILE:HD12	12:N:161:VAL:HB	1.98	0.45
14:P:93:VAL:HG11	14:P:140:ILE:HD13	1.98	0.45
9:K:154:ARG:NH1	9:K:157:GLU:HG3	2.30	0.45
1:A:1877:U:N3	1:A:1897:A:C2	2.84	0.45
1:A:2466:A:H2'	1:A:2467:A:O4'	2.16	0.45
13:O:94:ALA:HB3	13:O:95:PRO:CD	2.46	0.45
10:L:119:ILE:HG21	10:L:123:ILE:HD11	1.98	0.45
28:3:118:HIS:CD2	28:3:169:ARG:HG2	2.52	0.45
13:O:41:ARG:HG3	13:O:124:GLU:HB3	1.98	0.45
1:A:2336:U:C2	1:A:2337:A:C8	3.05	0.45
20:V:94:HIS:CD2	20:V:113:ALA:HB2	2.51	0.45
16:R:50:PHE:O	16:R:54:THR:HG23	2.16	0.45
17:S:171:ILE:HD12	17:S:184:ARG:HG2	1.97	0.45
1:A:1810:A:H2'	1:A:1811:A:C8	2.52	0.45
2:B:1611:G:C6	2:B:1612:C:N4	2.85	0.45
28:3:110:VAL:HG13	28:3:158:LEU:HD22	1.97	0.45
28:3:125:ARG:HD2	28:3:129:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2755:A:H5"	1:A:2756:C:OP2	2.17	0.45
23:Y:109:ARG:CZ	23:Y:136:VAL:HG22	2.47	0.45
1:A:1861:U:C2	1:A:1862:U:C5	3.05	0.45
23:Y:141:ALA:O	23:Y:145:VAL:HG23	2.17	0.45
1:A:2004:G:C5	1:A:2005:C:C4	3.04	0.45
32:7:74:ASP:N	32:7:75:PRO:HD3	2.31	0.45
1:A:1839:C:H2'	1:A:1840:C:C6	2.51	0.45
1:A:2372:U:O4'	1:A:2372:U:O2	2.33	0.45
1:A:1864:A:C6	1:A:1865:C:C5	3.05	0.45
8:J:70:ILE:HD13	8:J:80:ILE:HG12	1.98	0.45
1:A:2712:G:C2	1:A:2713:C:C2	3.04	0.45
1:A:3042:U:C4	1:A:3043:C:H1'	2.52	0.45
30:5:98:LEU:HD22	30:5:272:ASP:OD1	2.16	0.45
1:A:2756:C:P	22:X:112:ARG:HH22	2.40	0.45
1:A:2660:U:C2	1:A:2661:U:C6	3.04	0.45
1:A:1865:C:C4	1:A:1866:U:C5	3.04	0.45
1:A:2733:G:C2	1:A:2929:C:N3	2.85	0.45
1:A:2688:C:C2	1:A:2702:G:N2	2.85	0.45
1:A:2607:U:O2	1:A:2618:U:O4'	2.35	0.45
16:R:50:PHE:CD2	17:S:170:ILE:HG21	2.51	0.45
1:A:2233:U:C2	4:E:248:ILE:HD12	2.51	0.45
11:M:61:THR:HG22	11:M:61:THR:O	2.16	0.45
1:A:2022:G:C2	1:A:2023:U:C5	3.03	0.45
13:O:36:LEU:HD12	13:O:52:MET:HE2	1.97	0.45
1:A:2536:G:H5'	3:D:276:HIS:CD2	2.52	0.45
16:R:24:VAL:HG11	16:R:43:VAL:HG22	1.98	0.45
32:7:199:LEU:O	32:7:203:THR:HG23	2.17	0.45
22:X:42:HIS:ND1	22:X:86:ILE:HD11	2.31	0.45
5:F:227:PRO:O	5:F:230:ILE:HG22	2.17	0.45
21:W:61:VAL:HG13	21:W:65:ASN:HB2	1.99	0.45
1:A:2558:A:H3'	1:A:2559:U:O4'	2.17	0.45
1:A:2466:A:N1	1:A:2661:U:C4	2.85	0.45
1:A:1834:U:C4	18:T:206:ARG:HA	2.51	0.45
1:A:1907:A:H2'	1:A:1908:A:C8	2.51	0.45
7:I:125:VAL:HG23	7:I:152:MET:SD	2.57	0.45
18:T:141:TYR:CE1	18:T:179:VAL:HB	2.52	0.45
14:P:76:PHE:O	14:P:76:PHE:CD2	2.70	0.45
1:A:2559:U:H2'	1:A:2560:G:OP2	2.17	0.45
1:A:1876:U:H2'	1:A:1877:U:H6	1.80	0.45
18:T:94:ILE:HD11	18:T:106:LEU:HD21	1.99	0.45
15:Q:224:MET:SD	15:Q:243:ILE:CG2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2726:C:N3	1:A:2727:C:C5	2.85	0.45
1:A:2540:C:C4	1:A:2541:C:C6	3.05	0.45
7:I:83:ARG:HG2	7:I:134:PHE:CD1	2.52	0.45
1:A:1809:U:O2	1:A:1809:U:C2'	2.65	0.45
1:A:1750:G:O2'	1:A:1751:A:P	2.75	0.45
11:M:78:ILE:O	28:3:113:ARG:HD3	2.17	0.45
13:O:152:LEU:HD11	32:7:315:LYS:HB3	1.98	0.45
1:A:3069:A:C2	1:A:3070:G:C8	3.05	0.45
34:9:97:ALA:N	34:9:98:PRO:HD2	2.32	0.45
1:A:2490:C:C2	1:A:2646:G:N2	2.85	0.44
25:0:121:VAL:HG12	25:0:122:LEU:O	2.18	0.44
7:I:115:GLN:O	7:I:118:LYS:HB2	2.16	0.44
15:Q:133:PHE:CD2	15:Q:162:ILE:HD12	2.52	0.44
19:U:10:TYR:CE2	34:9:55:GLU:HB2	2.52	0.44
30:5:177:CYS:N	30:5:178:PRO:HD2	2.33	0.44
15:Q:176:VAL:HG11	15:Q:179:LEU:HG	2.00	0.44
1:A:3030:A:O2'	1:A:3031:G:H5'	2.18	0.44
1:A:1862:U:C2	1:A:1863:A:C8	3.05	0.44
1:A:2253:U:N3	1:A:2254:C:C5	2.84	0.44
22:X:42:HIS:CG	22:X:86:ILE:HD11	2.53	0.44
1:A:2341:C:N4	34:9:25:ARG:HA	2.32	0.44
1:A:3105:A:H2'	1:A:3106:C:O4'	2.17	0.44
1:A:2453:G:C2	1:A:2454:G:C8	3.05	0.44
1:A:2898:U:O2	1:A:2898:U:O4'	2.33	0.44
15:Q:111:PHE:CZ	15:Q:117:LEU:HD11	2.52	0.44
7:I:167:ILE:O	7:I:170:THR:HG22	2.18	0.44
1:A:2971:A:C2	1:A:2972:A:C8	3.06	0.44
1:A:3131:G:O6	1:A:3132:G:C2	2.70	0.44
22:X:127:VAL:HG13	22:X:127:VAL:O	2.17	0.44
1:A:3002:G:C2	1:A:3057:C:C2	3.05	0.44
1:A:2333:G:C6	1:A:2334:C:N4	2.86	0.44
1:A:2652:G:C6	1:A:2653:C:C4	3.05	0.44
32:7:214:LEU:HD12	32:7:257:ILE:HG22	1.99	0.44
30:5:104:CYS:SG	30:5:105:TYR:N	2.91	0.44
1:A:2198:A:N6	8:J:150:SER:OG	2.47	0.44
1:A:2722:A:C6	1:A:2990:A:C2	3.05	0.44
1:A:3004:C:C4	1:A:3029:A:C5	3.06	0.44
1:A:1870:A:N7	1:A:1902:C:C2	2.85	0.44
1:A:2999:C:H4'	4:E:224:PHE:CE2	2.52	0.44
4:E:208:ALA:HB3	4:E:290:PRO:HB2	2.00	0.44
1:A:3128:A:H2'	1:A:3129:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1864:A:C5	1:A:1865:C:C5	3.05	0.44
1:A:2161:A:H2'	1:A:2162:C:O4'	2.17	0.44
1:A:2420:U:H2'	1:A:2421:G:H5'	1.99	0.44
31:6:139:TRP:CE2	31:6:144:GLY:HA2	2.53	0.44
1:A:2606:U:C4	1:A:2608:G:O4'	2.70	0.44
28:3:125:ARG:NH2	28:3:145:ARG:O	2.49	0.44
15:Q:148:THR:HG22	15:Q:165:GLU:HA	2.00	0.44
1:A:2418:A:C2	1:A:2419:C:C6	3.05	0.44
22:X:148:ALA:CB	22:X:153:LEU:CD2	2.96	0.44
1:A:1671:G:C2	1:A:1672:C:C4	3.05	0.44
1:A:3149:C:C2	1:A:3163:G:N2	2.85	0.44
15:Q:183:LEU:HD11	15:Q:219:GLU:HG3	1.98	0.44
1:A:2302:U:C2	1:A:2303:A:C8	3.06	0.44
1:A:2876:G:C2	1:A:2877:C:C2	3.06	0.44
19:U:99:LEU:HD21	23:Y:64:LEU:CD1	2.46	0.44
1:A:1993:A:N1	1:A:1995:A:C8	2.86	0.44
10:L:114:PRO:HB3	10:L:137:VAL:HG22	2.00	0.44
1:A:1947:C:C2	1:A:1970:G:C2	3.06	0.44
4:E:286:ASN:C	4:E:286:ASN:OD1	2.56	0.44
1:A:2254:C:C2	1:A:2255:C:C6	3.06	0.44
1:A:2876:G:C6	1:A:2877:C:C4	3.05	0.44
4:E:120:THR:HG22	4:E:287:GLY:O	2.17	0.44
29:4:76:CYS:SG	29:4:98:HIS:NE2	2.90	0.44
1:A:3008:C:C2	1:A:3032:G:C2	3.06	0.44
30:5:211:ALA:HB3	30:5:222:VAL:HG22	2.00	0.44
11:M:178:PHE:C	11:M:179:TYR:HD1	2.20	0.44
25:0:119:LYS:O	25:0:120:HIS:ND1	2.51	0.44
7:I:135:LEU:HD11	7:I:147:PHE:CE2	2.53	0.44
21:W:57:GLU:HG3	21:W:98:ARG:HA	2.00	0.44
15:Q:245:PHE:O	15:Q:246:ASP:C	2.57	0.44
1:A:3131:G:O6	1:A:3132:G:C6	2.70	0.43
15:Q:240:ILE:HG21	15:Q:243:ILE:HD11	2.00	0.43
1:A:1884:G:N3	1:A:1895:C:O2'	2.44	0.43
11:M:164:ILE:HA	11:M:174:VAL:HG21	2.00	0.43
7:I:144:LEU:N	7:I:145:PRO:CD	2.81	0.43
1:A:2100:C:H1'	1:A:2135:A:C8	2.53	0.43
14:P:47:PHE:HB3	31:6:342:PHE:CE2	2.53	0.43
1:A:2307:U:O2'	1:A:2308:A:H5'	2.18	0.43
11:M:51:ARG:HB3	11:M:58:GLN:HA	2.00	0.43
5:F:212:TRP:CZ3	5:F:260:VAL:HG21	2.53	0.43
1:A:2590:A:O2'	1:A:2591:A:O5'	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2702:G:C2	1:A:2703:C:C2	3.06	0.43
1:A:2471:G:C2	1:A:2654:U:C5	3.06	0.43
1:A:2527:A:C8	3:D:104:TYR:CE2	3.05	0.43
30:5:401:VAL:O	30:5:401:VAL:HG12	2.18	0.43
32:7:143:TRP:HE3	32:7:143:TRP:HA	1.80	0.43
24:Z:67:HIS:O	24:Z:99:VAL:HA	2.18	0.43
1:A:2171:U:C5	1:A:2173:G:O4'	2.71	0.43
17:S:135:LEU:HD21	17:S:144:LEU:HD22	2.00	0.43
30:5:115:GLU:O	30:5:119:GLN:NE2	2.51	0.43
1:A:2244:U:C4	16:R:128:PHE:CE2	3.06	0.43
1:A:2286:A:H2'	1:A:2287:U:C6	2.54	0.43
12:N:127:PRO:HA	12:N:152:THR:HG22	1.99	0.43
1:A:3034:U:C6	1:A:3053:A:C5	3.06	0.43
1:A:2663:C:C2	1:A:2664:U:C5	3.06	0.43
19:U:26:ILE:HD11	19:U:44:ILE:HD13	2.00	0.43
1:A:1786:C:C2	1:A:1792:G:C2	3.07	0.43
9:K:154:ARG:CZ	9:K:157:GLU:OE2	2.62	0.43
13:O:32:LEU:HB3	13:O:52:MET:HG3	1.99	0.43
1:A:2726:C:H2'	1:A:2726:C:O2	2.19	0.43
9:K:42:LEU:HD23	9:K:47:TYR:CD2	2.53	0.43
14:P:80:LEU:HD23	14:P:80:LEU:C	2.39	0.43
4:E:243:VAL:HG11	4:E:251:VAL:HG22	2.00	0.43
30:5:121:LEU:O	30:5:125:LYS:N	2.51	0.43
1:A:2756:C:C5'	1:A:2756:C:C6	3.01	0.43
32:7:167:VAL:HG13	32:7:182:ASP:HB2	2.00	0.43
15:Q:240:ILE:HD13	15:Q:243:ILE:HD11	2.00	0.43
1:A:1816:G:C6	1:A:1817:C:C4	3.07	0.43
5:F:94:ASP:OD2	11:M:30:ASN:HB2	2.19	0.43
25:0:130:VAL:HG22	25:0:184:TRP:CZ3	2.54	0.43
1:A:1698:C:O2'	1:A:1702:A:N3	2.49	0.43
29:4:84:ARG:HB3	29:4:85:ARG:HD2	2.00	0.43
34:9:131:TYR:HB3	34:9:132:PRO:CD	2.48	0.43
1:A:3131:G:H2'	1:A:3132:G:H8	1.83	0.43
