



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Oct 2, 2017 – 04:52 AM EDT

PDB ID : 5NGM
EMDB ID: : EMD-3637
Title : 2.9S structure of the 70S ribosome composing the S. aureus 100S complex
Authors : Matzov, D.; Aibara, S.; Zimmerman, E.; Bashan, A.; Amunts, A.; Yonath, A.
Deposited on : unknown
Resolution : 2.90 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

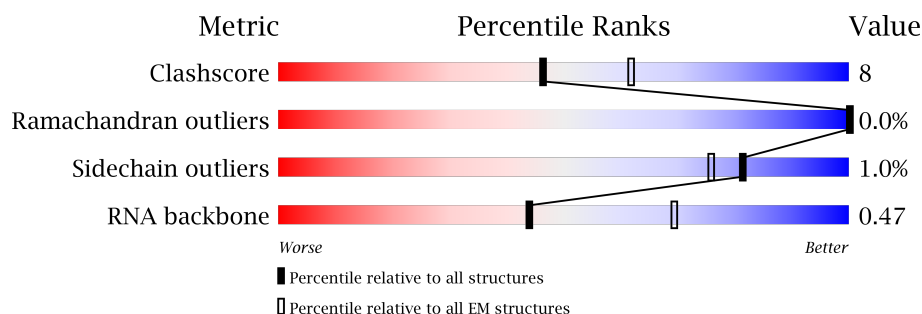
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.




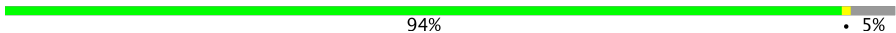

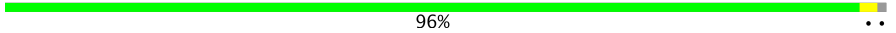

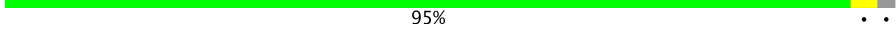
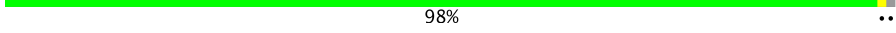
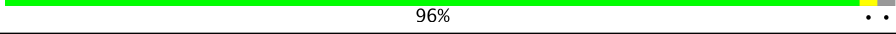



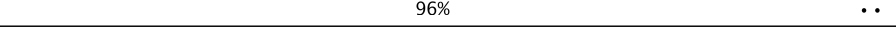

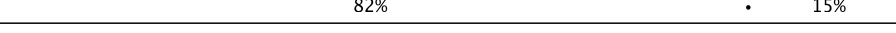
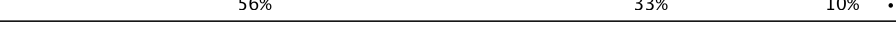


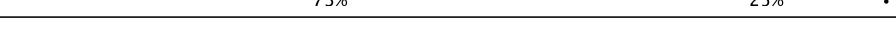


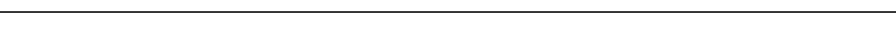




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	Aa	1555	68% 29% ..
2	Ab	255	88% 11%
3	Ac	217	93% 7%
4	Ad	200	98% ..
5	Ae	166	93% 6%
6	Af	98	96% ..
7	Ag	156	97% .
8	Ah	132	98% ..









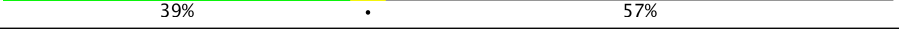


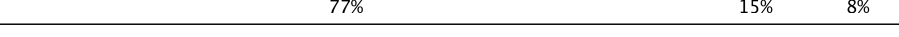

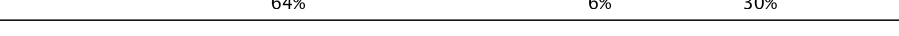


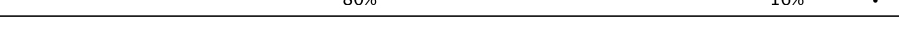

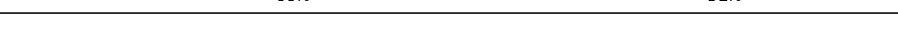
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Mol	Chain	Length	Quality of chain
9	Ai	132	 93% . .
10	Aj	102	 94% . 5%
11	Ak	129	 88% 12%
12	Al	137	 96% . .
13	Am	121	 85% . 14%
14	An	61	 95% . .
15	Ao	89	 98% . .
16	Ap	91	 96% . .
17	Aq	87	 92% 8%
18	Ar	80	 66% . 33%
19	As	92	 86% . 13%
20	At	83	 96% . .
21	Au	58	 90% 10%
22	Av	190	 82% . 15%
23	AA	2923	 56% 33% 10% . .
24	AB	115	 72% 23% . .
25	AC	277	 75% 24% .
26	AD	220	 73% 25% .
27	AE	207	 83% 16%
28	AF	179	 78% 20% .
29	AG	178	 83% 15% . .
30	AH	145	 90% 10%
31	AI	122	 67% 32% .
32	AJ	146	 76% 24%
33	AK	144	 76% 18% . 5%

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Mol	Chain	Length	Quality of chain
34	AL	122	
35	AM	119	
36	AN	116	
37	AO	118	
38	AP	102	
39	AQ	117	
40	AR	91	
41	AS	105	
42	AT	217	
43	AU	94	
44	AV	62	
45	AW	73	
46	AX	59	
47	AY	84	
48	AZ	57	
49	A1	49	
50	A2	45	
51	A3	66	
52	A4	37	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 140965 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	1539	Total	C	N	O	P	0	0
			32969	14719	6017	10694	1539		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ab	226	Total	C	N	O	S	0	0
			1819	1159	317	335	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ac	202	Total	C	N	O	S	0	0
			1501	945	284	271	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ad	198	Total	C	N	O	S	0	0
			1497	952	275	268	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ae	156	Total	C	N	O	S	0	0
			1145	723	211	209	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Af	95	Total	C	N	O	S	0	0
			778	493	138	145	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Ag	152	Total	C	N	O	S	0	0
			1161	722	218	217	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ah	131	Total	C	N	O	S	0	0
			1026	650	183	189	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ai	127	Total	C	N	O	S	0	0
			922	576	179	166	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Aj	97	Total	C	N	O	S	0	0
			752	475	140	136	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Ak	114	Total	C	N	O	S	0	0
			810	498	151	159	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Al	135	Total	C	N	O	S	0	0
			1037	646	211	178	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Am	104	Total	C	N	O	0	0
			727	453	139	135		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	An	60	Total	C	N	O	S	0	0
			487	307	98	77	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ao	88	Total	C	N	O	S	0	0
			723	448	150	124	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ap	89	Total	C	N	O	S	0	0
			694	436	128	129	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Aq	80	Total	C	N	O	S	0	0
			621	392	112	117			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Ar	54	Total	C	N	O	S	0	0
			445	284	86	73	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	As	80	Total	C	N	O	S	0	0
			636	410	113	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	At	81	Total	C	N	O	S	0	0
			591	358	117	115	1		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Au	52	Total	C	N	O	0	0
			400	249	79	72		

- Molecule 22 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Av	162	Total	C	N	O	S	0	0
			1333	835	242	254	2		

- Molecule 23 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AA	2905	Total	C	N	O	P	0	0
			62277	27803	11387	20182	2905		

- Molecule 24 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AB	115	Total	C	N	O	P	0	0
			2445	1094	436	801	114		

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AC	274	Total	C	N	O	S	0	0
			2094	1303	415	371	5		

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AD	215	Total	C	N	O	S	0	0
			1627	1018	299	305	5		

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AE	206	Total	C	N	O	S	0	0
			1572	986	288	296	2		

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AF	175	Total	C	N	O	S	0	0
			1325	837	227	255	6		

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AG	175	Total	C	N	O	S	0	0
			1263	790	239	231	3		

- Molecule 30 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AH	145	Total	C	N	O	S	0	0
			1143	714	208	218	3		

- Molecule 31 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AI	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AJ	146	Total	C	N	O	S	0	0
			1086	674	214	197	1		

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AK	137	Total	C	N	O	S	0	0
			1071	689	203	175	4		

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AL	120	Total	C	N	O	S	0	0
			932	576	182	173	1		

- Molecule 35 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AM	119	Total	C	N	O	S	0	0
			891	557	174	159	1		

- Molecule 36 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AN	114	Total	C	N	O	S	0	0
			889	563	175	151			

- Molecule 37 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AO	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

- Molecule 38 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	AP	102	Total	C	N	O	S	0	0
			790	503	142	144	1		

- Molecule 39 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	AQ	112	Total	C	N	O	S	0	0
			854	534	164	153	3		

- Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	AR	89	Total	C	N	O	S	0	0
			715	453	127	131	4		

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AS	103	Total	C	N	O	S	0	0
			770	486	142	141	1		

- Molecule 42 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	AT	94	Total	C	N	O	0	0
			722	463	130	129		

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	AU	82	Total	C	N	O	0	0
			622	385	122	115		

- Molecule 44 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	AV	58	Total	C	N	O	0	0
			445	277	96	72		

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	AW	67	Total	C	N	O	0	0
			541	333	102	106		

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	AX	58	Total	C	N	O	0	0
			449	280	85	84		

- Molecule 47 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AY	59	Total	C	N	O	S	0	0
			370	225	68	76	1		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AZ	48	Total	C	N	O	S	0	0
			360	222	77	59	2		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	A1	47	Total	C	N	O	S	0	0
			390	238	78	70	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	A2	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	A3	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	A4	37	Total	C	N	O	S	0	0
			295	186	60	44	5		

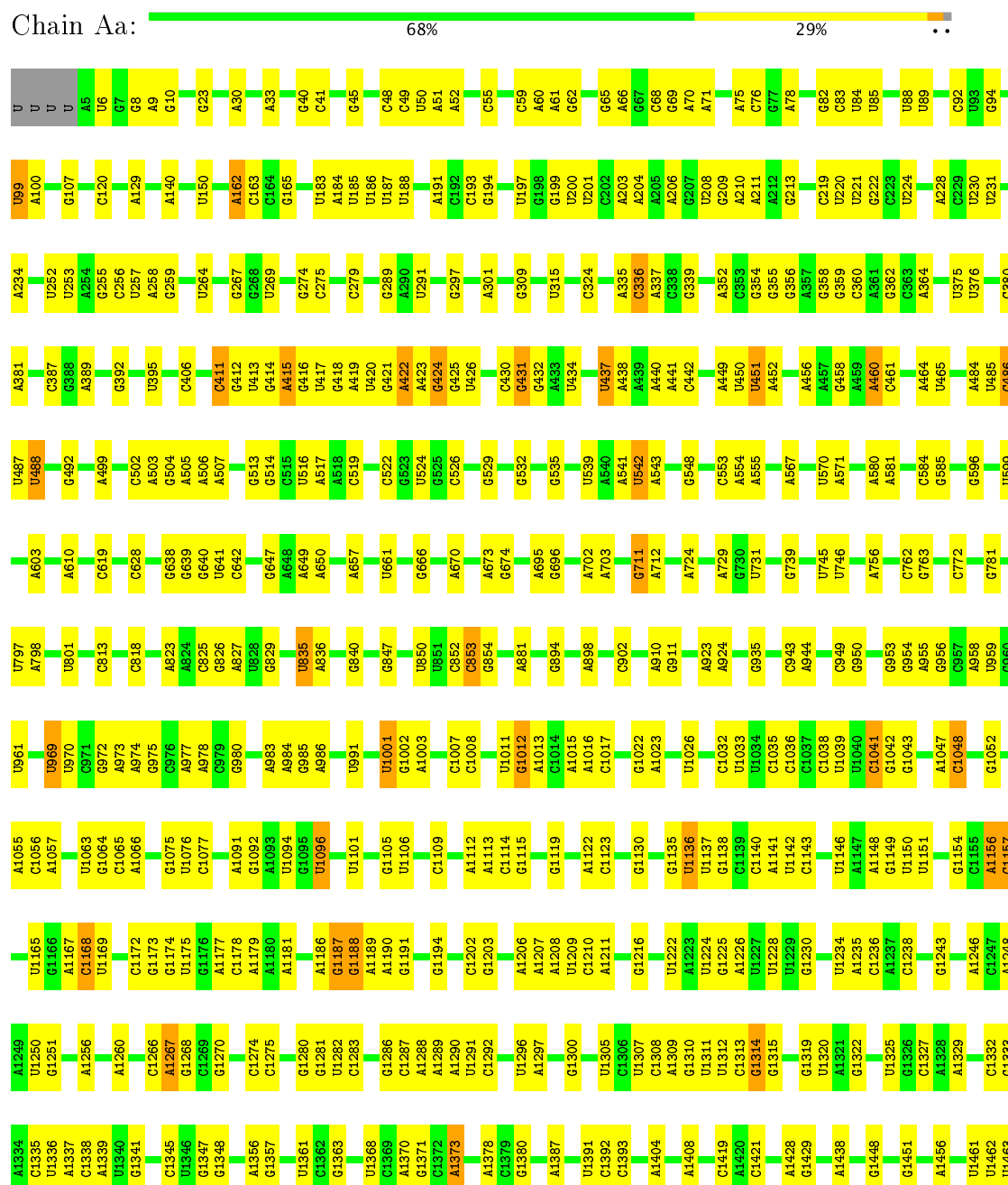
- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	AB	2	Total	Mg	0
			2	2	
53	AA	199	Total	Mg	0
			199	199	
53	AZ	1	Total	Mg	0
			1	1	
53	AC	2	Total	Mg	0
			2	2	
53	AU	1	Total	Mg	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

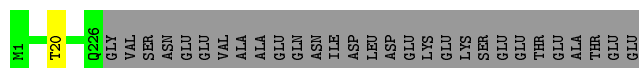
• Molecule 1: 16S ribosomal RNA





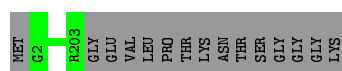
- Molecule 2: 30S ribosomal protein S2

Chain Ab: 88% 11%



- Molecule 3: 30S ribosomal protein S3

Chain Ac: 93% 7%



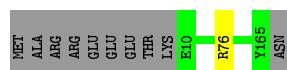
- Molecule 4: 30S ribosomal protein S4

Chain Ad: 98% ..