4:E:97:VAL:HG22	4:E:145:LEU:HD12	1.99	0.43
30:5:107:PHE:CZ	30:5:315:LEU:HD13	2.54	0.43
1:A:2537:G:C2	1:A:2538:C:C2	3.07	0.43
1:A:2024:C:H2'	1:A:2025:C:H6	1.84	0.43
1:A:2993:U:H5'	1:A:3063:G:O6	2.19	0.43
4:E:48:TRP:CE2	4:E:51:GLU:HB3	2.54	0.43
1:A:3023:C:C4	1:A:3024:U:C5	3.07	0.43
1:A:3025:A:C2	1:A:3026:U:C5	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:5:318:PHE:CZ	30:5:322:LEU:HD13	2.54	0.43
1:A:1975:U:O5'	1:A:1975:U:C6	2.71	0.43
22:X:87:LEU:HD23	22:X:104:VAL:HG22	2.00	0.43
4:E:316:PHE:HB3	4:E:317:PRO:HD3	2.01	0.43
1:A:2695:G:N7	1:A:2941:G:O2'	2.45	0.43
23:Y:91:ARG:O	23:Y:149:ARG:NH2	2.51	0.43
1:A:2493:C:C4	1:A:2540:C:C1'	2.98	0.43
31:6:259:PRO:CB	31:6:266:HIS:CD2	3.00	0.43
5:F:91:PRO:O	5:F:176:VAL:HG13	2.19	0.43
9:K:7:ALA:N	9:K:8:PRO:HD2	2.34	0.43
3:D:125:LYS:HB3	30:5:259:ILE:HD11	2.01	0.43
1:A:2677:A:H2'	1:A:2678:A:C8	2.54	0.43
5:F:116:THR:HG23	5:F:118:ALA:H	1.82	0.43
30:5:295:ASP:N	30:5:347:THR:HB	2.34	0.43
22:X:177:HIS:HB3	22:X:178:PRO:HD2	2.01	0.43
10:L:123:ILE:HD12	10:L:141:ALA:HB2	2.00	0.43
4:E:64:LEU:HD22	32:7:315:LYS:HE2	2.00	0.43
19:U:26:ILE:HD11	19:U:44:ILE:CD1	2.49	0.43
30:5:230:LEU:HD13	30:5:289:HIS:HD2	1.84	0.43
1:A:2201:G:C2	1:A:2202:C:C2	3.07	0.43
1:A:2321:A:N7	25:0:142:GLY:HA3	2.34	0.43
23:Y:93:LYS:HE3	34:9:70:LEU:HD11	2.01	0.43
18:T:108:PHE:CD1	18:T:108:PHE:N	2.87	0.43
1:A:2193:U:C3'	1:A:2194:U:C5'	2.94	0.43
1:A:2112:A:C8	1:A:2114:C:C6	3.06	0.43
11:M:115:PRO:CA	11:M:153:ASN:HD21	2.32	0.43
1:A:2254:C:C4	1:A:2255:C:C5	3.07	0.43
23:Y:95:ASN:OD1	23:Y:149:ARG:NH1	2.48	0.43
1:A:2456:U:H2'	1:A:2457:A:O4'	2.18	0.43
1:A:3147:G:C6	1:A:3148:C:C4	3.07	0.43
1:A:3147:G:C2	1:A:3148:C:C2	3.07	0.43
1:A:2408:U:O3'	30:5:108:HIS:CE1	2.72	0.43
7:I:37:ARG:HG2	12:N:245:PHE:CZ	2.54	0.43
15:Q:155:ILE:HD11	15:Q:160:VAL:HG21	2.00	0.43
1:A:3124:U:C4	1:A:3132:G:N2	2.87	0.42
1:A:2686:G:C2	1:A:2687:C:C5	3.07	0.42
1:A:1671:G:C6	1:A:1672:C:C4	3.07	0.42
1:A:2615:A:C6	10:L:58:ILE:HG23	2.53	0.42
1:A:1750:G:H4'	11:M:76:ILE:HD11	2.01	0.42
1:A:1786:C:C2	1:A:1792:G:N2	2.87	0.42
17:S:159:THR:HG23	17:S:196:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2493:C:O2'	1:A:2494:C:H5'	2.19	0.42
1:A:2541:C:N3	1:A:2542:G:C8	2.87	0.42
22:X:177:HIS:CB	22:X:178:PRO:CD	2.97	0.42
1:A:2301:U:H2'	1:A:2302:U:C6	2.54	0.42
1:A:2247:C:N3	1:A:2248:U:C5	2.87	0.42
8:J:121:ALA:HB2	8:J:144:ILE:CD1	2.49	0.42
1:A:2172:A:C5	8:J:23:ILE:HG22	2.54	0.42
21:W:110:ASN:C	21:W:110:ASN:ND2	2.73	0.42
1:A:2044:A:C6	1:A:2045:A:C5	3.07	0.42
1:A:2125:C:C6	1:A:2263:C:H1'	2.54	0.42
23:Y:132:LEU:O	23:Y:136:VAL:HG23	2.19	0.42
21:W:61:VAL:HG21	21:W:97:VAL:CG2	2.49	0.42
1:A:2800:U:N3	1:A:2801:A:N7	2.67	0.42
1:A:2542:G:C2	1:A:2543:C:C2	3.07	0.42
1:A:2660:U:C2	1:A:2661:U:C5	3.07	0.42
13:O:30:ARG:HD2	13:O:81:THR:HG23	2.00	0.42
1:A:3054:G:H2'	1:A:3055:U:C6	2.53	0.42
1:A:2025:C:C2	1:A:2269:G:C2	3.07	0.42
1:A:3117:C:C2	1:A:3118:U:C5	3.08	0.42
1:A:3070:G:N3	1:A:3070:G:H2'	2.33	0.42
14:P:80:LEU:CD2	14:P:82:VAL:HG23	2.50	0.42
4:E:58:VAL:N	4:E:59:PRO:HD2	2.34	0.42
31:6:330:ILE:HG22	31:6:335:LEU:HD13	2.01	0.42
1:A:3019:G:C2	1:A:3020:C:C2	3.07	0.42
1:A:2042:U:C4	1:A:2043:C:C5	3.08	0.42
1:A:2748:A:H2'	1:A:2749:A:N9	2.34	0.42
10:L:73:ILE:HD12	10:L:75:LEU:HD13	2.01	0.42
1:A:2279:U:N3	1:A:2280:C:C6	2.88	0.42
3:D:218:ARG:HD2	3:D:225:ILE:HD12	2.01	0.42
1:A:3216:C:C2	1:A:3225:G:C2	3.08	0.42
1:A:2709:A:C5	1:A:2710:C:C5	3.08	0.42
1:A:2541:C:C2	1:A:2542:G:C8	3.07	0.42
12:N:82:PHE:HE1	12:N:88:ALA:HB2	1.84	0.42
30:5:380:GLN:HB3	30:5:410:THR:HG22	2.02	0.42
1:A:2728:C:C2	1:A:2729:U:C5	3.08	0.42
1:A:2481:A:C6	1:A:2482:A:N6	2.88	0.42
1:A:2398:A:H2'	1:A:2399:A:O4'	2.20	0.42
1:A:3131:G:O6	1:A:3132:G:N1	2.53	0.42
22:X:153:LEU:C	22:X:153:LEU:CD1	2.88	0.42
1:A:2115:U:N3	1:A:2116:C:C5	2.87	0.42
18:T:99:ILE:HD11	18:T:178:LEU:CD1	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:111:THR:CG2	21:W:112:GLU:N	2.83	0.42
11:M:114:GLN:HG3	11:M:115:PRO:HD2	2.00	0.42
1:A:2571:G:C6	1:A:2572:C:C4	3.07	0.42
1:A:2182:G:N2	1:A:2183:C:C2	2.88	0.42
1:A:1947:C:H2'	1:A:1948:C:O4'	2.19	0.42
11:M:229:PHE:N	11:M:230:PRO:HD2	2.34	0.42
13:O:80:LEU:HD11	13:O:89:LEU:HD12	2.02	0.42
4:E:109:LEU:HD21	4:E:337:VAL:HG22	2.02	0.42
34:9:53:ILE:HD12	34:9:56:MET:HE3	2.01	0.42
5:F:284:TYR:HB2	5:F:285:PRO:CD	2.50	0.42
1:A:2599:U:O2	1:A:2599:U:O4'	2.36	0.42
13:O:44:ALA:HB3	13:O:49:VAL:HG22	2.02	0.42
1:A:2194:U:P	7:I:124:LYS:HZ1	2.43	0.42
1:A:2686:G:C4	1:A:2687:C:C5	3.07	0.42
1:A:2749:A:C5	1:A:2750:U:C5	3.08	0.42
1:A:1671:G:C6	1:A:1672:C:N4	2.88	0.42
17:S:136:VAL:HG21	17:S:154:VAL:HG21	2.01	0.42
1:A:2546:G:N2	1:A:2547:C:C2	2.87	0.42
1:A:3163:G:C6	1:A:3164:C:C4	3.08	0.42
1:A:1998:U:OP1	1:A:2001:C:N4	2.52	0.42
1:A:2201:G:N2	1:A:2202:C:C2	2.88	0.42
1:A:2508:C:H2'	1:A:2509:A:O4'	2.20	0.42
22:X:153:LEU:C	22:X:153:LEU:HD13	2.39	0.42
1:A:1790:A:C2	1:A:2006:C:H1'	2.55	0.42
1:A:2492:G:C1'	1:A:2506:A:H5'	2.46	0.42
22:X:112:ARG:HB2	22:X:127:VAL:HG11	2.01	0.42
30:5:173:ARG:HA	30:5:176:TYR:CE2	2.55	0.42
13:O:86:ILE:HB	13:O:87:PRO:HD3	2.00	0.42
13:O:44:ALA:HB3	13:O:49:VAL:CG2	2.50	0.42
3:D:67:LYS:HB2	30:5:35:VAL:HG21	2.01	0.42
32:7:85:ILE:N	32:7:85:ILE:HD12	2.35	0.42
1:A:2555:C:H2'	1:A:2556:A:O4'	2.19	0.42
1:A:3024:U:N3	1:A:3025:A:N7	2.67	0.42
8:J:112:VAL:O	8:J:156:VAL:N	2.52	0.42
1:A:2114:C:C4	1:A:2115:U:C5	3.08	0.42
3:D:126:VAL:HG22	3:D:163:ILE:HD11	2.00	0.42
1:A:2618:U:C5	1:A:3039:U:O2'	2.66	0.42
1:A:2418:A:N3	1:A:2419:C:C6	2.88	0.42
1:A:2073:A:OP2	31:6:27:ARG:N	2.53	0.42
19:U:56:TYR:OH	23:Y:106:LEU:HD11	2.20	0.42
1:A:1692:A:N1	23:Y:176:ILE:HD12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1897:A:C2	1:A:1898:A:C5	3.08	0.41
1:A:2600:A:HO2'	1:A:2601:A:H3'	1.85	0.41
1:A:1959:C:O2	1:A:1959:C:C2'	2.66	0.41
13:O:36:LEU:HD13	13:O:125:TYR:CE2	2.55	0.41
4:E:275:ARG:HG2	4:E:284:TYR:CD1	2.55	0.41
30:5:161:ALA:CB	30:5:180:ILE:CG1	2.98	0.41
1:A:2548:C:C2	1:A:2568:G:C2	3.08	0.41
24:Z:84:ASP:O	24:Z:88:MET:HG3	2.20	0.41
31:6:273:PHE:HA	31:6:313:PRO:HA	2.02	0.41
1:A:2459:A:C4	1:A:2460:A:C8	3.07	0.41
1:A:1708:A:N3	23:Y:190:LEU:HD13	2.35	0.41
15:Q:79:GLU:CD	15:Q:147:ALA:HB1	2.41	0.41
7:I:175:PRO:O	7:I:177:LEU:N	2.52	0.41
31:6:379:ILE:HG23	31:6:379:ILE:O	2.20	0.41
12:N:105:MET:SD	12:N:105:MET:N	2.93	0.41
1:A:3031:G:N1	1:A:3032:G:C5	2.88	0.41
1:A:2493:C:C2'	1:A:2494:C:H5'	2.50	0.41
1:A:2493:C:H2'	1:A:2494:C:H5'	2.01	0.41
1:A:2493:C:C2'	1:A:2494:C:C5'	2.97	0.41
1:A:2109:A:C8	1:A:2111:C:O4'	2.73	0.41
6:H:55:ILE:HG22	6:H:83:VAL:HG12	2.02	0.41
1:A:2737:U:O2'	1:A:3084:A:N3	2.53	0.41
16:R:12:ASN:OD1	16:R:12:ASN:N	2.53	0.41
19:U:65:VAL:HG13	19:U:97:VAL:HG13	2.01	0.41
1:A:1988:G:C2	1:A:1997:C:C2	3.08	0.41
30:5:300:ARG:N	30:5:301:PRO:HD2	2.35	0.41
4:E:230:THR:O	4:E:231:HIS:CB	2.68	0.41
4:E:145:LEU:HD13	4:E:187:ILE:HD11	2.02	0.41
1:A:2493:C:H42	1:A:2540:C:H1'	1.82	0.41
1:A:1826:G:N2	1:A:2686:G:C8	2.88	0.41
1:A:2753:A:O2'	6:H:88:HIS:ND1	2.52	0.41
1:A:2670:C:C2	1:A:2671:C:C6	3.08	0.41
1:A:1865:C:OP2	16:R:17:ARG:NH2	2.53	0.41
1:A:1780:U:O2'	1:A:1781:A:P	2.77	0.41
15:Q:111:PHE:CE2	15:Q:117:LEU:HD11	2.55	0.41
1:A:1795:A:H2'	1:A:1796:A:O4'	2.20	0.41
14:P:101:VAL:HG22	31:6:154:TYR:CD2	2.55	0.41
1:A:2686:G:C2	1:A:2687:C:C2	3.09	0.41
1:A:2497:U:O2'	1:A:2498:U:H5'	2.21	0.41
6:H:97:ILE:HD13	6:H:132:ALA:HA	2.02	0.41
8:J:116:HIS:O	8:J:120:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2291:A:C2	1:A:2293:A:C4	3.08	0.41