- Molecule 5: 30S ribosomal protein S5

Chain Ae: 93% • 6%



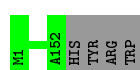
- Molecule 6: 30S ribosomal protein S6

Chain Af: 96% ..



- Molecule 7: 30S ribosomal protein S7

Chain Ag: 97% •



- Molecule 8: 30S ribosomal protein S8

Chain Ah: 98% ..



- Molecule 9: 30S ribosomal protein S9

Chain Ai:  93% . .



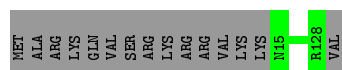
- Molecule 10: 30S ribosomal protein S10

Chain Aj:  94% . 5%



- Molecule 11: 30S ribosomal protein S11

Chain Ak:  88% 12%



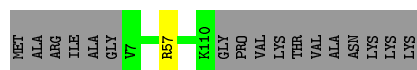
- Molecule 12: 30S ribosomal protein S12

Chain Al:  96% ..



- Molecule 13: 30S ribosomal protein S13

Chain Am:  85% . 14%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain An:  95% . .



- Molecule 15: 30S ribosomal protein S15

Chain Ao:  98% ..



- Molecule 16: 30S ribosomal protein S16

Chain Ap:  96% ..



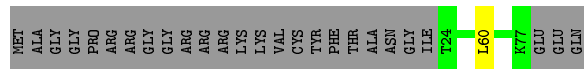
- Molecule 17: 30S ribosomal protein S17

Chain Aq:  92% 8%




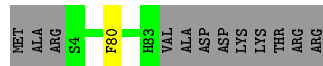
- Molecule 18: 30S ribosomal protein S18

Chain Ar:  66% 33%



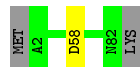
- Molecule 19: 30S ribosomal protein S19

Chain As:  86% 13%



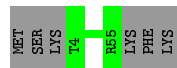
- Molecule 20: 30S ribosomal protein S20

Chain At:  96% ..




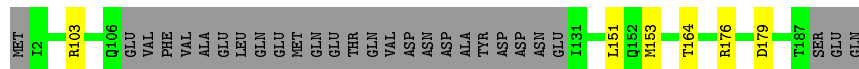
- Molecule 21: 30S ribosomal protein S21

Chain Au:  90% 10%



- Molecule 22: Ribosome hibernation promoting factor

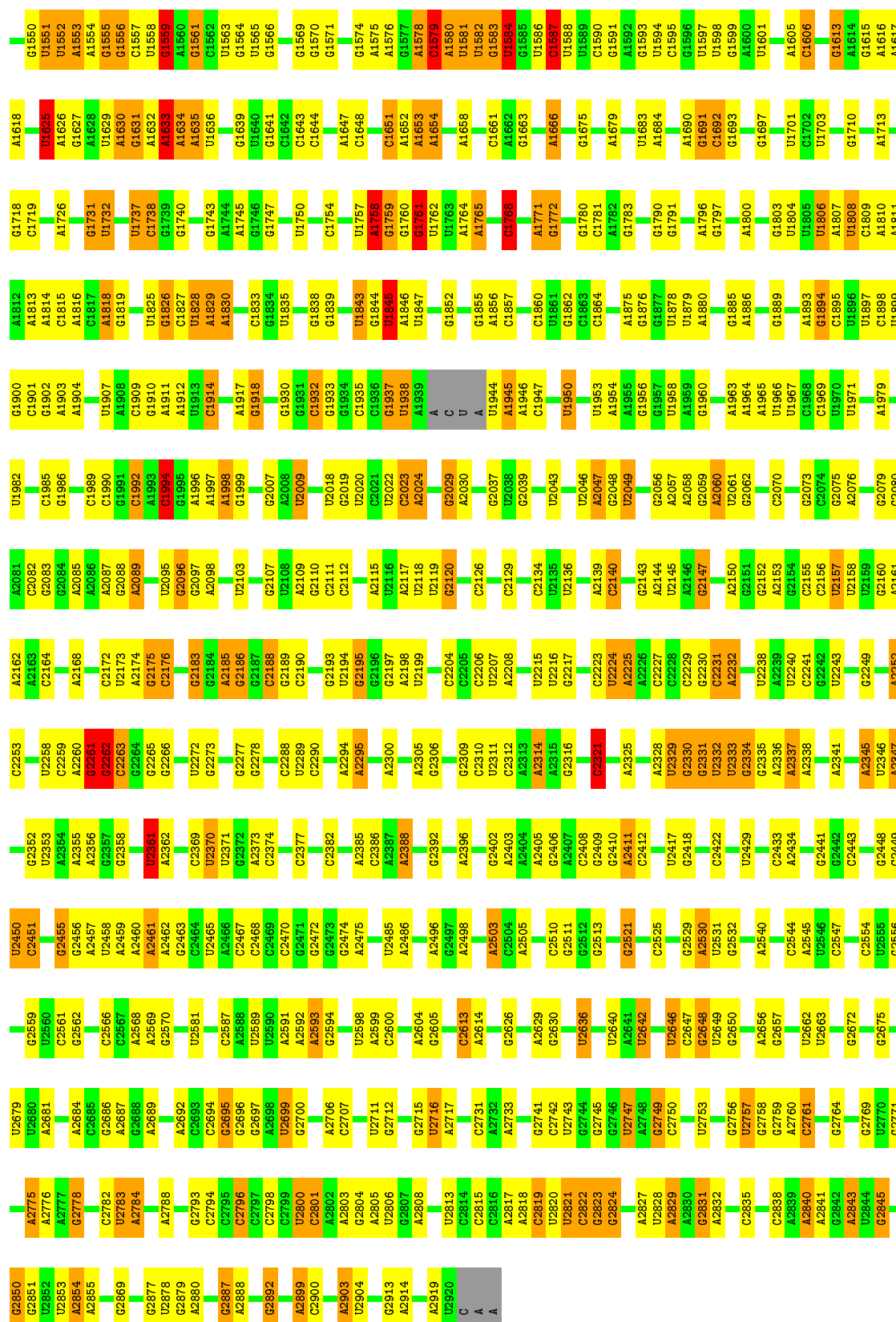
Chain Av:  82% 15%

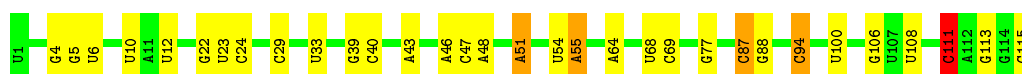


- Molecule 23: 23S Ribosomal RNA

Chain AA:  56% 33% 10% ..

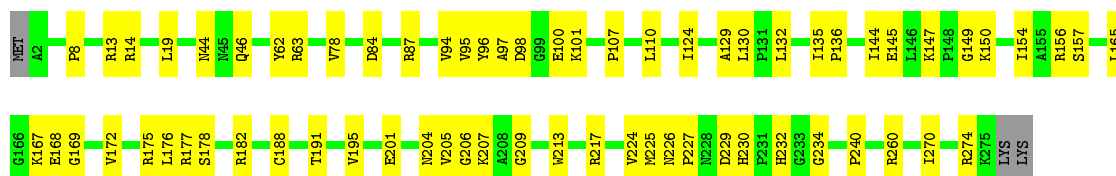




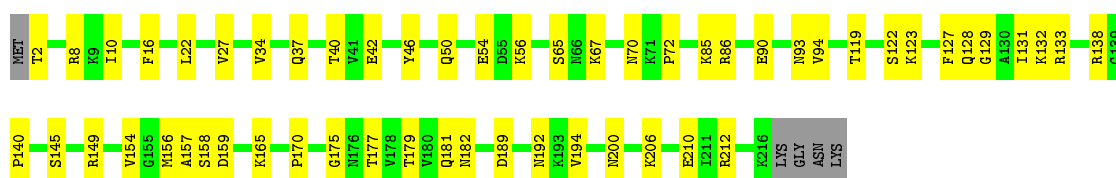
- Molecule 25: 50S ribosomal protein L2

Chain AC: 75% 24%



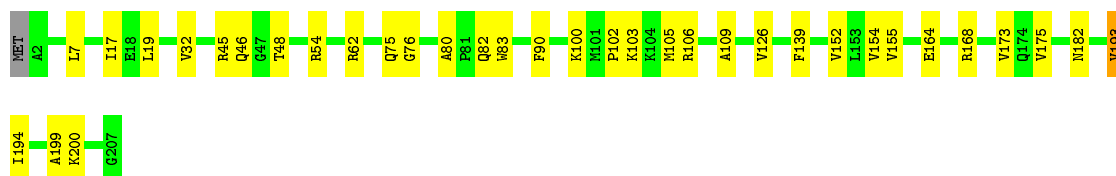
- Molecule 26: 50S ribosomal protein L3

Chain AD: 73% 25%



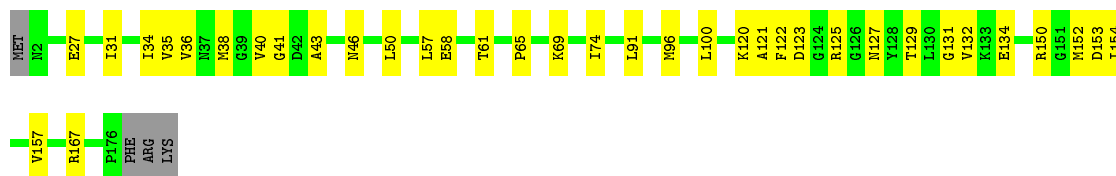
- Molecule 27: 50S ribosomal protein L4

Chain AE: 83% 16%



- Molecule 28: 50S ribosomal protein L5

Chain AF: 78% 20%



- Molecule 29: 50S ribosomal protein L6

Chain AG: 83% 15%



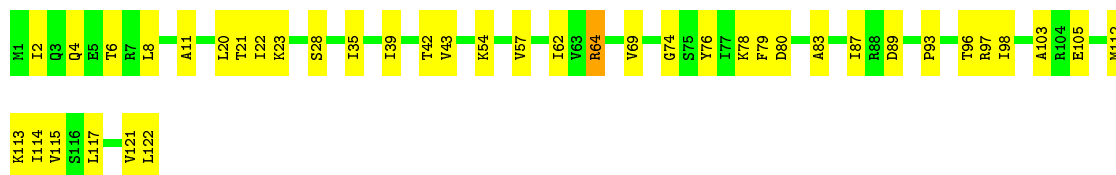
- Molecule 30: 50S ribosomal protein L13

Chain AH:  90% 10%




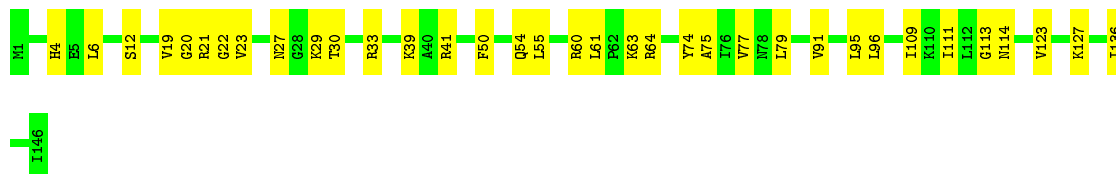
- Molecule 31: 50S ribosomal protein L14

Chain AI:  67% 32%




- Molecule 32: 50S ribosomal protein L15

Chain AJ:  76% 24%




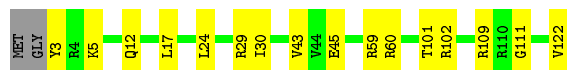
- Molecule 33: 50S ribosomal protein L16