1:A:1846:C:H2'	1:A:1847:U:O4'	2.20	0.41
6:H:59:TRP:O	6:H:60:TRP:HB2	2.21	0.41
1:A:2194:U:H2'	1:A:2195:A:H8	1.66	0.41
1:A:1995:A:C4	1:A:1996:C:C5	3.08	0.41
16:R:83:TYR:N	16:R:84:PRO:CD	2.82	0.41
12:N:53:ILE:HG21	12:N:102:PHE:CD2	2.56	0.41
17:S:133:VAL:HG11	17:S:156:VAL:HG23	2.01	0.41
18:T:95:ARG:O	18:T:142:ILE:O	2.38	0.41
1:A:1751:A:H2'	1:A:1752:U:O4'	2.21	0.41
22:X:227:PHE:HB3	23:Y:156:LEU:O	2.21	0.41
19:U:35:GLN:HB3	19:U:36:PRO:HD2	2.02	0.41
1:A:1679:U:O4	1:A:1772:A:O2'	2.29	0.41
1:A:2211:U:O2	1:A:2211:U:H2'	2.20	0.41
30:5:336:LEU:HD21	30:5:362:THR:CG2	2.49	0.41
1:A:2670:C:C2	1:A:2671:C:C5	3.09	0.41
1:A:2395:A:C1'	30:5:385:HIS:HB2	2.49	0.41
1:A:2733:G:N1	1:A:2929:C:C4	2.89	0.41
7:I:93:ASN:HD22	7:I:93:ASN:C	2.24	0.41
16:R:54:THR:HG21	17:S:172:MET:N	2.35	0.41
1:A:2842:C:O4'	12:N:63:ARG:NH1	2.53	0.41
1:A:2017:U:C2	1:A:2018:G:C8	3.09	0.41
4:E:96:ARG:NH1	4:E:315:PRO:O	2.54	0.41
29:4:80:TYR:CE1	29:4:91:TYR:HB2	2.56	0.41
1:A:1992:C:C4	3:D:274:ARG:HB2	2.56	0.41
1:A:2275:U:C2	1:A:2276:C:C5	3.09	0.41
1:A:2653:C:H2'	1:A:2654:U:O4'	2.21	0.41
1:A:2201:G:C6	1:A:2202:C:C4	3.08	0.41
1:A:2305:U:C2	1:A:2306:A:C8	3.09	0.41
2:B:1609:U:O2	2:B:1609:U:H2'	2.20	0.41
1:A:3024:U:O2	1:A:3025:A:C8	2.74	0.41
22:X:154:CYS:O	22:X:154:CYS:SG	2.78	0.41
6:H:56:VAL:HG11	6:H:80:TYR:CB	2.51	0.41
12:N:96:TYR:HB3	12:N:151:VAL:CG1	2.45	0.41
1:A:1877:U:N3	1:A:1878:U:C5	2.89	0.41
1:A:2751:G:N1	1:A:2752:C:C4	2.89	0.41
11:M:179:TYR:CD1	11:M:179:TYR:N	2.89	0.41
1:A:3077:C:C2'	1:A:3077:C:O2	2.69	0.41
1:A:2079:C:C4	1:A:2080:U:C2	3.08	0.41
1:A:2253:U:C2	1:A:2254:C:C6	3.09	0.41
7:I:102:VAL:HG13	7:I:103:ALA:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3181:U:OP2	1:A:3182:A:O2'	2.29	0.41
1:A:2055:U:C2	1:A:2056:G:C8	3.09	0.41
1:A:2898:U:H2'	1:A:2899:C:O4'	2.20	0.41
4:E:218:VAL:HG12	4:E:224:PHE:HB2	2.03	0.41
1:A:2017:U:O2'	1:A:2723:A:N1	2.48	0.41
32:7:108:VAL:HB	32:7:113:TRP:CD1	2.56	0.41
1:A:2834:C:C4	1:A:2835:C:C5	3.08	0.41
1:A:2016:C:OP2	11:M:59:ARG:NH1	2.52	0.41
22:X:90:ILE:HD11	22:X:103:LYS:HG2	2.03	0.41
1:A:3201:A:N3	1:A:3201:A:H2'	2.36	0.41
5:F:217:LEU:HD13	5:F:256:HIS:ND1	2.36	0.41
1:A:2995:G:H5'	1:A:2996:G:OP2	2.21	0.41
1:A:1671:G:H4'	18:T:51:TRP:HE3	1.86	0.41
18:T:80:ILE:CG2	18:T:116:ILE:HD13	2.50	0.41
1:A:2333:G:C6	1:A:2334:C:C4	3.09	0.41
31:6:219:THR:HG22	31:6:233:LEU:HA	2.03	0.41
18:T:82:TYR:O	18:T:172:CYS:SG	2.76	0.41
2:B:1641:G:OP2	14:P:121:VAL:HG23	2.21	0.41
14:P:91:ALA:HB1	14:P:131:LEU:HD12	2.01	0.41
33:8:87:MET:O	33:8:91:THR:HG23	2.20	0.41
32:7:313:TRP:CE3	32:7:313:TRP:HA	2.56	0.41
1:A:2166:C:H2'	1:A:2167:A:C8	2.56	0.41
1:A:2557:C:O2'	1:A:2558:A:P	2.79	0.40
1:A:2686:G:C6	1:A:2687:C:C4	3.09	0.40
3:D:181:ALA:HA	3:D:243:THR:HA	2.03	0.40
6:H:55:ILE:HG22	6:H:83:VAL:CG1	2.50	0.40
1:A:2796:G:C2	1:A:2797:C:C2	3.09	0.40
1:A:3115:U:H2'	1:A:3116:C:H6	1.85	0.40
28:3:169:ARG:HG3	28:3:169:ARG:HH11	1.86	0.40
26:1:45:HIS:HB3	26:1:56:PHE:CD1	2.55	0.40
1:A:2128:G:C2	1:A:2138:U:C2	3.09	0.40
1:A:2558:A:C4'	1:A:2559:U:OP2	2.69	0.40
1:A:3019:G:H2'	1:A:3020:C:O4'	2.21	0.40
1:A:2756:C:C5'	1:A:2757:A:OP2	2.70	0.40
18:T:51:TRP:CD1	18:T:76:CYS:SG	3.15	0.40
5:F:83:HIS:CG	5:F:274:LEU:HD11	2.56	0.40
24:Z:71:ARG:HD3	24:Z:91:LEU:O	2.22	0.40
30:5:121:LEU:CD2	30:5:126:THR:HG23	2.51	0.40
1:A:1941:G:N1	1:A:1942:C:C4	2.90	0.40
1:A:2998:U:H2'	1:A:2999:C:O4'	2.21	0.40
1:A:2418:A:C5	34:9:50:PHE:CD2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2301:U:C2	1:A:2302:U:C5	3.10	0.40
1:A:2134:A:O2'	1:A:2135:A:O5'	2.40	0.40
16:R:83:TYR:CZ	16:R:87:ILE:HG13	2.56	0.40
5:F:263:LEU:N	5:F:264:PRO:HD2	2.37	0.40
3:D:109:PHE:CE1	3:D:208:ARG:HD2	2.56	0.40
1:A:1725:C:C5	1:A:1726:C:C5	3.09	0.40
23:Y:110:ASN:O	23:Y:114:THR:HG23	2.22	0.40
1:A:1843:U:C2	1:A:1853:A:C8	3.09	0.40
1:A:2114:C:N3	1:A:2115:U:C5	2.89	0.40
1:A:2591:A:H2'	1:A:2592:G:O4'	2.21	0.40
4:E:61:ILE:O	4:E:65:VAL:HG23	2.21	0.40
7:I:116:LEU:HB3	7:I:121:ILE:O	2.21	0.40
1:A:2571:G:C2	1:A:2572:C:C2	3.09	0.40
30:5:297:ALA:HB3	30:5:303:ARG:HG2	2.03	0.40
1:A:2201:G:N1	1:A:2202:C:C4	2.90	0.40
6:H:97:ILE:N	6:H:97:ILE:HD12	2.37	0.40
1:A:2264:A:C2	1:A:2265:A:C8	3.09	0.40
1:A:3119:C:H2'	1:A:3120:C:O4'	2.21	0.40
21:W:76:HIS:CD2	21:W:128:LYS:HG2	2.57	0.40
7:I:176:LEU:HD12	7:I:191:PHE:CE2	2.56	0.40
13:O:46:TRP:HD1	13:O:121:ALA:HB2	1.86	0.40
15:Q:221:LYS:HB3	15:Q:244:ARG:HG3	1.99	0.40
1:A:2194:U:C2'	1:A:2194:U:O2	2.69	0.40
1:A:2493:C:N3	1:A:2540:C:C1'	2.85	0.40
1:A:2041:U:H2'	1:A:2042:U:H6	1.84	0.40
6:H:54:VAL:C	6:H:55:ILE:HD12	2.42	0.40
7:I:82:LEU:O	7:I:86:ILE:HD13	2.21	0.40
10:L:77:ILE:HG22	10:L:78:LYS:HE2	2.04	0.40
1:A:1861:U:H2'	1:A:1862:U:H6	1.87	0.40
1:A:2934:G:HO2'	1:A:2987:U:H5	1.70	0.40
1:A:2418:A:C4	1:A:2419:C:C5	3.10	0.40
8:J:94:ALA:HB1	8:J:116:HIS:NE2	2.35	0.40
1:A:3078:C:C2	1:A:3079:G:C8	3.10	0.40
13:O:104:TYR:O	13:O:105:THR:OG1	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	D	234/305 (77%)	222 (95%)	11 (5%)	1 (0%)	39 79
4	E	296/348 (85%)	268 (90%)	21 (7%)	7 (2%)	7 44
5	F	248/311 (80%)	228 (92%)	17 (7%)	3 (1%)	16 59
6	H	93/267 (35%)	81 (87%)	10 (11%)	2 (2%)	8 46
7	I	154/261 (59%)	143 (93%)	6 (4%)	5 (3%)	5 38
8	J	138/192 (72%)	115 (83%)	16 (12%)	7 (5%)	2 24
9	K	175/178 (98%)	157 (90%)	10 (6%)	8 (5%)	3 26
10	L	113/145 (78%)	100 (88%)	10 (9%)	3 (3%)	6 41
11	M	285/296 (96%)	256 (90%)	23 (8%)	6 (2%)	9 47
12	N	203/251 (81%)	186 (92%)	15 (7%)	2 (1%)	19 63
13	O	150/175 (86%)	133 (89%)	15 (10%)	2 (1%)	15 57
14	P	129/179 (72%)	115 (89%)	12 (9%)	2 (2%)	12 53
15	Q	200/292 (68%)	179 (90%)	17 (8%)	4 (2%)	9 48
16	R	138/149 (93%)	128 (93%)	7 (5%)	3 (2%)	8 46
17	S	154/205 (75%)	144 (94%)	9 (6%)	1 (1%)	30 72
18	T	164/212 (77%)	152 (93%)	9 (6%)	3 (2%)	11 50
19	U	109/153 (71%)	96 (88%)	12 (11%)	1 (1%)	21 65
20	V	183/216 (85%)	161 (88%)	15 (8%)	7 (4%)	4 32
21	W	105/148 (71%)	102 (97%)	2 (2%)	1 (1%)	19 63
22	X	241/256 (94%)	220 (91%)	16 (7%)	5 (2%)	9 47
23	Y	174/250 (70%)	157 (90%)	17 (10%)	0	100 100
24	Z	118/161 (73%)	107 (91%)	9 (8%)	2 (2%)	11 51
25	0	94/188 (50%)	81 (86%)	7 (7%)	6 (6%)	2 17
26	1	50/65 (77%)	46 (92%)	2 (4%)	2 (4%)	4 31
27	2	41/92 (45%)	40 (98%)	0	1 (2%)	7 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	3	93/188 (50%)	88 (95%)	5 (5%)	0	100	100
29	4	34/103 (33%)	34 (100%)	0	0	100	100
30	5	368/423 (87%)	329 (89%)	26 (7%)	13 (4%)	4	35
31	6	313/380 (82%)	274 (88%)	30 (10%)	9 (3%)	6	40
32	7	258/338 (76%)	236 (92%)	21 (8%)	1 (0%)	39	79
33	8	55/206 (27%)	53 (96%)	2 (4%)	0	100	100
34	9	105/137 (77%)	93 (89%)	9 (9%)	3 (3%)	6	40
35	a	37/142 (26%)	35 (95%)	2 (5%)	0	100	100
36	b	146/155 (94%)	125 (86%)	17 (12%)	4 (3%)	6	41
37	c	271/332 (82%)	238 (88%)	27 (10%)	6 (2%)	8	46
38	d	156/306 (51%)	139 (89%)	11 (7%)	6 (4%)	4	32
39	e	132/279 (47%)	103 (78%)	25 (19%)	4 (3%)	5	39
40	f	71/211 (34%)	63 (89%)	7 (10%)	1 (1%)	14	55
41	g	127/166 (76%)	116 (91%)	8 (6%)	3 (2%)	7	44
42	h	96/158 (61%)	82 (85%)	10 (10%)	4 (4%)	3	29
43	i	94/128 (73%)	80 (85%)	13 (14%)	1 (1%)	17	61
44	j	83/123 (68%)	79 (95%)	3 (4%)	1 (1%)	16	59
45	k	82/112 (73%)	64 (78%)	13 (16%)	5 (6%)	2	18
46	o	92/102 (90%)	80 (87%)	9 (10%)	3 (3%)	5	37
47	p	79/206 (38%)	73 (92%)	5 (6%)	1 (1%)	15	57
48	q	126/222 (57%)	120 (95%)	5 (4%)	1 (1%)	24	67
49	r	140/196 (71%)	125 (89%)	12 (9%)	3 (2%)	9	47
50	s	366/439 (83%)	326 (89%)	32 (9%)	8 (2%)	8	46
All	All	7313/10347 (71%)	6572 (90%)	580 (8%)	161 (2%)	13	46