Chain AK:  76% 18% 5%




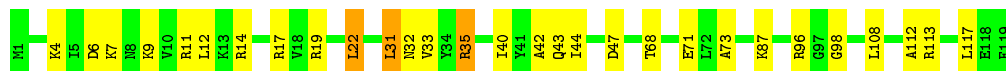
- Molecule 34: 50S ribosomal protein L17

Chain AL:  85% 13%




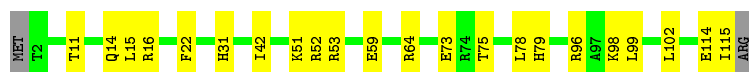
- Molecule 35: 50S ribosomal protein L18

Chain AM:  76% 22%

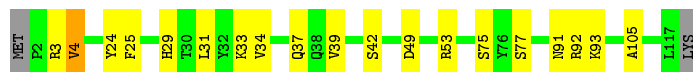
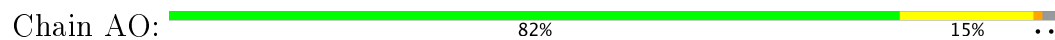


- Molecule 36: 50S ribosomal protein L19

Chain AN:  79% 19%



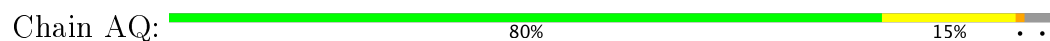
- Molecule 37: 50S ribosomal protein L20



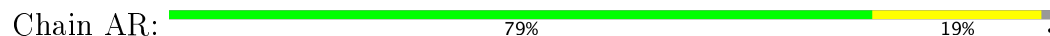
- Molecule 38: 50S ribosomal protein L21



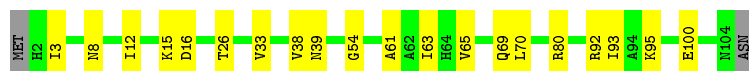
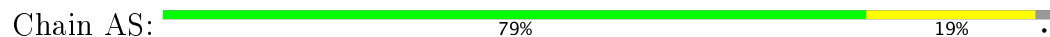
- Molecule 39: 50S ribosomal protein L22



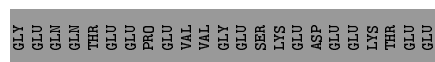
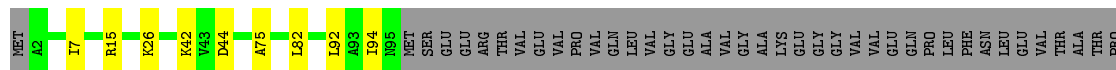
- Molecule 40: 50S ribosomal protein L23




- Molecule 41: 50S ribosomal protein L24



- Molecule 42: 50S ribosomal protein L25




- Molecule 43: 50S ribosomal protein L27

Chain AU:  73% 13% • 13%




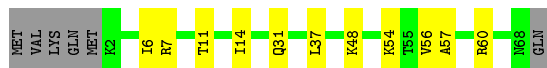
- Molecule 44: 50S ribosomal protein L28

Chain AV:  81% 11% • 6%




- Molecule 45: 50S ribosomal protein L29

Chain AW:  77% 15% 8%



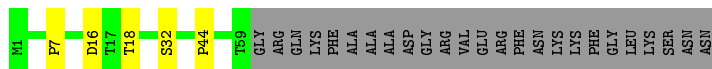
- Molecule 46: 50S ribosomal protein L30

Chain AX:  81% 17% •



- Molecule 47: 50S ribosomal protein L31 type B

Chain AY:  64% 6% 30%




- Molecule 48: 50S ribosomal protein L32

Chain AZ:  67% 18% 16%




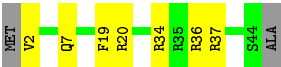
- Molecule 49: 50S ribosomal protein L33

Chain A1:  80% 16% •

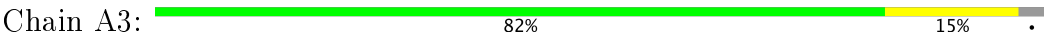


- Molecule 50: 50S ribosomal protein L34

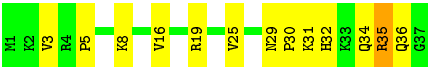
Chain A2:  80% 16% •



- Molecule 51: 50S ribosomal protein L35



- Molecule 52: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	224554	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.3	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	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: 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	Aa	0.38	0/36913	0.95	102/57564 (0.2%)
10	Aj	0.27	0/764	0.56	0/1034
11	Ak	0.29	0/824	0.59	0/1119
12	Al	0.30	0/1054	0.63	1/1415 (0.1%)
13	Am	0.26	0/732	0.56	0/991
14	An	0.32	0/497	0.63	0/662
15	Ao	0.26	0/732	0.53	0/979
16	Ap	0.33	0/705	0.57	0/952
17	Aq	0.31	0/629	0.58	0/849
18	Ar	0.28	0/452	0.65	1/604 (0.2%)
19	As	0.31	0/654	0.58	0/879
2	Ab	0.26	0/1846	0.54	1/2477 (0.0%)
20	At	0.23	0/591	0.50	0/793
21	Au	0.27	0/403	0.51	0/535
22	Av	0.49	0/1350	0.81	2/1812 (0.1%)
23	AA	0.74	3/69738 (0.0%)	1.02	202/108747 (0.2%)
24	AB	0.61	0/2732	1.16	20/4253 (0.5%)
25	AC	0.48	0/2129	0.67	3/2858 (0.1%)
26	AD	0.49	0/1651	0.66	0/2215
27	AE	0.47	0/1595	0.66	0/2154
28	AF	0.31	0/1339	0.63	0/1805
29	AG	0.35	0/1281	0.58	0/1736
3	Ac	0.27	0/1523	0.59	0/2062
30	AH	0.48	0/1165	0.65	0/1570
31	AI	0.47	0/925	0.73	3/1242 (0.2%)
32	AJ	0.45	0/1100	0.71	2/1467 (0.1%)
33	AK	0.46	0/1095	0.61	0/1472
34	AL	0.43	0/936	0.71	0/1253
35	AM	0.43	0/900	0.68	2/1205 (0.2%)
36	AN	0.43	0/901	0.65	1/1209 (0.1%)
37	AO	0.52	0/954	0.64	0/1264
38	AP	0.47	0/800	0.67	0/1070

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	AQ	0.45	0/862	0.70	0/1161
4	Ad	0.28	0/1526	0.62	1/2063 (0.0%)
40	AR	0.43	0/723	0.63	0/966
41	AS	0.39	0/779	0.67	0/1043
42	AT	0.37	0/730	0.66	1/981 (0.1%)
43	AU	0.54	0/628	0.68	1/833 (0.1%)
44	AV	0.38	0/451	0.66	0/603
45	AW	0.39	0/542	0.69	0/722
46	AX	0.40	0/451	0.61	0/606
47	AY	0.25	0/378	0.53	0/521
48	AZ	0.43	0/366	0.65	0/489
49	A1	0.34	0/395	0.60	0/530
5	Ae	0.28	0/1159	0.59	0/1566
50	A2	0.48	0/371	0.67	0/484
51	A3	0.40	0/526	0.61	0/690
52	A4	0.52	0/298	0.63	0/392
6	Af	0.30	0/789	0.60	1/1060 (0.1%)
7	Ag	0.26	0/1176	0.54	0/1588
8	Ah	0.31	0/1038	0.63	0/1395
9	Ai	0.27	0/937	0.67	1/1269 (0.1%)
All	All	0.58	3/153035 (0.0%)	0.92	345/229209 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	Al	0	1
19	As	0	1
20	At	0	1
26	AD	0	1
38	AP	0	1
5	Ae	0	1
9	Ai	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AA	1584	U	C1'-N1	5.36	1.56	1.48
23	AA	1065	A	N9-C4	-5.35	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AA	1186	A	N9-C4	-5.08	1.34	1.37

All (345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	87	C	N1-C2-O2	12.65	126.49	118.90
24	AB	87	C	C2-N1-C1'	12.12	132.13	118.80
23	AA	576	U	C2-N1-C1'	11.98	132.08	117.70
1	Aa	745	U	OP1-P-O3'	-11.40	80.13	105.20
23	AA	2150	A	N7-C8-N9	10.80	119.20	113.80
24	AB	111	C	N1-C2-O2	10.61	125.27	118.90
23	AA	576	U	N1-C2-O2	10.61	130.22	122.80
24	AB	87	C	N3-C2-O2	-10.51	114.55	121.90
23	AA	1179	C	N1-C2-O2	10.45	125.17	118.90
23	AA	576	U	N3-C2-O2	-10.00	115.20	122.20
23	AA	2150	A	C5-N7-C8	9.88	108.84	103.90
23	AA	1994	C	N1-C2-O2	9.73	124.74	118.90
23	AA	1994	C	C2-N1-C1'	9.61	129.37	118.80
23	AA	1932	C	N1-C2-O2	9.48	124.59	118.90
23	AA	1932	C	C2-N1-C1'	9.36	129.10	118.80
24	AB	87	C	C6-N1-C1'	-9.05	109.94	120.80
23	AA	1179	C	N3-C2-O2	-8.75	115.77	121.90
23	AA	1179	C	C2-N1-C1'	8.72	128.39	118.80
24	AB	111	C	N3-C2-O2	-8.69	115.82	121.90
23	AA	593	U	C2-N1-C1'	8.62	128.04	117.70
24	AB	111	C	C2-N1-C1'	8.59	128.24	118.80
24	AB	108	U	N3-C2-O2	-8.42	116.31	122.20
23	AA	439	U	C2-N1-C1'	8.36	127.73	117.70
23	AA	1894	G	C4-N9-C1'	8.34	137.35	126.50
23	AA	576	U	C6-N1-C1'	-8.33	109.54	121.20
9	Ai	66	LEU	CA-CB-CG	8.30	134.39	115.30
23	AA	1378	U	N3-C2-O2	-8.23	116.44	122.20
23	AA	1804	U	C2-N1-C1'	8.16	127.50	117.70
1	Aa	55	C	N1-C2-O2	8.13	123.78	118.90
1	Aa	99	U	C2-N1-C1'	8.07	127.39	117.70
24	AB	108	U	C2-N1-C1'	8.04	127.34	117.70
1	Aa	599	U	C2-N1-C1'	8.03	127.33	117.70
23	AA	1378	U	N1-C2-O2	8.02	128.41	122.80
24	AB	100	U	C2-N1-C1'	8.02	127.32	117.70
23	AA	759	U	N1-C2-O2	8.01	128.41	122.80
1	Aa	55	C	C2-N1-C1'	7.99	127.59	118.80
23	AA	1994	C	N3-C2-O2	-7.99	116.31	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AA	759	U	C2-N1-C1'	7.98	127.28	117.70
1	Aa	1187	G	C4-N9-C1'	7.94	136.82	126.50
23	AA	439	U	N3-C2-O2	-7.83	116.72	122.20
23	AA	439	U	N1-C2-O2	7.82	128.27	122.80
23	AA	1227	U	N3-C2-O2	-7.82	116.73	122.20
1	Aa	745	U	OP2-P-O3'	-7.80	88.05	105.20
23	AA	2370	U	N3-C2-O2	-7.73	116.79	122.20
23	AA	882	C	C2-N1-C1'	7.70	127.27	118.80
23	AA	1378	U	C2-N1-C1'	7.65	126.88	117.70
24	AB	108	U	N1-C2-O2	7.59	128.11	122.80
23	AA	1932	C	N3-C2-O2	-7.58	116.60	121.90
31	AI	20	LEU	CA-CB-CG	7.56	132.69	115.30
23	AA	1894	G	C8-N9-C1'	-7.53	117.21	127.00
1	Aa	1136	U	C2-N1-C1'	7.45	126.64	117.70
35	AM	31	LEU	CA-CB-CG	7.44	132.40	115.30
23	AA	1599	G	N3-C2-N2	-7.37	114.74	119.90
1	Aa	415	A	P-O3'-C3'	7.32	128.49	119.70
23	AA	1692	C	C2-N1-C1'	7.25	126.78	118.80
23	AA	1579	C	N1-C2-O2	7.22	123.23	118.90
1	Aa	835	U	C2-N1-C1'	7.14	126.27	117.70
1	Aa	902	C	C2-N1-C1'	7.13	126.64	118.80
23	AA	1994	C	C6-N1-C1'	-7.13	112.25	120.80
23	AA	2223	C	N1-C2-O2	7.11	123.17	118.90
1	Aa	746	U	OP1-P-OP2	7.09	130.24	119.60
23	AA	1597	U	N3-C2-O2	-7.08	117.25	122.20
1	Aa	99	U	N3-C2-O2	-7.07	117.25	122.20
1	Aa	99	U	N1-C2-O2	7.07	127.75	122.80
23	AA	1932	C	C6-N1-C1'	-7.05	112.34	120.80
1	Aa	460	A	P-O3'-C3'	6.97	128.06	119.70
23	AA	2261	G	P-O3'-C3'	-6.97	111.34	119.70
23	AA	759	U	N3-C2-O2	-6.96	117.32	122.20
1	Aa	1187	G	N3-C4-N9	6.95	130.17	126.00
23	AA	1914	C	N1-C2-O2	6.93	123.06	118.90
23	AA	2819	C	N1-C2-O2	6.90	123.04	118.90
23	AA	575	G	C4-N9-C1'	6.88	135.44	126.50
23	AA	1894	G	N3-C4-N9	6.87	130.12	126.00
1	Aa	431	G	C4-N9-C1'	6.85	135.41	126.50
1	Aa	424	G	C4-N9-C1'	6.85	135.41	126.50
23	AA	1160	C	N1-C2-O2	6.85	123.01	118.90
23	AA	1214	C	N1-C2-O2	6.85	123.01	118.90
23	AA	2361	U	C2-N1-C1'	6.82	125.88	117.70
22	Av	176	ARG	NE-CZ-NH1	6.81	123.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	853	C	P-O3'-C3'	6.76	127.81	119.70
1	Aa	55	C	N3-C2-O2	-6.72	117.19	121.90
1	Aa	1187	G	N3-C4-C5	-6.67	125.26	128.60
1	Aa	431	G	N3-C4-N9	6.65	129.99	126.00
23	AA	1227	U	N1-C2-O2	6.64	127.45	122.80
1	Aa	424	G	N3-C4-C5	-6.60	125.30	128.60
1	Aa	711	G	P-O3'-C3'	6.60	127.62	119.70
1	Aa	451	U	P-O3'-C3'	6.57	127.58	119.70
1	Aa	1041	C	P-O3'-C3'	6.57	127.58	119.70
1	Aa	65	G	P-O3'-C3'	6.57	127.58	119.70
1	Aa	1187	G	C8-N9-C1'	-6.53	118.52	127.00
4	Ad	101	LEU	CA-CB-CG	6.51	130.27	115.30
1	Aa	1075	G	P-O3'-C3'	6.50	127.50	119.70
23	AA	1597	U	N1-C2-O2	6.50	127.35	122.80
1	Aa	1136	U	N3-C2-O2	-6.49	117.66	122.20
1	Aa	336	C	C2-N1-C1'	6.49	125.93	118.80
23	AA	2049	U	C2-N1-C1'	6.48	125.48	117.70
1	Aa	835	U	N3-C2-O2	-6.44	117.69	122.20
1	Aa	315	U	C2-N1-C1'	6.44	125.42	117.70
23	AA	268	A	P-O3'-C3'	6.43	127.41	119.70
23	AA	1213	C	N1-C2-O2	6.42	122.75	118.90
23	AA	2223	C	N3-C2-O2	-6.42	117.41	121.90
23	AA	1731	G	P-O3'-C3'	6.41	127.39	119.70
23	AA	2699	U	N1-C2-O2	6.41	127.28	122.80
23	AA	2450	U	P-O3'-C3'	6.40	127.38	119.70
23	AA	1651	C	N1-C2-O2	6.38	122.73	118.90
23	AA	1992	C	C2-N1-C1'	6.36	125.80	118.80
24	AB	111	C	C6-N1-C1'	-6.36	113.17	120.80
1	Aa	1136	U	N1-C2-O2	6.36	127.25	122.80
23	AA	1552	U	N3-C2-O2	-6.34	117.76	122.20
23	AA	74	U	N1-C2-O2	6.34	127.24	122.80
1	Aa	902	C	N3-C2-O2	-6.33	117.47	121.90
23	AA	1804	U	C6-N1-C1'	-6.33	112.33	121.20
23	AA	1804	U	N3-C2-O2	-6.33	117.77	122.20
1	Aa	431	G	N3-C4-C5	-6.33	125.44	128.60
23	AA	975	U	N1-C2-O2	6.31	127.22	122.80
23	AA	2262	G	O5'-P-OP1	-6.30	100.03	105.70
23	AA	2747	U	C2-N1-C1'	6.30	125.26	117.70
23	AA	1692	C	N1-C2-O2	6.29	122.68	118.90
1	Aa	424	G	N3-C4-N9	6.29	129.78	126.00
23	AA	575	G	N3-C4-N9	6.29	129.78	126.00
1	Aa	762	C	C2-N1-C1'	6.26	125.69	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AA	862	C	N1-C2-O2	6.26	122.66	118.90
23	AA	988	C	N1-C2-O2	6.26	122.66	118.90
1	Aa	902	C	N1-C2-O2	6.26	122.65	118.90
1	Aa	797	U	C2-N1-C1'	6.24	125.19	117.70
24	AB	94	C	N1-C2-O2	6.22	122.63	118.90
23	AA	1804	U	N1-C2-O2	6.21	127.15	122.80
1	Aa	599	U	N1-C2-O2	6.20	127.14	122.80
23	AA	184	C	C2-N1-C1'	6.19	125.61	118.80
23	AA	1953	U	C2-N1-C1'	6.18	125.12	117.70
23	AA	1227	U	C2-N1-C1'	6.18	125.11	117.70
23	AA	1579	C	N3-C2-O2	-6.17	117.58	121.90
1	Aa	1168	C	N1-C2-O2	6.17	122.60	118.90
23	AA	1914	C	N3-C2-O2	-6.17	117.58	121.90
1	Aa	835	U	N1-C2-O2	6.17	127.12	122.80
18	Ar	60	LEU	CA-CB-CG	6.16	129.48	115.30
1	Aa	387	C	C2-N1-C1'	6.16	125.57	118.80
1	Aa	460	A	C2-N3-C4	6.14	113.67	110.60
1	Aa	1001	U	P-O3'-C3'	6.14	127.07	119.70
23	AA	2845	G	N3-C2-N2	-6.14	115.60	119.90
1	Aa	502	C	C2-N1-C1'	6.13	125.54	118.80
23	AA	882	C	C6-N1-C1'	-6.13	113.45	120.80
1	Aa	524	U	C2-N1-C1'	6.12	125.04	117.70
23	AA	593	U	C6-N1-C1'	-6.09	112.67	121.20
1	Aa	762	C	N1-C2-O2	6.09	122.55	118.90
23	AA	2845	G	N3-C4-N9	-6.08	122.36	126.00
23	AA	575	G	C8-N9-C1'	-6.07	119.11	127.00
23	AA	2112	C	N1-C2-O2	6.04	122.53	118.90
36	AN	15	LEU	CA-CB-CG	6.04	129.18	115.30
1	Aa	1140	C	N1-C2-O2	6.02	122.51	118.90
1	Aa	162	A	C2-N3-C4	6.02	113.61	110.60
1	Aa	1314	G	P-O3'-C3'	6.01	126.92	119.70
1	Aa	969	U	P-O3'-C3'	6.01	126.92	119.70
1	Aa	1096	U	C2-N1-C1'	5.99	124.88	117.70
23	AA	2347	A	C2-N3-C4	5.97	113.58	110.60
1	Aa	1096	U	N1-C2-O2	5.97	126.98	122.80
23	AA	882	C	N3-C2-O2	-5.97	117.72	121.90
23	AA	463	C	N1-C2-O2	5.96	122.48	118.90
23	AA	987	U	P-O3'-C3'	5.96	126.86	119.70
23	AA	882	C	N1-C2-O2	5.96	122.48	118.90
23	AA	576	U	P-O3'-C3'	5.95	126.84	119.70
23	AA	2223	C	C2-N1-C1'	5.95	125.34	118.80
23	AA	1179	C	C6-N1-C1'	-5.95	113.66	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1267	A	P-O3'-C3'	5.95	126.84	119.70
1	Aa	1325	U	C2-N1-C1'	5.93	124.82	117.70
23	AA	439	U	C6-N1-C1'	-5.93	112.89	121.20
24	AB	87	C	C6-N1-C2	-5.93	117.93	120.30
23	AA	1731	G	OP1-P-O3'	5.93	118.25	105.20
23	AA	577	A	P-O3'-C3'	5.93	126.81	119.70
23	AA	1179	C	C6-N1-C2	-5.92	117.93	120.30
1	Aa	431	G	C8-N9-C1'	-5.91	119.32	127.00
24	AB	100	U	C6-N1-C1'	-5.90	112.93	121.20
31	AI	89	ASP	CB-CG-OD1	5.90	123.61	118.30
23	AA	2049	U	N1-C2-O2	5.89	126.93	122.80
1	Aa	315	U	N1-C2-O2	5.89	126.92	122.80