All (161) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	I	102	VAL
8	J	70	ILE
12	N	67	LYS
16	R	12	ASN
22	X	69	ILE
22	X	127	VAL

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Mol	Chain	Res	Type
24	Z	146	VAL
26	1	39	GLU
30	5	383	TYR
30	5	420	HIS
31	6	344	PHE
36	b	69	PRO
37	c	123	GLN
38	d	164	VAL
38	d	187	GLU
38	d	268	PRO
38	d	272	PRO
39	e	221	LYS
42	h	65	ASP
42	h	147	ASN
45	k	61	GLU
45	k	62	PRO
49	r	76	ASN
49	r	158	SER
4	E	231	HIS
4	E	317	PRO
5	F	223	HIS
9	K	115	ASN
15	Q	264	TRP
17	S	94	ARG
20	V	155	PRO
22	X	177	HIS
25	0	146	GLY
25	0	178	ASP
30	5	35	VAL
30	5	263	ILE
30	5	359	LEU
31	6	379	ILE
37	c	64	PRO
37	c	264	THR
38	d	195	VAL
41	g	145	GLY
44	j	40	TYR
45	k	18	VAL
46	o	15	ARG
48	q	43	GLU
50	s	345	PHE
3	D	67	LYS

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Mol	Chain	Res	Type
7	I	120	LYS
7	I	172	PRO
7	I	178	GLY
8	J	61	LYS
9	K	3	SER
9	K	15	ALA
11	M	287	ASP
13	O	112	ASN
15	Q	76	LEU
18	T	209	VAL
20	V	118	ARG
20	V	178	SER
30	5	272	ASP
31	6	51	TYR
31	6	72	ARG
34	9	46	SER
34	9	131	TYR
36	b	14	VAL
36	b	116	ARG
40	f	182	VAL
42	h	146	SER
46	o	50	SER
47	p	139	SER
50	s	85	LYS
50	s	250	PHE
50	s	407	ASP
4	E	82	ASP
4	E	127	CYS
4	E	141	LYS
7	I	176	LEU
9	K	151	ILE
11	M	125	ARG
11	M	208	GLU
12	N	240	LYS
15	Q	215	VAL
18	T	158	TYR
20	V	171	ILE
21	W	127	TYR
22	X	34	GLU
25	0	177	ARG
25	0	184	TRP
26	1	60	LYS