23	AA	1768	C	N1-C2-O2	5.88	122.43	118.90
1	Aa	415	A	OP1-P-O3'	5.87	118.12	105.20
23	AA	402	C	N1-C2-O2	5.87	122.42	118.90
1	Aa	415	A	C2-N3-C4	5.86	113.53	110.60
43	AU	53	ILE	C-N-CA	5.86	136.34	121.70
1	Aa	387	C	N1-C2-O2	5.84	122.41	118.90
1	Aa	599	U	N3-C2-O2	-5.84	118.11	122.20
1	Aa	315	U	N3-C2-O2	-5.84	118.11	122.20
23	AA	897	A	C5-C6-N6	-5.84	119.03	123.70
23	AA	2370	U	N1-C2-O2	5.84	126.89	122.80
23	AA	688	A	P-O3'-C3'	5.82	126.68	119.70
1	Aa	336	C	N1-C2-O2	5.80	122.38	118.90
23	AA	2796	C	N1-C2-O2	5.80	122.38	118.90
23	AA	828	A	C4-N9-C1'	5.79	136.72	126.30
23	AA	74	U	N3-C2-O2	-5.79	118.15	122.20
1	Aa	437	U	P-O3'-C3'	5.78	126.64	119.70
23	AA	268	A	O4'-C1'-N9	5.78	112.83	108.20
23	AA	2369	C	N1-C2-O2	5.77	122.36	118.90
1	Aa	1156	A	P-O3'-C3'	5.77	126.62	119.70
23	AA	755	C	N1-C2-O2	5.77	122.36	118.90
23	AA	2742	C	N1-C2-O2	5.76	122.35	118.90
23	AA	1287	U	N1-C2-O2	5.72	126.81	122.80
23	AA	1588	U	O4'-C1'-N1	5.72	112.78	108.20
23	AA	1213	C	N3-C2-O2	-5.70	117.91	121.90
23	AA	759	U	C6-N1-C1'	-5.69	113.24	121.20
23	AA	2749	G	P-O3'-C3'	5.67	126.51	119.70
23	AA	943	C	N1-C2-O2	5.67	122.30	118.90
23	AA	1552	U	N1-C2-O2	5.66	126.76	122.80
23	AA	2361	U	N1-C2-O2	5.66	126.76	122.80
23	AA	1287	U	C2-N1-C1'	5.66	124.49	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1370	A	P-O3'-C3'	5.65	126.48	119.70
23	AA	1287	U	N3-C2-O2	-5.65	118.24	122.20
1	Aa	486	C	N1-C2-O2	5.65	122.29	118.90
1	Aa	65	G	C4-N9-C1'	5.65	133.84	126.50
23	AA	975	U	N3-C2-O2	-5.63	118.26	122.20
23	AA	1803	G	C4-N9-C1'	5.63	133.82	126.50
23	AA	2370	U	C2-N1-C1'	5.62	124.45	117.70
23	AA	1214	C	N3-C2-O2	-5.61	117.97	121.90
1	Aa	599	U	C6-N1-C1'	-5.61	113.35	121.20
23	AA	593	U	C5-C6-N1	5.60	125.50	122.70
23	AA	1228	A	N7-C8-N9	5.60	116.60	113.80
23	AA	872	U	N1-C2-O2	5.60	126.72	122.80
23	AA	577	A	C2-N3-C4	5.59	113.40	110.60
23	AA	862	C	N3-C2-O2	-5.59	117.99	121.90
1	Aa	1136	U	P-O3'-C3'	5.59	126.40	119.70
23	AA	1845	U	P-O3'-C3'	5.59	126.40	119.70
23	AA	754	U	N1-C2-O2	5.58	126.71	122.80
1	Aa	424	G	C8-N9-C1'	-5.58	119.75	127.00
22	Av	153	MET	CG-SD-CE	-5.56	91.30	100.20
23	AA	1579	C	C6-N1-C2	-5.56	118.08	120.30
23	AA	2761	C	N1-C2-O2	5.56	122.23	118.90
24	AB	69	C	N1-C2-O2	5.56	122.23	118.90
23	AA	1633	A	C2-N3-C4	5.55	113.37	110.60
23	AA	1343	U	C2-N1-C1'	5.54	124.35	117.70
35	AM	22	LEU	CA-CB-CG	5.54	128.05	115.30
23	AA	1692	C	C6-N1-C1'	-5.54	114.16	120.80
1	Aa	553	C	O4'-C1'-N1	5.53	112.63	108.20
1	Aa	1048	C	N1-C2-O2	5.53	122.22	118.90
1	Aa	1122	A	P-O3'-C3'	5.52	126.32	119.70
23	AA	1451	U	N1-C2-O2	5.51	126.66	122.80
23	AA	862	C	C6-N1-C2	-5.51	118.10	120.30
23	AA	256	C	N1-C2-O2	5.50	122.20	118.90
23	AA	1992	C	N1-C2-O2	5.50	122.20	118.90
23	AA	1894	G	C6-C5-N7	-5.49	127.11	130.40
1	Aa	55	C	C6-N1-C1'	-5.49	114.22	120.80
23	AA	2699	U	N3-C2-O2	-5.48	118.36	122.20
1	Aa	387	C	N3-C2-O2	-5.48	118.07	121.90
23	AA	2408	C	N1-C2-O2	5.48	122.19	118.90
23	AA	398	C	N1-C2-O2	5.47	122.18	118.90
23	AA	1049	C	N1-C2-O2	5.45	122.17	118.90
23	AA	1815	C	N1-C2-O2	5.44	122.17	118.90
23	AA	1514	A	N1-C6-N6	5.44	121.86	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AA	975	U	C2-N1-C1'	5.43	124.22	117.70
23	AA	1216	U	C2-N1-C1'	5.43	124.21	117.70
23	AA	872	U	N3-C2-O2	-5.41	118.41	122.20
1	Aa	1168	C	C2-N1-C1'	5.41	124.75	118.80
23	AA	2747	U	N3-C2-O2	-5.41	118.42	122.20
24	AB	115	C	N1-C2-O2	5.41	122.14	118.90
1	Aa	486	C	N3-C2-O2	-5.39	118.12	121.90
23	AA	327	G	O4'-C1'-N9	5.39	112.51	108.20
1	Aa	1157	C	N1-C2-O2	5.38	122.13	118.90
23	AA	2321	C	N1-C2-O2	5.38	122.13	118.90
24	AB	94	C	N3-C2-O2	-5.35	118.15	121.90
23	AA	1692	C	N3-C2-O2	-5.34	118.16	121.90
24	AB	100	U	N1-C2-O2	5.34	126.54	122.80
23	AA	2249	G	O4'-C1'-N9	5.34	112.47	108.20
23	AA	2112	C	N3-C2-O2	-5.34	118.16	121.90
25	AC	130	LEU	CA-CB-CG	5.34	127.57	115.30
23	AA	2361	U	N3-C2-O2	-5.33	118.47	122.20
23	AA	1732	U	O5'-P-OP2	-5.33	100.90	105.70
31	AI	64	ARG	CA-CB-CG	5.33	125.13	113.40
1	Aa	411	C	C6-N1-C2	-5.32	118.17	120.30
25	AC	19	LEU	CA-CB-CG	5.32	127.53	115.30
23	AA	2636	U	C2-N1-C1'	5.32	124.08	117.70
23	AA	988	C	N3-C2-O2	-5.31	118.19	121.90
1	Aa	422	A	C2-N3-C4	5.30	113.25	110.60
23	AA	2049	U	N3-C2-O2	-5.30	118.49	122.20
23	AA	340	C	N1-C2-O2	5.30	122.08	118.90
1	Aa	1012	G	C4-N9-C1'	5.29	133.38	126.50
23	AA	575	G	N3-C4-C5	-5.29	125.95	128.60
23	AA	1101	A	C2-N3-C4	5.29	113.25	110.60
23	AA	1758	A	C2-N3-C4	5.28	113.24	110.60
23	AA	2796	C	N3-C2-O2	-5.28	118.20	121.90
1	Aa	55	C	C6-N1-C2	-5.28	118.19	120.30
23	AA	1894	G	N3-C4-C5	-5.28	125.96	128.60
23	AA	2731	C	N1-C2-O2	5.28	122.07	118.90
23	AA	460	C	N1-C2-O2	5.27	122.06	118.90
23	AA	971	U	N1-C2-O2	5.27	126.49	122.80
23	AA	1551	U	O5'-P-OP1	-5.27	100.95	105.70
23	AA	1557	C	N1-C2-O2	5.26	122.06	118.90
23	AA	714	G	C4-N9-C1'	5.26	133.34	126.50
23	AA	394	U	N1-C2-O2	5.23	126.46	122.80
23	AA	2263	C	N1-C2-O2	5.22	122.03	118.90
23	AA	1950	U	N1-C2-O2	5.22	126.45	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AA	1451	U	N3-C2-O2	-5.21	118.56	122.20
12	Al	62	LEU	CA-CB-CG	5.20	127.27	115.30
25	AC	13	ARG	CA-CB-CG	5.20	124.84	113.40
23	AA	1101	A	C4-N9-C1'	5.20	135.65	126.30
23	AA	1228	A	O4'-C1'-N9	5.19	112.35	108.20
1	Aa	1063	U	C2-N1-C1'	5.18	123.92	117.70
1	Aa	1188	G	C4-N9-C1'	5.18	133.24	126.50
23	AA	1101	A	N7-C8-N9	5.18	116.39	113.80
23	AA	1214	C	C2-N1-C1'	5.18	124.50	118.80
1	Aa	1096	U	N3-C2-O2	-5.18	118.58	122.20
1	Aa	797	U	N1-C2-O2	5.17	126.42	122.80
32	AJ	6	LEU	CA-CB-CG	5.17	127.19	115.30
32	AJ	61	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	Aa	502	C	N1-C2-O2	5.15	121.99	118.90
23	AA	2263	C	C6-N1-C2	-5.15	118.24	120.30
1	Aa	324	C	C6-N1-C2	-5.14	118.24	120.30
1	Aa	1186	A	C2-N3-C4	5.14	113.17	110.60
6	Af	54	ASP	CB-CG-OD1	5.14	122.92	118.30
1	Aa	99	U	C5-C6-N1	5.14	125.27	122.70
23	AA	1160	C	N3-C2-O2	-5.13	118.31	121.90
23	AA	57	C	N1-C2-O2	5.13	121.98	118.90
23	AA	1587	C	N1-C2-O2	5.13	121.98	118.90
23	AA	1651	C	N3-C2-O2	-5.13	118.31	121.90
23	AA	1953	U	N3-C2-O2	-5.13	118.61	122.20
23	AA	556	U	N1-C2-O2	5.13	126.39	122.80
23	AA	1385	G	P-O3'-C3'	5.13	125.85	119.70
23	AA	1625	U	N3-C2-O2	-5.12	118.62	122.20
23	AA	576	U	C5-C6-N1	5.11	125.25	122.70
1	Aa	542	U	C2-N1-C1'	5.11	123.83	117.70
23	AA	1758	A	C4-N9-C1'	5.10	135.48	126.30
24	AB	108	U	C6-N1-C1'	-5.10	114.06	121.20
23	AA	1803	G	C8-N9-C1'	-5.10	120.38	127.00
23	AA	754	U	N3-C2-O2	-5.09	118.63	122.20
1	Aa	1114	C	C6-N1-C2	-5.08	118.27	120.30
23	AA	1761	G	N3-C4-C5	5.08	131.14	128.60
1	Aa	488	U	C2-N1-C1'	5.08	123.80	117.70
1	Aa	797	U	N3-C2-O2	-5.08	118.65	122.20
1	Aa	460	A	N3-C4-N9	5.07	131.46	127.40
23	AA	1216	U	N1-C2-O2	5.07	126.35	122.80
42	AT	82	LEU	C-N-CA	5.07	134.38	121.70
23	AA	1380	G	C4-N9-C1'	5.07	133.09	126.50
23	AA	256	C	N3-C2-O2	-5.06	118.36	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AA	2819	C	C2-N1-C1'	5.06	124.36	118.80
23	AA	530	C	N1-C2-O2	5.05	121.93	118.90
23	AA	1552	U	C6-N1-C2	-5.04	117.98	121.00
1	Aa	99	U	P-O3'-C3'	5.04	125.74	119.70
23	AA	2369	C	N3-C2-O2	-5.03	118.38	121.90
23	AA	1559	G	N3-C2-N2	-5.03	116.38	119.90
23	AA	1992	C	N3-C2-O2	-5.03	118.38	121.90
2	Ab	20	THR	C-N-CA	5.02	134.26	121.70
1	Aa	1373	A	C2-N3-C4	5.02	113.11	110.60
23	AA	2095	U	N1-C2-O2	5.02	126.31	122.80
23	AA	2224	U	N3-C2-O2	-5.01	118.69	122.20
1	Aa	599	U	O4'-C1'-N1	5.01	112.20	108.20
23	AA	2742	C	N3-C2-O2	-5.00	118.40	121.90
1	Aa	65	G	OP2-P-O3'	5.00	116.21	105.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	AD	158	SER	Peptide
38	AP	50	ALA	Peptide
5	Ae	76	ARG	Peptide
9	Ai	108	ARG	Peptide
12	Al	126	GLY	Peptide
19	As	80	PHE	Peptide
20	At	58	ASP	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	Aa	32969	0	16595	0	0
2	Ab	1819	0	1886	0	0
3	Ac	1501	0	1464	0	0
4	Ad	1497	0	1449	0	0
5	Ae	1145	0	1202	0	0
6	Af	778	0	775	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Ag	1161	0	1165	0	0
8	Ah	1026	0	1078	0	0
9	Ai	922	0	890	0	0
10	Aj	752	0	775	0	0
11	Ak	810	0	784	0	0
12	Al	1037	0	1091	0	0
13	Am	727	0	674	0	0
14	An	487	0	492	0	0
15	Ao	723	0	749	0	0
16	Ap	694	0	709	0	0
17	Aq	621	0	615	0	0
18	Ar	445	0	482	0	0
19	As	636	0	626	0	0
20	At	591	0	616	0	0
21	Au	400	0	407	0	0
22	Av	1333	0	1349	0	0
23	AA	62277	0	31301	700	0
24	AB	2445	0	1241	14	0
25	AC	2094	0	2203	86	0
26	AD	1627	0	1667	56	0
27	AE	1572	0	1619	39	0
28	AF	1325	0	1342	52	0
29	AG	1263	0	1225	24	0
30	AH	1143	0	1134	16	0
31	AI	918	0	980	25	0
32	AJ	1086	0	1125	27	0
33	AK	1071	0	1123	23	0
34	AL	932	0	983	26	0
35	AM	891	0	925	21	0
36	AN	889	0	937	15	0
37	AO	942	0	1014	31	0
38	AP	790	0	830	12	0
39	AQ	854	0	914	17	0
40	AR	715	0	748	21	0
41	AS	770	0	809	17	0
42	AT	722	0	766	5	0
43	AU	622	0	643	8	0
44	AV	445	0	466	6	0
45	AW	541	0	563	8	0
46	AX	449	0	491	8	0
47	AY	370	0	243	3	0
48	AZ	360	0	358	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	A1	390	0	394	7	0
50	A2	367	0	415	10	0
51	A3	521	0	586	10	0
52	A4	295	0	340	14	0
53	AA	199	0	0	2	0
53	AB	2	0	0	0	0
53	AC	2	0	0	0	0
53	AU	1	0	0	0	0
53	AZ	1	0	0	0	0
All	All	140965	0	93258	923	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 (923) 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)
23:AA:2717:A:N7	34:AL:3:TYR:CD1	1.68	1.60
23:AA:1533:A:N7	25:AC:96:TYR:C	1.79	1.36
23:AA:2717:A:N7	34:AL:3:TYR:CE1	1.94	1.36
23:AA:581:A:OP1	30:AH:1:MET:CE	1.72	1.35
23:AA:581:A:OP1	30:AH:1:MET:HE1	1.18	1.25
23:AA:2046:U:OP2	48:AZ:6:ARG:NH1	1.72	1.22
23:AA:2332:U:H1'	28:AF:132:VAL:O	1.05	1.19
23:AA:2648:G:OP1	26:AD:133:ARG:NH2	1.79	1.15
23:AA:2717:A:C8	34:AL:3:TYR:CE1	2.35	1.14
23:AA:1818:A:O2'	25:AC:206:GLY:HA2	1.49	1.13
23:AA:1819:G:OP1	25:AC:205:VAL:N	1.81	1.12
23:AA:2332:U:C1'	28:AF:132:VAL:O	1.99	1.09
23:AA:1663:G:HO2'	50:A2:2:VAL:N	1.49	1.09
23:AA:1818:A:O2'	25:AC:206:GLY:CA	2.00	1.09
23:AA:2717:A:N6	34:AL:3:TYR:HB2	1.67	1.09
23:AA:2331:G:H4'	28:AF:129:THR:O	1.54	1.08
27:AE:17:ILE:HD11	27:AE:200:LYS:HE3	1.35	1.08
23:AA:1533:A:N7	25:AC:97:ALA:N	1.91	1.06
23:AA:2338:A:H8	28:AF:40:VAL:HG21	1.13	1.05
23:AA:1613:G:C4	25:AC:213:TRP:CE3	2.23	1.04
23:AA:2312:C:OP2	49:A1:2:ARG:NH2	1.92	1.02
23:AA:513:G:OP1	50:A2:34:ARG:NH1	1.94	1.00
23:AA:2332:U:C6	28:AF:152:MET:O	2.14	1.00
23:AA:1613:G:C5	25:AC:213:TRP:CE3	2.36	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AA:492:G:OP1	37:AO:3:ARG:HB3	1.66	0.95
23:AA:2776:A:H1'	29:AG:63:THR:HG22	1.46	0.95
23:AA:2330:G:H5''	28:AF:122:PHE:O	1.65	0.94
23:AA:1533:A:N6	25:AC:96:TYR:O	2.00	0.93
23:AA:606:G:H21	37:AO:37:GLN:HE22	1.09	0.92
23:AA:74:U:OP1	45:AW:48:LYS:NZ	2.02	0.92
23:AA:2642:U:C2	48:AZ:4:PRO:HA	2.05	0.92
23:AA:2800:U:OP1	26:AD:179:THR:HG23	1.68	0.91
23:AA:660:A:H8	27:AE:182:ASN:HB3	1.33	0.91
23:AA:2717:A:N7	34:AL:3:TYR:CG	2.40	0.90
23:AA:1377:U:OP2	40:AR:58:TYR:OH	1.88	0.90
23:AA:2338:A:C8	28:AF:40:VAL:HG21	2.05	0.89
23:AA:2775:A:H1'	29:AG:67:THR:HG22	1.55	0.89
23:AA:2717:A:C8	34:AL:3:TYR:CZ	2.62	0.88
23:AA:581:A:OP1	30:AH:1:MET:SD	2.33	0.87
23:AA:1781:C:H5	36:AN:96:ARG:HH21	1.22	0.86
23:AA:372:A:H61	41:AS:15:LYS:HG2	1.40	0.86
23:AA:731:U:O2	50:A2:7:GLN:O	1.94	0.86
23:AA:2717:A:C5	34:AL:3:TYR:CD1	2.63	0.85
27:AE:17:ILE:CD1	27:AE:200:LYS:HE3	2.07	0.85
23:AA:1533:A:N7	25:AC:96:TYR:O	2.10	0.84
23:AA:2338:A:C8	28:AF:40:VAL:HG11	2.11	0.84
23:AA:2231:C:H5''	25:AC:147:LYS:CE	2.08	0.84
23:AA:2231:C:H5''	25:AC:147:LYS:HE3	1.60	0.83
23:AA:2333:U:H3	28:AF:40:VAL:CG2	1.91	0.83
23:AA:1324:A:H5'	34:AL:109:ARG:HD2	1.58	0.83
23:AA:2332:U:N1	28:AF:152:MET:O	2.13	0.82
23:AA:1040:A:OP2	38:AP:10:LYS:HD3	1.81	0.81
23:AA:1701:U:OP1	26:AD:149:ARG:N	2.13	0.81
23:AA:54:G:O2'	50:A2:36:ARG:NH1	2.13	0.81
23:AA:2800:U:OP1	26:AD:179:THR:CG2	2.28	0.80
35:AM:19:ARG:HH21	35:AM:47:ASP:CG	1.83	0.80
23:AA:2337:A:H2	28:AF:74:ILE:CG2	1.93	0.80
23:AA:2706:A:H2	26:AD:200:ASN:HD21	1.27	0.80
23:AA:2717:A:C6	34:AL:3:TYR:HB2	2.16	0.80
23:AA:2337:A:C2	28:AF:74:ILE:HG21	2.16	0.79
23:AA:1290:G:H1	37:AO:37:GLN:HE21	1.27	0.79
23:AA:902:A:OP1	43:AU:85:LYS:NZ	2.10	0.79
23:AA:1498:U:P	34:AL:59:ARG:HH12	2.06	0.78
23:AA:967:C:O2'	43:AU:34:ALA:HB2	1.82	0.78
23:AA:1819:G:P	25:AC:205:VAL:HG22	2.23	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AA:2835:C:O2'	48:AZ:40:HIS:HD2	1.67	0.78
23:AA:1818:A:HO2'	25:AC:206:GLY:HA2	1.47	0.78
23:AA:492:G:OP1	37:AO:3:ARG:HD3	1.84	0.78
23:AA:1514:A:H61	23:AA:1566:G:H1	1.30	0.78
23:AA:1185:U:OP2	30:AH:66:THR:OG1	2.01	0.77
23:AA:2048:G:N2	37:AO:25:PHE:CD2	2.52	0.77
23:AA:1710:G:O2'	31:AI:6:THR:HG22	1.83	0.77
23:AA:2333:U:O2	28:AF:40:VAL:HB	1.84	0.77
23:AA:2694:C:N3	29:AG:110:SER:OG	2.17	0.77
23:AA:247:A:OP2	51:A3:8:ARG:NH2	2.17	0.77
23:AA:1613:G:C5	25:AC:213:TRP:CZ3	2.62	0.77
23:AA:2337:A:H2	28:AF:74:ILE:HG21	1.48	0.75
23:AA:1582:U:H3	23:AA:1587:C:HO2'	1.32	0.75
23:AA:703:A:O2'	27:AE:102:PRO:HG3	1.84	0.75
23:AA:2039:G:N7	39:AQ:16:LYS:NZ	2.31	0.75
23:AA:351:G:O2'	41:AS:15:LYS:NZ	2.20	0.74
23:AA:1533:A:C5	25:AC:96:TYR:O	2.39	0.74
23:AA:2332:U:O5'	28:AF:131:GLY:HA3	1.88	0.74
23:AA:2288:C:OP1	43:AU:27:LYS:HE3	1.89	0.73
23:AA:2835:C:O2'	48:AZ:40:HIS:CD2	2.42	0.73
23:AA:1449:A:N7	23:AA:1635:A:N6	2.37	0.73
27:AE:17:ILE:HD11	27:AE:200:LYS:CE	2.18	0.72
23:AA:2231:C:H5'	25:AC:147:LYS:HD2	1.71	0.72
23:AA:1515:G:H1	23:AA:1565:U:H3	1.37	0.72
23:AA:1998:A:C2	25:AC:240:PRO:HD3	2.25	0.72
23:AA:1261:G:OP1	38:AP:67:ARG:NH2	2.23	0.72
23:AA:252:C:O2	51:A3:12:LYS:NZ	2.24	0.71
23:AA:1533:A:C6	25:AC:96:TYR:O	2.43	0.71
23:AA:651:A:OP1	27:AE:100:LYS:NZ	2.18	0.71
23:AA:660:A:C8	27:AE:182:ASN:HB3	2.22	0.71
23:AA:529:A:O2'	41:AS:54:GLY:O	2.08	0.70
23:AA:2455:G:N2	32:AJ:54:GLN:HE21	1.89	0.70
23:AA:2801:C:OP1	26:AD:177:THR:OG1	2.09	0.70
23:AA:1287:U:H5'	37:AO:4:VAL:CG1	2.22	0.70
23:AA:2259:C:OP2	44:AV:27:ARG:NH2	2.24	0.70
24:AB:5:G:H21	35:AM:43:GLN:HE22	1.40	0.69
23:AA:2331:G:O2'	28:AF:153:ASP:OD1	2.10	0.69
23:AA:1498:U:P	34:AL:59:ARG:NH1	2.66	0.69
23:AA:1641:G:OP1	40:AR:39:LYS:NZ	2.18	0.69
23:AA:2049:U:OP2	48:AZ:12:ARG:NH2	2.26	0.69
23:AA:252:C:O2'	32:AJ:63:LYS:NZ	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:AI:76:TYR:HB2	36:AN:75:THR:HB	1.74	0.68
28:AF:132:VAL:HG12	28:AF:134:GLU:H	1.58	0.67
33:AK:82:ARG:HH11	43:AU:12:LYS:HE3	1.58	0.67
23:AA:2314:A:H62	23:AA:2371:U:H3	1.40	0.67
23:AA:2904:U:H5	48:AZ:40:HIS:CE1	2.12	0.67
23:AA:1663:G:O2'	50:A2:2:VAL:N	2.26	0.67
23:AA:2554:C:H5''	52:A4:30:PRO:HB2	1.76	0.66
23:AA:2277:G:N2	33:AK:84:GLY:HA3	2.11	0.66
23:AA:606:G:N2	37:AO:37:GLN:HE22	1.89	0.66
23:AA:721:A:H8	23:AA:2096:G:H21	1.42	0.66
23:AA:2646:U:H5'	26:AD:165:LYS:HB3	1.78	0.65
36:AN:59:GLU:HG2	36:AN:78:LEU:HD23	1.79	0.65
23:AA:2046:U:OP1	48:AZ:7:ARG:HD3	1.97	0.65
23:AA:1701:U:OP1	26:AD:149:ARG:HB2	1.97	0.65
23:AA:2037:G:H5''	39:AQ:42:ALA:HB2	1.76	0.65
23:AA:2904:U:O4	48:AZ:40:HIS:N	2.24	0.65
23:AA:502:C:H5	40:AR:68:TYR:CD1	2.15	0.65
23:AA:498:G:H21	23:AA:503:A:H8	1.45	0.65
23:AA:2841:A:OP1	26:AD:123:LYS:O	2.14	0.65
23:AA:2225:A:N7	23:AA:2252:A:N6	2.45	0.64
23:AA:75:G:O2'	45:AW:48:LYS:NZ	2.26	0.64
23:AA:1510:U:H3	23:AA:1571:G:H1	1.44	0.64
23:AA:492:G:OP1	37:AO:3:ARG:CB	2.42	0.64
23:AA:1287:U:H5'	37:AO:4:VAL:HG13	1.80	0.64
23:AA:1578:A:N6	23:AA:1590:C:N3	2.44	0.64
25:AC:167:LYS:HG2	25:AC:172:VAL:HG12	1.78	0.64
23:AA:539:G:H4'	39:AQ:6:VAL:HG22	1.80	0.63
23:AA:17:G:OP1	48:AZ:11:THR:HG22	1.99	0.63
23:AA:2039:G:OP1	39:AQ:11:ARG:NH1	2.30	0.63