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Mol	Chain	Res	Type
30	5	296	LYS
30	5	297	ALA
31	6	165	ALA
31	6	307	HIS
36	b	117	LYS
37	c	35	PHE
39	e	160	PHE
43	i	65	ASN
45	k	37	VAL
45	k	60	SER
50	s	248	ALA
50	s	264	ILE
4	E	126	ASP
4	E	324	ASP
5	F	74	GLN
8	J	60	ILE
8	J	84	GLN
8	J	109	ALA
9	K	14	PHE
9	K	24	LYS
9	K	143	GLU
14	P	173	GLU
14	P	177	ILE
15	Q	171	VAL
16	R	137	GLU
16	R	143	SER
19	U	12	LEU
20	V	142	GLU
20	V	185	ARG
30	5	70	LEU
30	5	170	ILE
30	5	256	PHE
31	6	68	PRO
31	6	351	HIS
32	7	157	ALA
34	9	39	LYS
37	c	314	TRP
39	e	219	TYR
41	g	137	VAL
42	h	66	LEU
6	H	61	LYS
9	K	23	GLY

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Mol	Chain	Res	Type
10	L	113	ASN
10	L	131	GLU
11	M	110	VAL
11	M	242	TYR
22	X	52	ILE
25	0	113	CYS
25	0	116	LEU
27	2	51	ASN
30	5	381	LEU
37	c	229	PHE
39	e	178	ARG
41	g	136	PRO
50	s	284	VAL
50	s	364	GLY
30	5	305	GLN
49	r	61	PRO
6	H	71	PRO
38	d	208	VAL
5	F	128	TRP
8	J	74	PRO
8	J	136	PRO
10	L	112	GLY
31	6	130	VAL
11	M	265	ILE
13	O	12	GLY
18	T	69	ARG
20	V	110	PRO
24	Z	143	GLY
46	o	13	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
3	D	190/245 (78%)	175 (92%)	15 (8%)	15 52
4	E	255/290 (88%)	234 (92%)	21 (8%)	14 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	F	217/262 (83%)	193 (89%)	24 (11%)	8 33
6	H	86/228 (38%)	81 (94%)	5 (6%)	25 65
7	I	145/232 (62%)	135 (93%)	10 (7%)	19 59
8	J	113/150 (75%)	101 (89%)	12 (11%)	8 36
9	K	155/156 (99%)	144 (93%)	11 (7%)	18 58
10	L	98/124 (79%)	93 (95%)	5 (5%)	29 69
11	M	245/249 (98%)	218 (89%)	27 (11%)	8 34
12	N	172/211 (82%)	158 (92%)	14 (8%)	15 51
13	O	133/150 (89%)	113 (85%)	20 (15%)	3 20
14	P	115/154 (75%)	108 (94%)	7 (6%)	23 63
15	Q	186/256 (73%)	171 (92%)	15 (8%)	15 51
16	R	118/126 (94%)	108 (92%)	10 (8%)	13 48
17	S	141/180 (78%)	125 (89%)	16 (11%)	7 32
18	T	146/182 (80%)	131 (90%)	15 (10%)	9 37
19	U	99/135 (73%)	91 (92%)	8 (8%)	15 51
20	V	169/191 (88%)	154 (91%)	15 (9%)	12 45
21	W	87/119 (73%)	78 (90%)	9 (10%)	9 37
22	X	217/227 (96%)	198 (91%)	19 (9%)	12 46
23	Y	159/223 (71%)	144 (91%)	15 (9%)	11 42
24	Z	111/147 (76%)	105 (95%)	6 (5%)	27 67
25	0	88/164 (54%)	74 (84%)	14 (16%)	3 17
26	1	49/60 (82%)	41 (84%)	8 (16%)	3 16
27	2	38/72 (53%)	34 (90%)	4 (10%)	8 36
28	3	88/166 (53%)	83 (94%)	5 (6%)	25 65
29	4	35/89 (39%)	33 (94%)	2 (6%)	25 65
30	5	337/368 (92%)	306 (91%)	31 (9%)	11 43
31	6	266/332 (80%)	230 (86%)	36 (14%)	5 24
32	7	242/303 (80%)	231 (96%)	11 (4%)	34 73
33	8	51/190 (27%)	49 (96%)	2 (4%)	39 76
34	9	91/112 (81%)	87 (96%)	4 (4%)	35 73
35	a	37/133 (28%)	34 (92%)	3 (8%)	15 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	b	130/135 (96%)	120 (92%)	10 (8%)	16 53
37	c	241/288 (84%)	227 (94%)	14 (6%)	25 65
38	d	151/274 (55%)	148 (98%)	3 (2%)	63 87
39	e	114/236 (48%)	99 (87%)	15 (13%)	5 25
40	f	70/173 (40%)	64 (91%)	6 (9%)	13 48
41	g	119/148 (80%)	109 (92%)	10 (8%)	14 49
42	h	95/148 (64%)	83 (87%)	12 (13%)	5 27
43	i	85/110 (77%)	71 (84%)	14 (16%)	3 15
44	j	68/97 (70%)	63 (93%)	5 (7%)	17 55
45	k	74/90 (82%)	67 (90%)	7 (10%)	11 41
46	o	80/87 (92%)	72 (90%)	8 (10%)	9 38
47	p	75/181 (41%)	67 (89%)	8 (11%)	8 35
48	q	110/178 (62%)	104 (94%)	6 (6%)	27 66
49	r	133/169 (79%)	119 (90%)	14 (10%)	8 36
50	s	326/381 (86%)	300 (92%)	26 (8%)	15 51
All	All	6550/8921 (73%)	5973 (91%)	577 (9%)	17 46

All (577) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	71	LYS
3	D	74	ILE
3	D	115	GLU
3	D	177	ARG
3	D	195	ASN
3	D	202	ARG
3	D	232	ARG
3	D	240	CYS
3	D	243	THR
3	D	244	VAL
3	D	262	ARG
3	D	274	ARG
3	D	277	ARG
3	D	284	ARG
3	D	293	LYS
4	E	54	SER
4	E	57	ASN

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Mol	Chain	Res	Type
4	E	60	PHE
4	E	86	PRO
4	E	120	THR
4	E	154	ARG
4	E	156	ARG
4	E	164	PHE
4	E	168	LEU
4	E	187	ILE
4	E	207	THR
4	E	213	LYS
4	E	227	GLN
4	E	233	GLN
4	E	271	LEU
4	E	278	THR
4	E	286	ASN
4	E	300	LYS
4	E	301	ASP
4	E	304	LEU
4	E	330	GLU
5	F	59	ARG
5	F	76	ARG
5	F	89	THR
5	F	96	LEU
5	F	98	GLN
5	F	101	MET
5	F	108	ARG
5	F	110	SER
5	F	121	ARG
5	F	125	ARG
5	F	126	LYS
5	F	140	SER
5	F	145	LEU
5	F	184	GLN
5	F	185	ASP
5	F	187	LEU
5	F	194	GLU
5	F	203	LEU
5	F	221	LEU
5	F	228	GLN
5	F	258	THR
5	F	259	LEU
5	F	277	ASP

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Mol	Chain	Res	Type
5	F	283	LEU
6	H	75	ARG
6	H	76	ARG
6	H	82	LEU
6	H	94	LEU
6	H	98	LEU
7	I	44	ARG
7	I	47	LEU
7	I	93	ASN
7	I	101	ASN
7	I	116	LEU
7	I	130	VAL
7	I	136	GLU
7	I	151	ASN
7	I	170	THR
7	I	191	PHE
8	J	23	ILE
8	J	50	CYS
8	J	56	ARG
8	J	71	LEU
8	J	75	ASP
8	J	86	THR
8	J	123	ILE
8	J	124	LYS
8	J	130	PHE
8	J	141	VAL
8	J	142	ARG
8	J	150	SER
9	K	5	SER
9	K	10	GLN
9	K	13	THR
9	K	20	LEU
9	K	38	ARG
9	K	60	MET
9	K	95	LEU
9	K	125	LEU
9	K	145	LEU
9	K	154	ARG
9	K	158	TYR
10	L	37	ARG
10	L	38	VAL
10	L	89	HIS

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Mol	Chain	Res	Type
10	L	104	ASN
10	L	130	ARG
11	M	19	LEU
11	M	28	LYS
11	M	41	ARG
11	M	57	ARG
11	M	64	ARG
11	M	87	HIS
11	M	96	LEU
11	M	100	ARG
11	M	101	LEU
11	M	114	GLN
11	M	118	LEU
11	M	130	GLN
11	M	132	LEU
11	M	142	GLU
11	M	156	VAL
11	M	162	LEU
11	M	179	TYR
11	M	182	ARG
11	M	184	LEU
11	M	195	LEU
11	M	208	GLU
11	M	222	TYR
11	M	233	ARG
11	M	234	LEU
11	M	255	MET
11	M	273	TRP
11	M	279	ASP
12	N	50	LEU
12	N	54	GLU
12	N	90	LEU
12	N	103	GLU
12	N	105	MET
12	N	113	MET
12	N	123	ARG
12	N	151	VAL
12	N	158	ARG
12	N	168	GLU
12	N	198	MET
12	N	206	GLU
12	N	226	ILE

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Mol	Chain	Res	Type
12	N	250	ARG
13	O	14	VAL
13	O	17	ARG
13	O	20	LEU
13	O	23	GLU
13	O	26	ILE
13	O	30	ARG
13	O	33	LEU
13	O	36	LEU
13	O	75	MET
13	O	89	LEU
13	O	104	TYR
13	O	112	ASN
13	O	123	ILE
13	O	129	CYS
13	O	138	ARG
13	O	141	HIS
13	O	144	LEU
13	O	146	ASN
13	O	152	LEU
13	O	153	ARG
14	P	50	ARG
14	P	134	ARG
14	P	137	GLU
14	P	141	ASN
14	P	146	GLN
14	P	155	ASP
14	P	160	LEU
15	Q	75	PHE
15	Q	87	THR
15	Q	88	ASP
15	Q	102	ARG
15	Q	129	LYS
15	Q	156	GLU
15	Q	158	GLN
15	Q	194	LEU
15	Q	220	LEU
15	Q	235	ARG
15	Q	237	ASN
15	Q	244	ARG
15	Q	246	ASP
15	Q	251	GLU

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Mol	Chain	Res	Type
15	Q	261	ASN
16	R	10	LEU
16	R	12	ASN
16	R	34	ARG
16	R	36	ASN
16	R	67	LEU
16	R	98	ASN
16	R	102	LEU
16	R	119	LEU
16	R	123	ARG
16	R	124	ARG
17	S	84	ASN
17	S	101	PHE
17	S	107	LYS
17	S	112	ASP
17	S	118	ASN
17	S	131	GLU
17	S	134	LEU
17	S	135	LEU
17	S	144	LEU
17	S	153	LEU
17	S	155	ARG
17	S	167	TRP
17	S	172	MET
17	S	173	ARG
17	S	184	ARG
17	S	194	ARG
18	T	83	SER
18	T	92	LYS
18	T	95	ARG
18	T	100	ASP
18	T	127	MET
18	T	137	ARG
18	T	149	ARG
18	T	159	HIS
18	T	161	ARG
18	T	163	ARG
18	T	168	GLU
18	T	180	GLU
18	T	201	GLN
18	T	206	ARG
18	T	207	THR

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Mol	Chain	Res	Type
19	U	3	ARG
19	U	17	LEU
19	U	25	PHE
19	U	28	LEU
19	U	38	ASP
19	U	53	LEU
19	U	71	ARG
19	U	101	HIS
20	V	20	ARG
20	V	40	ARG
20	V	63	GLU
20	V	83	ARG
20	V	101	THR
20	V	104	TYR
20	V	108	MET
20	V	120	VAL
20	V	145	ARG
20	V	149	ARG
20	V	152	ARG
20	V	185	ARG
20	V	193	THR
20	V	197	GLU
20	V	209	LYS
21	W	45	LYS
21	W	70	GLN
21	W	71	ARG
21	W	72	HIS
21	W	88	CYS
21	W	105	VAL
21	W	110	ASN
21	W	112	GLU
21	W	139	GLU
22	X	60	GLU
22	X	63	GLU
22	X	69	ILE
22	X	77	ARG
22	X	89	GLN
22	X	95	ASP
22	X	101	LEU
22	X	130	ARG
22	X	141	LEU
22	X	143	PHE

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Mol	Chain	Res	Type
22	X	153	LEU
22	X	154	CYS
22	X	189	ASP
22	X	208	LEU
22	X	213	GLU
22	X	219	GLU
22	X	226	LEU
22	X	234	LEU
22	X	241	GLN
23	Y	88	GLN
23	Y	90	LEU
23	Y	91	ARG
23	Y	98	LEU
23	Y	108	GLU
23	Y	115	LEU
23	Y	117	GLN
23	Y	150	GLU
23	Y	157	GLN
23	Y	169	ARG
23	Y	175	ARG
23	Y	190	LEU
23	Y	204	TYR
23	Y	213	ARG
23	Y	226	LEU
24	Z	77	ARG
24	Z	110	LEU
24	Z	134	MET
24	Z	138	CYS
24	Z	139	LEU
24	Z	144	GLU
25	0	85	ARG
25	0	86	THR
25	0	94	ARG
25	0	96	ASN
25	0	98	GLN
25	0	105	ASN
25	0	113	CYS
25	0	115	HIS
25	0	116	LEU
25	0	117	LYS
25	0	136	GLU
25	0	154	ILE

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Mol	Chain	Res	Type
25	0	178	ASP
25	0	185	PHE
26	1	18	VAL
26	1	22	SER
26	1	30	PHE
26	1	34	ARG
26	1	41	LEU
26	1	47	ASP
26	1	58	GLU
26	1	65	LEU
27	2	54	GLN
27	2	72	THR
27	2	87	ARG
27	2	92	HIS
28	3	94	LEU
28	3	112	ASP
28	3	129	TYR
28	3	168	ARG
28	3	169	ARG
29	4	76	CYS
29	4	85	ARG
30	5	55	LEU
30	5	96	HIS
30	5	98	LEU
30	5	106	ILE
30	5	110	ARG
30	5	113	LEU
30	5	167	THR
30	5	168	GLU
30	5	201	ARG
30	5	218	LEU
30	5	220	LEU
30	5	223	ARG
30	5	229	ARG
30	5	230	LEU
30	5	256	PHE
30	5	269	ASN
30	5	272	ASP
30	5	293	LEU
30	5	294	LEU
30	5	305	GLN
30	5	309	LEU

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Mol	Chain	Res	Type
30	5	312	LYS
30	5	315	LEU
30	5	322	LEU
30	5	345	VAL
30	5	358	GLN
30	5	365	ASP
30	5	371	LYS
30	5	375	TRP
30	5	381	LEU
30	5	382	LEU
31	6	40	ILE
31	6	42	LEU
31	6	51	TYR
31	6	52	ARG
31	6	60	ARG
31	6	73	THR
31	6	74	TYR
31	6	130	VAL
31	6	136	ARG
31	6	142	THR
31	6	146	TYR
31	6	157	LEU
31	6	173	LEU
31	6	182	ASP
31	6	185	MET
31	6	192	GLU
31	6	200	GLN
31	6	206	TYR
31	6	218	LEU
31	6	222	ASP
31	6	233	LEU
31	6	235	TRP
31	6	267	ARG
31	6	272	LEU
31	6	292	GLN
31	6	298	PHE
31	6	303	PHE
31	6	318	PHE
31	6	324	ASP
31	6	334	LEU
31	6	339	GLU
31	6	354	GLN

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Mol	Chain	Res	Type
31	6	356	ARG
31	6	370	ARG
31	6	371	ASP
31	6	372	SER
32	7	54	ARG
32	7	55	GLN
32	7	64	LYS
32	7	65	ILE
32	7	81	MET
32	7	114	ASP
32	7	143	TRP
32	7	168	ARG
32	7	234	LYS
32	7	300	VAL
32	7	313	TRP
33	8	77	TRP
33	8	85	ARG
34	9	17	ARG
34	9	23	SER
34	9	54	LYS
34	9	96	VAL
35	a	109	ILE
35	a	122	ARG
35	a	132	CYS
36	b	15	LEU
36	b	26	LEU
36	b	62	VAL
36	b	68	ARG
36	b	71	CYS
36	b	81	ASN
36	b	96	GLU
36	b	103	LYS
36	b	131	HIS
36	b	135	ASN
37	c	65	ASN
37	c	88	LEU
37	c	94	ASN
37	c	123	GLN
37	c	145	TYR
37	c	180	LEU
37	c	202	LEU
37	c	203	LEU

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Mol	Chain	Res	Type
37	c	211	THR
37	c	227	GLU
37	c	269	LEU
37	c	271	PHE
37	c	283	GLU
37	c	315	ASN
38	d	124	ARG
38	d	166	GLU
38	d	209	TYR
39	e	111	ARG
39	e	121	PHE
39	e	131	GLN
39	e	140	LEU
39	e	146	ARG
39	e	148	LEU
39	e	156	MET
39	e	163	ASN
39	e	168	HIS
39	e	175	GLN
39	e	188	PHE
39	e	219	TYR
39	e	220	LEU
39	e	225	LEU
39	e	227	GLN
40	f	54	HIS
40	f	113	LEU
40	f	114	CYS
40	f	154	GLU
40	f	169	ILE
40	f	172	GLU
41	g	46	GLN
41	g	55	THR
41	g	76	ARG
41	g	94	ILE
41	g	104	ASN
41	g	107	MET
41	g	126	ASP
41	g	141	ASN
41	g	147	LEU
41	g	155	GLN
42	h	70	LEU
42	h	73	TYR