23:AA:2325:A:H62	23:AA:2345:A:H8	1.45	0.63
23:AA:1042:C:OP1	37:AO:92:ARG:NH2	2.31	0.63
23:AA:1555:G:N2	23:AA:1556:G:O6	2.32	0.63
23:AA:2338:A:H8	28:AF:40:VAL:CG2	2.00	0.63
23:AA:2904:U:C5	48:AZ:40:HIS:CE1	2.87	0.63
26:AD:16:PHE:O	36:AN:14:GLN:NE2	2.32	0.63
41:AS:12:ILE:HD11	41:AS:69:GLN:HB2	1.81	0.63
23:AA:2733:A:O2'	34:AL:60:ARG:NH1	2.32	0.62
35:AM:31:LEU:HB3	35:AM:44:ILE:HD13	1.81	0.62
23:AA:1522:G:H1	23:AA:1558:U:H3	1.46	0.62
23:AA:1533:A:C8	25:AC:98:ASP:HB2	2.35	0.62
36:AN:31:HIS:HB3	36:AN:42:ILE:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AA:1076:A:OP1	52:A4:8:LYS:HG2	2.00	0.62
23:AA:1818:A:O2'	25:AC:206:GLY:C	2.37	0.62
33:AK:51:ARG:HG3	33:AK:66:ILE:HD11	1.82	0.62
41:AS:3:ILE:HD11	41:AS:33:VAL:HG11	1.82	0.62
23:AA:2717:A:H8	34:AL:3:TYR:CZ	2.16	0.62
25:AC:107:PRO:HA	25:AC:195:VAL:HA	1.82	0.62
46:AX:12:VAL:HG22	46:AX:20:ARG:HG2	1.82	0.62
23:AA:1492:G:N3	23:AA:1574:G:N2	2.48	0.62
23:AA:2043:U:O2	48:AZ:4:PRO:HG2	1.99	0.62
23:AA:1581:U:O5'	23:AA:1584:U:H5	1.83	0.61
23:AA:1967:U:O2	23:AA:1969:C:N4	2.33	0.61
23:AA:2663:U:O2'	26:AD:46:TYR:OH	2.16	0.61
23:AA:1651:C:N4	23:AA:1666:A:OP2	2.33	0.61
25:AC:230:HIS:HD2	25:AC:232:HIS:H	1.47	0.61
35:AM:19:ARG:NH2	35:AM:47:ASP:CG	2.53	0.61
23:AA:2388:A:OP2	51:A3:24:ARG:NH2	2.32	0.61
23:AA:2784:A:N1	29:AG:67:THR:HG21	2.16	0.61
23:AA:2851:G:OP2	26:AD:65:SER:OG	2.13	0.61
23:AA:365:A:OP1	27:AE:168:ARG:NE	2.31	0.61
23:AA:2231:C:C5'	25:AC:147:LYS:HD2	2.29	0.61
31:AI:78:LYS:HB2	36:AN:73:GLU:HB2	1.83	0.61
23:AA:268:A:N6	23:AA:473:U:O2'	2.34	0.61
23:AA:2080:G:H5'	26:AD:157:ALA:O	2.01	0.61
23:AA:2046:U:P	48:AZ:6:ARG:HH12	2.22	0.61
39:AQ:11:ARG:O	39:AQ:11:ARG:NH2	2.33	0.61
23:AA:2295:A:OP1	53:AA:3178:MG:MG	1.43	0.61
23:AA:2330:G:H4'	28:AF:122:PHE:O	2.01	0.61
23:AA:2278:G:OP1	33:AK:82:ARG:NH2	2.34	0.61
23:AA:1533:A:C8	25:AC:98:ASP:CB	2.47	0.60
23:AA:1833:C:O2'	25:AC:46:GLN:OE1	2.19	0.60
23:AA:1037:A:H62	23:AA:1205:U:H3	1.49	0.60
23:AA:2403:A:N3	35:AM:113:ARG:NH2	2.47	0.60
23:AA:2089:A:N6	23:AA:2530:A:N7	2.50	0.60
23:AA:611:U:OP1	23:AA:989:A:N6	2.33	0.60
23:AA:583:A:O2'	30:AH:8:ASN:OD1	2.20	0.60
23:AA:2120:G:N3	23:AA:2225:A:N6	2.49	0.60
23:AA:579:U:H5'	37:AO:42:SER:HB2	1.84	0.60
35:AM:68:THR:HG1	35:AM:71:GLU:H	1.48	0.60
23:AA:1498:U:OP2	34:AL:59:ARG:NH1	2.29	0.60
26:AD:128:GLN:HE21	26:AD:132:LYS:HG2	1.67	0.60
23:AA:2330:G:C5'	28:AF:122:PHE:O	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:AF:41:GLY:HA3	28:AF:150:ARG:HH22	1.67	0.60
23:AA:2333:U:H3	28:AF:40:VAL:HG21	1.65	0.60
23:AA:1533:A:C5	25:AC:96:TYR:C	2.71	0.60
23:AA:1521:A:H61	23:AA:1559:G:H1	1.50	0.60
23:AA:2333:U:N3	28:AF:40:VAL:CG2	2.64	0.60
23:AA:2649:U:O3'	23:AA:2845:G:N2	2.33	0.60
29:AG:164:TYR:HB2	29:AG:167:GLU:HB2	1.84	0.60
23:AA:648:G:N3	23:AA:702:U:O2'	2.35	0.59
23:AA:795:A:N1	23:AA:803:C:N4	18.43	0.59
23:AA:1043:U:OP2	53:AA:3110:MG:MG	1.44	0.59
23:AA:2231:C:C5'	25:AC:147:LYS:HE3	2.32	0.59
41:AS:39:ASN:HB3	41:AS:61:ALA:HB3	1.84	0.59
23:AA:2047:A:H5'	48:AZ:9:SER:HB3	1.84	0.59
23:AA:1038:C:OP1	37:AO:53:ARG:NH2	2.35	0.59
27:AE:17:ILE:CG1	27:AE:200:LYS:HE3	2.32	0.59
23:AA:2717:A:C5	34:AL:3:TYR:CG	2.88	0.59
23:AA:1284:A:HO2'	27:AE:45:ARG:HH22	1.51	0.59
29:AG:57:ASP:OD1	29:AG:62:ARG:NH1	2.36	0.59
23:AA:2321:C:OP1	35:AM:96:ARG:NH2	2.35	0.59
23:AA:1040:A:O2'	37:AO:91:ASN:ND2	2.36	0.59
23:AA:1761:G:H1	23:AA:1768:C:H42	1.49	0.59
23:AA:2778:G:N2	29:AG:3:ARG:HH21	2.01	0.59
23:AA:1133:G:N2	23:AA:1145:U:O4	2.36	0.58
23:AA:2258:U:OP1	44:AV:30:ASN:N	2.35	0.58
25:AC:78:VAL:HG22	25:AC:94:VAL:HG12	1.84	0.58
23:AA:2333:U:C2	28:AF:40:VAL:HB	2.38	0.58
23:AA:856:U:OP2	32:AJ:20:GLY:C	2.41	0.58
23:AA:1122:U:O2'	23:AA:1132:A:N3	2.35	0.58
23:AA:2566:C:H5'	52:A4:3:VAL:HG21	1.85	0.58
23:AA:2232:A:OP1	25:AC:150:LYS:HG3	2.03	0.58
26:AD:129:GLY:HA2	26:AD:170:PRO:HB3	1.85	0.58
23:AA:1099:G:N2	23:AA:1149:U:O2	2.37	0.58
23:AA:1450:A:H61	23:AA:1635:A:H62	1.52	0.58
23:AA:2195:G:N1	23:AA:2197:G:N7	2.51	0.58
23:AA:635:G:H21	51:A3:4:MET:HE3	1.67	0.58
23:AA:761:A:C6	37:AO:39:VAL:O	136.41	0.58
23:AA:856:U:OP2	32:AJ:20:GLY:O	2.21	0.58
33:AK:39:THR:HG23	33:AK:98:LYS:HA	1.85	0.58
24:AB:77:G:O6	42:AT:15:ARG:NH2	2.37	0.58
23:AA:2136:U:H3	23:AA:2207:U:H3	1.52	0.58
23:AA:502:C:C5	40:AR:68:TYR:CD1	2.92	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AC:95:VAL:HG22	25:AC:101:LYS:HG2	1.86	0.58
23:AA:517:A:N7	23:AA:551:G:O2'	27.51	0.57
23:AA:1101:A:OP2	23:AA:1133:G:N2	2.36	0.57
23:AA:2706:A:H2	26:AD:200:ASN:ND2	1.97	0.57
43:AU:44:ILE:HD13	43:AU:47:ARG:HH21	1.69	0.57
23:AA:1091:G:O2'	23:AA:1155:A:N6	2.37	0.57
23:AA:1379:A:OP1	40:AR:35:LYS:NZ	2.37	0.57
23:AA:868:A:H62	23:AA:879:U:H3	1.50	0.57
24:AB:46:A:OP1	35:AM:35:ARG:NH1	2.37	0.57
29:AG:86:VAL:HG22	29:AG:132:LYS:HG2	1.85	0.57
23:AA:1917:A:C8	23:AA:2261:G:N2	2.72	0.57
23:AA:1450:A:N1	23:AA:1634:A:N6	2.52	0.57
41:AS:93:ILE:HG22	41:AS:95:LYS:H	1.69	0.57
42:AT:75:ALA:HB2	42:AT:92:LEU:HB2	1.86	0.57
23:AA:1287:U:C5'	37:AO:4:VAL:HG13	2.35	0.57
23:AA:2329:U:O2'	28:AF:123:ASP:HB2	2.04	0.57
23:AA:2877:G:N2	23:AA:2880:A:OP2	2.32	0.57
40:AR:50:VAL:HA	40:AR:82:LEU:HA	1.86	0.57
23:AA:1401:G:N2	23:AA:1404:A:OP2	2.37	0.57
23:AA:1063:U:H3	23:AA:1186:A:H62	1.51	0.56
23:AA:2046:U:OP1	48:AZ:7:ARG:CD	2.53	0.56
23:AA:344:U:OP2	41:AS:80:ARG:NH2	2.32	0.56
23:AA:1847:U:O2	25:AC:201:GLU:HB3	2.05	0.56
23:AA:1818:A:O3'	25:AC:205:VAL:HG22	2.05	0.56
23:AA:2510:C:O2	33:AK:124:LYS:HE2	2.06	0.56
23:AA:125:A:OP2	50:A2:19:PHE:N	2.38	0.56
23:AA:1527:A:OP1	23:AA:1556:G:N2	2.38	0.56
23:AA:1938:U:O2'	23:AA:1945:A:N6	2.36	0.56
23:AA:2869:G:N7	23:AA:2887:G:N2	2.53	0.56
23:AA:656:G:H21	23:AA:660:A:H2	1.54	0.56
45:AW:11:THR:OG1	45:AW:60:ARG:NH2	2.38	0.56
23:AA:506:A:H2	23:AA:515:G:H21	1.52	0.56
23:AA:191:A:H5'	44:AV:14:THR:HG21	1.88	0.56
23:AA:2694:C:O2	29:AG:110:SER:N	2.37	0.56
23:AA:1197:C:OP1	37:AO:92:ARG:NH2	2.29	0.56
23:AA:1845:U:OP2	25:AC:156:ARG:NH2	2.38	0.56
31:AI:21:THR:HG22	31:AI:39:ILE:HD13	1.87	0.56
23:AA:1109:U:O2'	23:AA:1118:G:N1	2.33	0.55
23:AA:713:A:H2'	23:AA:715:A:H62	1.71	0.55
23:AA:1020:G:HO2'	23:AA:1199:A:HO2'	1.53	0.55
23:AA:1107:G:N2	23:AA:1120:C:O3'	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AA:1488:A:H61	23:AA:1595:C:H42	1.53	0.55
23:AA:2695:G:H1'	29:AG:110:SER:HB2	1.88	0.55
23:AA:922:G:H2'	23:AA:923:A:H8	1.71	0.55
32:AJ:91:VAL:HA	32:AJ:95:LEU:HD12	1.87	0.55
23:AA:2136:U:O4	23:AA:2206:C:N4	2.39	0.55
23:AA:492:G:OP1	37:AO:3:ARG:CD	2.53	0.55
23:AA:1533:A:N7	25:AC:96:TYR:CB	2.70	0.55
23:AA:2162:A:H62	23:AA:2183:G:H21	1.55	0.55
29:AG:125:VAL:HG22	29:AG:131:VAL:HG22	1.89	0.55
23:AA:2717:A:H62	34:AL:3:TYR:HB2	1.66	0.55
35:AM:6:ASP:OD2	35:AM:9:LYS:HG3	2.06	0.55
23:AA:1521:A:N3	23:AA:1561:G:N2	2.54	0.55
23:AA:1648:C:O2'	23:AA:1654:A:N6	2.40	0.55
23:AA:608:C:OP2	38:AP:78:ARG:O	2.25	0.55
23:AA:1129:A:N3	23:AA:1148:C:O2'	2.35	0.54
23:AA:2332:U:H1'	28:AF:132:VAL:C	2.11	0.54
31:AI:69:VAL:HG21	31:AI:105:GLU:HG3	1.88	0.54
23:AA:124:A:H5''	50:A2:20:ARG:HB2	1.88	0.54
23:AA:1378:U:H1'	40:AR:54:ASN:HB3	1.88	0.54
23:AA:650:U:OP1	27:AE:102:PRO:HA	2.07	0.54
23:AA:2079:G:OP1	26:AD:154:VAL:HG22	2.07	0.54
49:A1:9:CYS:SG	49:A1:10:THR:N	2.80	0.54
23:AA:246:U:OP2	51:A3:8:ARG:NH1	2.40	0.54
23:AA:1487:G:H2'	23:AA:1488:A:H8	1.73	0.54
23:AA:1613:G:N2	25:AC:209:GLY:O	2.41	0.54
23:AA:502:C:H5	40:AR:68:TYR:CE1	2.25	0.54
23:AA:1864:C:O2'	23:AA:1954:A:N3	2.36	0.54
23:AA:2559:G:O2'	23:AA:2684:A:N1	2.40	0.54
23:AA:319:G:H22	23:AA:326:A:H61	1.54	0.54
23:AA:250:G:OP2	23:AA:252:C:N4	2.40	0.54
23:AA:816:G:HO2'	23:AA:1392:G:HO2'	1.41	0.54
23:AA:2314:A:H2	23:AA:2373:A:H62	1.56	0.54
23:AA:2758:G:OP1	26:AD:182:ASN:ND2	2.40	0.54