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Mol	Chain	Res	Type
42	h	92	GLU
42	h	96	LEU
42	h	100	LEU
42	h	107	ASP
42	h	117	LEU
42	h	120	MET
42	h	131	ASN
42	h	137	ARG
42	h	147	ASN
42	h	156	TRP
43	i	51	ARG
43	i	63	LEU
43	i	65	ASN
43	i	74	ILE
43	i	88	LEU
43	i	93	ARG
43	i	95	ARG
43	i	101	ARG
43	i	105	ASP
43	i	106	ASP
43	i	107	LEU
43	i	110	LEU
43	i	113	ARG
43	i	127	PHE
44	j	36	ASN
44	j	40	TYR
44	j	63	GLN
44	j	66	ARG
44	j	76	ARG
45	k	21	CYS
45	k	25	LYS
45	k	28	GLU
45	k	32	THR
45	k	43	ARG
45	k	81	LEU
45	k	87	LEU
46	o	22	ARG
46	o	23	ARG
46	o	59	GLU
46	o	60	ARG
46	o	68	ARG
46	o	69	GLU

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Mol	Chain	Res	Type
46	o	82	PHE
46	o	87	PHE
47	p	102	ARG
47	p	124	LYS
47	p	129	ARG
47	p	135	LEU
47	p	141	ARG
47	p	144	PHE
47	p	160	GLU
47	p	163	GLN
48	q	26	ARG
48	q	43	GLU
48	q	60	GLN
48	q	89	GLU
48	q	112	GLN
48	q	114	ARG
49	r	40	GLU
49	r	59	GLU
49	r	60	SER
49	r	65	ASN
49	r	77	LEU
49	r	84	ASP
49	r	85	ASP
49	r	88	LEU
49	r	117	GLU
49	r	152	THR
49	r	163	TYR
49	r	168	ARG
49	r	171	ARG
49	r	187	TYR
50	s	65	ARG
50	s	77	ASP
50	s	192	ASN
50	s	229	LEU
50	s	230	ARG
50	s	235	ASP
50	s	238	ASN
50	s	251	VAL
50	s	253	LEU
50	s	264	ILE
50	s	270	LYS
50	s	280	ASN

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Mol	Chain	Res	Type
50	s	281	HIS
50	s	284	VAL
50	s	301	LEU
50	s	304	ASP
50	s	333	PHE
50	s	358	GLN
50	s	360	VAL
50	s	368	SER
50	s	373	GLN
50	s	379	LEU
50	s	394	TRP
50	s	404	THR
50	s	414	ASN
50	s	427	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	276	HIS
4	E	57	ASN
4	E	128	HIS
4	E	231	HIS
5	F	58	HIS
5	F	74	GLN
5	F	97	HIS
5	F	228	GLN
5	F	249	ASN
7	I	189	GLN
10	L	64	ASN
11	M	26	ASN
11	M	102	GLN
13	O	146	ASN
14	P	78	HIS
14	P	95	HIS
14	P	120	ASN
15	Q	139	GLN
15	Q	258	GLN
15	Q	261	ASN
16	R	36	ASN
16	R	98	ASN
18	T	210	HIS
19	U	82	HIS

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Mol	Chain	Res	Type
19	U	101	HIS
21	W	80	HIS
21	W	110	ASN
22	X	241	GLN
23	Y	225	ASN
24	Z	47	GLN
26	1	15	ASN
29	4	98	HIS
30	5	102	GLN
30	5	119	GLN
30	5	186	GLN
30	5	251	HIS
30	5	305	GLN
30	5	358	GLN
30	5	380	GLN
30	5	384	GLN
31	6	292	GLN
32	7	246	GLN
32	7	298	GLN
33	8	99	GLN
34	9	129	GLN
36	b	24	GLN
36	b	131	HIS
37	c	193	GLN
37	c	222	GLN
38	d	235	GLN
38	d	286	GLN
39	e	124	GLN
39	e	182	ASN
40	f	158	GLN
41	g	104	ASN
42	h	99	ASN
42	h	103	HIS
42	h	147	ASN
46	o	62	HIS
46	o	85	HIS
47	p	96	ASN
47	p	146	ASN
48	q	60	GLN
48	q	137	GLN
50	s	71	HIS
50	s	164	HIS

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Mol	Chain	Res	Type
50	s	373	GLN
50	s	385	GLN
50	s	420	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1458/1559 (93%)	550 (37%)	118 (8%)
2	B	51/73 (69%)	21 (41%)	3 (5%)
All	All	1509/1632 (92%)	571 (37%)	121 (8%)

All (571) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1672	C
1	A	1674	A
1	A	1675	A
1	A	1676	A
1	A	1677	C
1	A	1678	C
1	A	1679	U
1	A	1680	A
1	A	1681	G
1	A	1685	C
1	A	1689	C
1	A	1694	U
1	A	1699	C
1	A	1700	U
1	A	1701	U
1	A	1702	A
1	A	1703	C
1	A	1704	U
1	A	1708	A
1	A	1709	G
1	A	1712	A
1	A	1713	A
1	A	1714	C
1	A	1715	C
1	A	1716	U
1	A	1717	U
1	A	1724	A

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Mol	Chain	Res	Type
1	A	1727	A
1	A	1728	U
1	A	1732	C
1	A	1741	A
1	A	1748	G
1	A	1750	G
1	A	1751	A
1	A	1767	G
1	A	1770	G
1	A	1773	A
1	A	1775	A
1	A	1777	A
1	A	1779	A
1	A	1780	U
1	A	1781	A
1	A	1794	A
1	A	1799	U
1	A	1805	A
1	A	1806	U
1	A	1807	U
1	A	1808	A
1	A	1809	U
1	A	1810	A
1	A	1812	C
1	A	1814	A
1	A	1817	C
1	A	1820	A
1	A	1821	A
1	A	1823	A
1	A	1824	U
1	A	1825	A
1	A	1827	C
1	A	1828	A
1	A	1829	A
1	A	1832	A
1	A	1836	A
1	A	1839	C
1	A	1843	U
1	A	1844	A
1	A	1849	C
1	A	1851	G
1	A	1852	C

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Mol	Chain	Res	Type
1	A	1853	A
1	A	1854	U
1	A	1856	A
1	A	1867	A
1	A	1869	A
1	A	1871	A
1	A	1872	U
1	A	1878	U
1	A	1882	A
1	A	1883	G
1	A	1886	G
1	A	1887	A
1	A	1888	G
1	A	1889	C
1	A	1893	A
1	A	1894	G
1	A	1901	C
1	A	1902	C
1	A	1903	C
1	A	1909	A
1	A	1918	G
1	A	1927	G
1	A	1935	A
1	A	1939	G
1	A	1940	A
1	A	1944	C
1	A	1947	C
1	A	1956	U
1	A	1961	A
1	A	1966	G
1	A	1972	A
1	A	1973	G
1	A	1974	A
1	A	1975	U
1	A	1985	G
1	A	1986	A
1	A	1987	G
1	A	1991	A
1	A	1992	C
1	A	1993	A
1	A	1994	A
1	A	1995	A

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Mol	Chain	Res	Type
1	A	1998	U
1	A	1999	A
1	A	2000	C
1	A	2001	C
1	A	2002	G
1	A	2010	U
1	A	2014	A
1	A	2015	G
1	A	2016	C
1	A	2020	U
1	A	2021	U
1	A	2022	G
1	A	2029	A
1	A	2030	U
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2034	A
1	A	2036	C
1	A	2037	U
1	A	2039	A
1	A	2044	A
1	A	2053	U
1	A	2054	U
1	A	2057	C
1	A	2059	C
1	A	2060	A
1	A	2065	A
1	A	2066	C
1	A	2074	A
1	A	2079	C
1	A	2083	U
1	A	2085	A
1	A	2092	C
1	A	2093	U
1	A	2095	U
1	A	2097	A
1	A	2098	G
1	A	2099	U
1	A	2105	G
1	A	2111	C
1	A	2113	G

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Mol	Chain	Res	Type
1	A	2124	A
1	A	2125	C
1	A	2126	U
1	A	2129	G
1	A	2132	A
1	A	2134	A
1	A	2135	A
1	A	2136	C
1	A	2141	U
1	A	2142	A
1	A	2143	G
1	A	2147	G
1	A	2150	U
1	A	2154	A
1	A	2156	A
1	A	2157	U
1	A	2158	U
1	A	2159	U
1	A	2160	A
1	A	2163	A
1	A	2165	C
1	A	2166	C
1	A	2168	U
1	A	2169	A
1	A	2170	G
1	A	2172	A
1	A	2173	G
1	A	2174	G
1	A	2175	C
1	A	2180	A
1	A	2181	A
1	A	2182	G
1	A	2183	C
1	A	2187	C
1	A	2189	C
1	A	2190	C
1	A	2191	A
1	A	2192	A
1	A	2193	U
1	A	2194	U
1	A	2195	A
1	A	2196	A

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Mol	Chain	Res	Type
1	A	2197	G
1	A	2198	A
1	A	2200	A
1	A	2202	C
1	A	2204	U
1	A	2210	C
1	A	2211	U
1	A	2216	A
1	A	2218	C
1	A	2229	A
1	A	2230	A
1	A	2232	A
1	A	2233	U
1	A	2237	A
1	A	2238	A
1	A	2239	A
1	A	2241	A
1	A	2242	U
1	A	2243	A
1	A	2244	U
1	A	2245	A
1	A	2246	A
1	A	2247	C
1	A	2259	C
1	A	2262	C
1	A	2263	C
1	A	2264	A
1	A	2269	G
1	A	2271	C
1	A	2275	U
1	A	2280	C
1	A	2281	A
1	A	2283	C
1	A	2284	C
1	A	2285	U
1	A	2290	A
1	A	2294	A
1	A	2297	A
1	A	2299	U
1	A	2300	G
1	A	2306	A
1	A	2308	A

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Mol	Chain	Res	Type
1	A	2309	A
1	A	2315	A
1	A	2320	A
1	A	2321	A
1	A	2322	C
1	A	2324	U
1	A	2331	C
1	A	2332	C
1	A	2335	A
1	A	2342	U
1	A	2345	G
1	A	2350	A
1	A	2364	C
1	A	2365	U
1	A	2370	A
1	A	2371	U
1	A	2372	U
1	A	2373	A
1	A	2374	A
1	A	2375	C
1	A	2379	C
1	A	2381	A
1	A	2384	A
1	A	2387	U
1	A	2389	C
1	A	2390	A
1	A	2392	U
1	A	2393	C
1	A	2394	A
1	A	2395	A
1	A	2396	C
1	A	2397	C
1	A	2401	A
1	A	2404	U
1	A	2405	C
1	A	2406	A
1	A	2407	U
1	A	2413	C
1	A	2414	C
1	A	2415	C
1	A	2416	U
1	A	2417	C

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Mol	Chain	Res	Type
1	A	2418	A
1	A	2419	C
1	A	2421	G
1	A	2422	U
1	A	2423	C
1	A	2426	C
1	A	2429	A
1	A	2432	A
1	A	2434	A
1	A	2435	G
1	A	2443	C
1	A	2444	A
1	A	2445	U
1	A	2446	A
1	A	2447	A
1	A	2449	G
1	A	2453	G
1	A	2455	U
1	A	2458	A
1	A	2464	G
1	A	2471	G
1	A	2478	G
1	A	2479	C
1	A	2483	U
1	A	2484	C
1	A	2485	U
1	A	2493	C
1	A	2494	C
1	A	2498	U
1	A	2500	A
1	A	2502	C
1	A	2506	A
1	A	2507	A
1	A	2508	C
1	A	2511	C
1	A	2514	C
1	A	2520	C
1	A	2521	A
1	A	2522	U
1	A	2523	C
1	A	2524	A
1	A	2527	A

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Mol	Chain	Res	Type
1	A	2530	A
1	A	2531	U
1	A	2536	G
1	A	2540	C
1	A	2546	G
1	A	2550	A
1	A	2556	A
1	A	2557	C
1	A	2558	A
1	A	2559	U
1	A	2560	G
1	A	2561	U
1	A	2563	U
1	A	2564	A
1	A	2570	C
1	A	2574	G
1	A	2581	A
1	A	2583	C
1	A	2587	G
1	A	2590	A
1	A	2591	A
1	A	2592	G
1	A	2593	G
1	A	2594	U
1	A	2599	U
1	A	2601	A
1	A	2602	U
1	A	2603	C
1	A	2604	A
1	A	2606	U
1	A	2607	U
1	A	2610	U
1	A	2614	U
1	A	2615	A
1	A	2616	A
1	A	2618	U
1	A	2626	U
1	A	2627	G
1	A	2629	A
1	A	2630	U
1	A	2632	A
1	A	2633	A

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Mol	Chain	Res	Type
1	A	2634	U
1	A	2635	G
1	A	2638	U
1	A	2645	G
1	A	2649	U
1	A	2650	C
1	A	2654	U
1	A	2656	U
1	A	2660	U
1	A	2661	U
1	A	2665	U
1	A	2677	A
1	A	2683	C
1	A	2684	C
1	A	2686	G
1	A	2693	A
1	A	2694	A
1	A	2695	G
1	A	2696	A
1	A	2706	A
1	A	2708	C
1	A	2709	A
1	A	2713	C
1	A	2718	C
1	A	2719	G
1	A	2723	A
1	A	2724	G
1	A	2725	A
1	A	2726	C
1	A	2731	U
1	A	2732	G
1	A	2733	G
1	A	2740	A
1	A	2744	U
1	A	2745	A
1	A	2746	U
1	A	2748	A
1	A	2749	A
1	A	2750	U
1	A	2756	C
1	A	2757	A
1	A	2758	G

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Mol	Chain	Res	Type
1	A	2795	U
1	A	2804	A
1	A	2807	U
1	A	2810	G
1	A	2813	U
1	A	2814	G
1	A	2830	A
1	A	2831	G
1	A	2832	A
1	A	2833	A
1	A	2834	C
1	A	2842	C
1	A	2844	G
1	A	2846	G
1	A	2847	C
1	A	2848	A
1	A	2851	A
1	A	2854	U
1	A	2855	G
1	A	2857	U
1	A	2858	A
1	A	2859	A
1	A	2864	U
1	A	2865	C
1	A	2870	G
1	A	2871	U
1	A	2879	A
1	A	2892	A
1	A	2895	U
1	A	2901	A
1	A	2906	C
1	A	2910	A
1	A	2912	C
1	A	2913	A
1	A	2914	A
1	A	2916	G
1	A	2917	G
1	A	2919	A
1	A	2921	A
1	A	2922	A
1	A	2926	A
1	A	2928	C

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Mol	Chain	Res	Type
1	A	2933	G
1	A	2935	A
1	A	2936	U
1	A	2937	A
1	A	2945	A
1	A	2946	A
1	A	2948	C
1	A	2955	U
1	A	2956	A
1	A	2960	U
1	A	2961	C
1	A	2962	C
1	A	2963	A
1	A	2964	U
1	A	2971	A
1	A	2978	U
1	A	2982	C
1	A	2985	C
1	A	2986	C
1	A	2989	G
1	A	2990	A
1	A	2991	U
1	A	2992	G
1	A	2993	U
1	A	2994	U
1	A	2995	G
1	A	3004	C
1	A	3005	A
1	A	3007	C
1	A	3010	G
1	A	3014	G
1	A	3016	G
1	A	3018	A
1	A	3022	G
1	A	3029	A
1	A	3030	A
1	A	3031	G
1	A	3040	G
1	A	3041	U
1	A	3042	U
1	A	3049	U
1	A	3053	A

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Mol	Chain	Res	Type
1	A	3054	G
1	A	3055	U
1	A	3056	C
1	A	3059	A
1	A	3060	C
1	A	3061	G
1	A	3063	G
1	A	3064	A
1	A	3065	U
1	A	3068	G
1	A	3069	A
1	A	3070	G
1	A	3072	U
1	A	3073	C
1	A	3074	A
1	A	3076	A
1	A	3077	C
1	A	3085	A
1	A	3086	U
1	A	3093	C
1	A	3096	U
1	A	3097	U
1	A	3098	U
1	A	3100	U
1	A	3101	A
1	A	3102	U
1	A	3108	U
1	A	3109	U
1	A	3114	U
1	A	3123	G
1	A	3128	A
1	A	3129	A
1	A	3131	G
1	A	3141	A
1	A	3150	U
1	A	3151	A
1	A	3155	C
1	A	3157	C
1	A	3158	A
1	A	3160	A
1	A	3162	C
1	A	3168	C

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Mol	Chain	Res	Type
1	A	3169	C
1	A	3172	C
1	A	3173	G
1	A	3180	A
1	A	3183	U
1	A	3185	A
1	A	3189	C
1	A	3190	A
1	A	3196	G
1	A	3202	U
1	A	3204	C
1	A	3206	C
1	A	3207	A
1	A	3213	A
1	A	3217	A
1	A	3218	A
1	A	3220	A
1	A	3223	A
1	A	3228	U
2	B	1604	G
2	B	1608	G
2	B	1609	U
2	B	1610	A
2	B	1611	G
2	B	1612	C
2	B	1614	U
2	B	1615	A
2	B	1625	A
2	B	1629	A
2	B	1631	C
2	B	1632	U
2	B	1634	A
2	B	1641	G
2	B	1644	G
2	B	1645	A
2	B	1650	A
2	B	1659	U
2	B	1665	C
2	B	1667	C
2	B	1669	G

All (121) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1677	C
1	A	1700	U
1	A	1702	A
1	A	1703	C
1	A	1708	A
1	A	1713	A
1	A	1715	C
1	A	1724	A
1	A	1727	A
1	A	1772	A
1	A	1780	U
1	A	1798	A
1	A	1805	A
1	A	1806	U
1	A	1807	U
1	A	1809	U
1	A	1820	A
1	A	1823	A
1	A	1824	U
1	A	1852	C
1	A	1870	A
1	A	1871	A
1	A	1882	A
1	A	1887	A
1	A	1888	G
1	A	1901	C
1	A	1918	G
1	A	1972	A
1	A	1974	A
1	A	1985	G
1	A	1998	U
1	A	2001	C
1	A	2021	U
1	A	2029	A
1	A	2059	C
1	A	2065	A
1	A	2109	A
1	A	2135	A
1	A	2154	A
1	A	2158	U
1	A	2160	A
1	A	2165	C
1	A	2172	A

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Mol	Chain	Res	Type
1	A	2174	G
1	A	2186	C
1	A	2189	C
1	A	2193	U
1	A	2196	A
1	A	2197	G
1	A	2209	G
1	A	2231	A
1	A	2243	A
1	A	2245	A
1	A	2251	A
1	A	2274	A
1	A	2284	C
1	A	2321	A
1	A	2370	A
1	A	2372	U
1	A	2373	A
1	A	2374	A
1	A	2380	C
1	A	2400	C
1	A	2404	U
1	A	2421	G
1	A	2422	U
1	A	2431	C
1	A	2444	A
1	A	2457	A
1	A	2506	A
1	A	2507	A
1	A	2519	G
1	A	2523	C
1	A	2530	A
1	A	2531	U
1	A	2540	C
1	A	2558	A
1	A	2559	U
1	A	2601	A
1	A	2606	U
1	A	2607	U
1	A	2615	A
1	A	2617	A
1	A	2618	U
1	A	2625	C

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Mol	Chain	Res	Type
1	A	2628	U
1	A	2649	U
1	A	2653	C
1	A	2693	A
1	A	2695	G
1	A	2744	U
1	A	2807	U
1	A	2813	U
1	A	2831	G
1	A	2839	C
1	A	2853	A
1	A	2865	C
1	A	2870	G
1	A	2905	A
1	A	2918	A
1	A	2936	U
1	A	2945	A
1	A	2955	U
1	A	2989	G
1	A	2990	A
1	A	2993	U
1	A	3016	G
1	A	3030	A
1	A	3041	U
1	A	3063	G
1	A	3068	G
1	A	3092	U
1	A	3096	U
1	A	3149	C
1	A	3160	A
1	A	3162	C
1	A	3168	C
1	A	3201	A
2	B	1607	U
2	B	1608	G
2	B	1628	C

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 70 ligands modelled in this entry, 69 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
52	A	A	3301	-	17,24,25	0.53	0	16,35,38	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	A	A	3301	-	-	0/3/25/26	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.