30:AH:2:ARG:HB2	37:AO:93:LYS:HZ3	1.72	0.54
48:AZ:34:GLY:HA3	48:AZ:47:GLY:HA2	1.90	0.54
23:AA:1035:C:O2'	23:AA:1046:G:N2	28.84	0.54
27:AE:32:VAL:HG12	27:AE:109:ALA:HB2	1.89	0.54
44:AV:38:ILE:HG22	44:AV:60:THR:HA	1.89	0.54
23:AA:1115:G:N1	23:AA:1136:C:OP2	2.36	0.54
23:AA:788:A:O2'	23:AA:1703:U:OP1	2.25	0.54
23:AA:706:U:H1'	32:AJ:12:SER:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:AJ:55:LEU:O	32:AJ:60:ARG:NH1	2.41	0.54
23:AA:1077:U:H3	23:AA:1166:G:H1	1.55	0.53
23:AA:2227:C:O2	23:AA:2253:C:N4	2.41	0.53
23:AA:2813:U:O2	26:AD:72:PRO:HB3	2.08	0.53
23:AA:1025:A:HO2'	23:AA:1227:U:HO2'	27.10	0.53
23:AA:718:C:OP1	27:AE:54:ARG:HD2	2.07	0.53
36:AN:51:LYS:HG3	36:AN:98:LYS:HE2	1.90	0.53
23:AA:1111:A:N1	23:AA:1139:A:O2'	2.36	0.53
23:AA:2782:C:H3'	52:A4:19:ARG:HH22	1.74	0.53
23:AA:299:U:O2'	23:AA:300:G:N2	2.41	0.53
23:AA:78:U:H5'	45:AW:7:ARG:HH22	1.73	0.53
23:AA:2029:G:OP1	34:AL:5:LYS:HD3	2.08	0.53
23:AA:2361:U:O3'	35:AM:17:ARG:HG2	2.09	0.53
23:AA:2642:U:O2	48:AZ:4:PRO:HA	2.09	0.53
23:AA:743:C:O2'	23:AA:779:A:N6	2.42	0.53
23:AA:2331:G:OP1	28:AF:121:ALA:HA	2.08	0.53
31:AI:22:ILE:HG22	31:AI:23:LYS:HG2	1.90	0.53
23:AA:2455:G:N2	32:AJ:54:GLN:NE2	2.57	0.53
23:AA:838:A:OP2	23:AA:2098:A:O2'	2.27	0.53
23:AA:2647:C:O2'	26:AD:170:PRO:O	2.18	0.53
23:AA:1101:A:N6	23:AA:1131:G:OP2	2.35	0.53
23:AA:2819:C:N4	23:AA:2822:C:O2	2.41	0.53
23:AA:735:C:O2'	23:AA:825:G:OP1	2.26	0.53
41:AS:16:ASP:HB2	41:AS:38:VAL:HG13	1.91	0.53
33:AK:75:THR:HA	33:AK:90:VAL:HA	1.89	0.53
23:AA:502:C:C5	40:AR:68:TYR:CG	2.97	0.53
42:AT:26:LYS:NZ	42:AT:44:ASP:OD1	2.37	0.53
23:AA:1022:G:N1	23:AA:1025:A:OP2	7.18	0.53
23:AA:1106:G:O2'	23:AA:1121:A:N6	2.42	0.53
23:AA:1102:U:H3	23:AA:1124:A:H61	1.56	0.53
23:AA:1449:A:H62	23:AA:1635:A:H61	1.57	0.53
23:AA:1960:G:H1	23:AA:1994:C:H5	1.55	0.53
23:AA:1843:U:C5	25:AC:62:TYR:CD2	2.97	0.53
23:AA:2778:G:N1	29:AG:3:ARG:NH2	2.56	0.53
23:AA:895:U:O2	46:AX:46:GLN:NE2	2.42	0.52
29:AG:38:ASN:ND2	29:AG:41:MET:SD	2.82	0.52
31:AI:42:THR:HG22	31:AI:57:VAL:HG22	1.91	0.52
23:AA:184:C:O2'	23:AA:185:A:N7	2.40	0.52
23:AA:2231:C:C5'	25:AC:147:LYS:CE	2.84	0.52
25:AC:227:PRO:HD3	25:AC:234:GLY:H	1.74	0.52
23:AA:1031:C:H5''	46:AX:10:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AA:1131:G:H1	23:AA:1133:G:H21	1.56	0.52
28:AF:127:ASN:HD22	28:AF:157:VAL:HA	1.74	0.52
31:AI:35:ILE:HG21	31:AI:103:ALA:HB3	1.91	0.52
36:AN:16:ARG:H	36:AN:79:HIS:HD2	1.57	0.52
49:A1:22:ASN:ND2	49:A1:25:ASN:OD1	2.40	0.52
23:AA:502:C:H5	40:AR:68:TYR:CG	2.28	0.52
32:AJ:79:LEU:HB2	32:AJ:113:GLY:HA2	1.92	0.52
45:AW:31:GLN:HG3	45:AW:37:LEU:HD12	1.90	0.52
23:AA:1451:U:H3	23:AA:1633:A:H62	1.57	0.52
23:AA:1581:U:O5'	23:AA:1584:U:C5	2.62	0.52
23:AA:842:U:OP1	27:AE:62:ARG:NH2	2.42	0.52
23:AA:2776:A:C1'	29:AG:63:THR:HG22	2.30	0.52
23:AA:1643:C:OP2	40:AR:35:LYS:HD3	2.09	0.52
23:AA:2715:G:N2	23:AA:2747:U:O2	2.43	0.52
23:AA:488:G:O4'	27:AE:46:GLN:NE2	2.43	0.52
50:A2:34:ARG:HG2	50:A2:37:ARG:HH22	1.74	0.52
23:AA:2778:G:C2	29:AG:3:ARG:NH2	2.71	0.52
23:AA:1304:G:OP2	39:AQ:15:ARG:NH2	2.43	0.52
27:AE:75:GLN:HE22	27:AE:82:GLN:HE21	1.58	0.52
23:AA:2140:C:N3	23:AA:2195:G:O2'	2.41	0.52
25:AC:144:ILE:HB	25:AC:154:ILE:HB	1.92	0.52
23:AA:1847:U:O2	25:AC:201:GLU:N	2.43	0.52
26:AD:93:ASN:HD21	26:AD:212:ARG:HB2	1.74	0.52
38:AP:24:LYS:HA	38:AP:93:THR:HG23	1.91	0.52
23:AA:2388:A:OP2	51:A3:24:ARG:NH1	2.43	0.51
52:A4:25:VAL:HG22	52:A4:34:GLN:HB2	1.92	0.51
23:AA:863:G:H21	23:AA:1228:A:H2	1.55	0.51
23:AA:926:G:O2'	23:AA:941:A:N1	2.41	0.51
23:AA:2850:G:P	26:AD:67:LYS:HB3	2.51	0.51
23:AA:1579:C:H3'	23:AA:1581:U:H3	1.75	0.51
23:AA:320:U:H5'	23:AA:321:U:H3'	1.92	0.51
23:AA:720:A:OP1	27:AE:76:GLY:CA	2.59	0.51
28:AF:46:ASN:O	28:AF:50:LEU:N	2.40	0.51
23:AA:492:G:OP1	37:AO:3:ARG:CG	2.58	0.51
40:AR:7:LEU:HD21	40:AR:42:VAL:HG12	1.91	0.51
23:AA:1325:U:O2'	23:AA:1691:G:N2	2.34	0.51
23:AA:2840:A:C6	26:AD:206:LYS:HD2	2.45	0.51
23:AA:650:U:O5'	27:AE:103:LYS:HE3	2.09	0.51
35:AM:112:ALA:HB1	35:AM:117:LEU:HD12	1.92	0.51
23:AA:1359:A:H62	23:AA:1383:G:H8	42.38	0.51
23:AA:2707:C:OP1	26:AD:123:LYS:HG2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:AF:57:LEU:HD22	28:AF:65:PRO:HG3	1.93	0.51
23:AA:2331:G:H5'	28:AF:129:THR:OG1	2.10	0.51
23:AA:522:G:N1	23:AA:525:A:OP2	2.44	0.51
23:AA:2843:A:OP1	26:AD:127:PHE:HB2	2.10	0.51
26:AD:22:LEU:HD13	31:AI:74:GLY:HA3	1.92	0.51
23:AA:2371:U:OP1	49:A1:33:LYS:HD2	2.09	0.51
23:AA:502:C:H41	40:AR:68:TYR:CB	2.24	0.51
34:AL:45:GLU:OE2	34:AL:101:THR:OG1	2.24	0.51
42:AT:7:ILE:HB	42:AT:42:LYS:HB2	1.93	0.51
23:AA:2686:G:N2	23:AA:2689:A:OP2	2.39	0.51
23:AA:2778:G:N2	29:AG:3:ARG:NH2	2.59	0.51
23:AA:2854:A:H2'	23:AA:2899:A:H61	1.75	0.51
23:AA:1376:G:H5''	40:AR:15:LYS:HG2	1.93	0.51
23:AA:1008:C:O2'	23:AA:2300:A:N3	2.38	0.51
23:AA:326:A:H1'	23:AA:327:G:H5'	1.93	0.51
25:AC:84:ASP:OD2	25:AC:87:ARG:NH1	2.41	0.51
23:AA:1286:G:C5	37:AO:3:ARG:HB2	2.45	0.51
23:AA:1701:U:OP1	26:AD:149:ARG:CA	2.57	0.51
23:AA:1844:G:OP1	25:AC:87:ARG:NH2	2.44	0.51
43:AU:55:PRO:HG3	43:AU:61:ARG:HB2	1.93	0.51
23:AA:1242:A:N3	32:AJ:4:HIS:HB3	2.27	0.50
23:AA:1781:C:N3	23:AA:2743:U:O2'	2.44	0.50
23:AA:503:A:H62	23:AA:516:A:H5''	1.76	0.50
30:AH:53:ASP:OD1	30:AH:53:ASP:N	2.44	0.50
36:AN:16:ARG:H	36:AN:79:HIS:CD2	2.29	0.50
46:AX:18:THR:HG22	46:AX:49:LYS:HZ1	1.75	0.50
23:AA:1369:G:N7	23:AA:1653:A:O2'	2.36	0.50
23:AA:12:U:O4	23:AA:13:A:N6	2.44	0.50
23:AA:2465:U:O2'	23:AA:2467:C:OP1	2.29	0.50
23:AA:85:G:OP1	41:AS:26:THR:HG21	2.11	0.50
23:AA:1472:C:N4	23:AA:1617:A:OP2	2.34	0.50
25:AC:165:LEU:HD11	25:AC:175:ARG:HB2	1.92	0.50
28:AF:31:ILE:HD11	28:AF:34:ILE:HD11	1.93	0.50
52:A4:5:PRO:O	52:A4:36:GLN:NE2	2.45	0.50
23:AA:1937:G:O6	23:AA:1946:A:N6	2.45	0.50
23:AA:1498:U:O5'	34:AL:59:ARG:NH1	2.45	0.50
23:AA:1492:G:N2	23:AA:1508:C:N3	2.59	0.50
23:AA:1818:A:O2'	25:AC:206:GLY:N	2.42	0.50
27:AE:80:ALA:HB3	27:AE:83:TRP:HD1	1.76	0.50
23:AA:1265:G:H2'	23:AA:1289:A:H61	23.14	0.50
23:AA:2782:C:H3'	52:A4:19:ARG:NH2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AA:1819:G:OP1	25:AC:204:ASN:HA	2.12	0.50
23:AA:2717:A:H8	34:AL:3:TYR:CE1	2.19	0.50
23:AA:1183:G:O2'	23:AA:1187:A:N1	2.40	0.50
23:AA:1508:C:N4	23:AA:1509:G:O6	2.45	0.50
23:AA:2147:G:O6	23:AA:2199:U:O2'	2.28	0.50
23:AA:2157:U:O2'	23:AA:2185:A:N1	2.42	0.50
23:AA:2706:A:C2	26:AD:200:ASN:ND2	2.77	0.50
23:AA:578:G:O6	23:AA:874:A:N6	57.12	0.50
23:AA:573:A:H5'	30:AH:114:ARG:HG2	1.93	0.50
23:AA:168:A:H5''	23:AA:169:G:C8	2.46	0.50
23:AA:2598:U:O2	26:AD:156:MET:HG2	2.12	0.50
23:AA:609:U:H5''	32:AJ:29:LYS:HD2	1.92	0.50
23:AA:826:A:OP1	25:AC:217:ARG:NH2	2.39	0.50
23:AA:720:A:OP1	27:AE:76:GLY:HA2	2.11	0.50
29:AG:87:LEU:HD13	29:AG:148:ILE:HD13	1.94	0.50
31:AI:80:ASP:OD2	36:AN:64:ARG:NH2	2.39	0.50
23:AA:1208:A:H62	23:AA:1224:U:H3	1.60	0.50
23:AA:2134:C:N4	23:AA:2208:A:OP2	2.41	0.50
31:AI:112:MET:N	31:AI:112:MET:SD	3.35	0.50
23:AA:1726:A:H61	23:AA:1750:U:H3	1.59	0.49
23:AA:878:C:OP1	32:AJ:39:LYS:HE3	2.12	0.49
28:AF:61:THR:HG21	28:AF:91:LEU:HD11	1.95	0.49
24:AB:29:C:OP1	35:AM:4:LYS:NZ	2.44	0.49
23:AA:1759:G:H21	23:AA:1772:G:H5'	1.77	0.49
26:AD:119:THR:HB	26:AD:210:GLU:HB2	1.93	0.49
23:AA:1055:A:P	37:AO:77:SER:HG	2.35	0.49
23:AA:1491:C:O2'	23:AA:1574:G:N2	2.39	0.49
23:AA:2341:A:H5'	28:AF:35:VAL:HG11	1.94	0.49
23:AA:2818:A:N6	23:AA:2824:G:O6	2.45	0.49
23:AA:2831:G:OP1	26:AD:70:ASN:HB2	2.11	0.49
25:AC:230:HIS:CD2	25:AC:232:HIS:H	2.27	0.49
23:AA:590:U:OP1	23:AA:1257:G:O2'	2.26	0.49
23:AA:1510:U:O2	23:AA:1571:G:N2	2.43	0.49
23:AA:1533:A:N7	25:AC:96:TYR:HB3	2.27	0.49
23:AA:2418:G:O2'	23:AA:2451:C:N4	2.46	0.49
23:AA:928:C:N4	23:AA:937:G:OP2	2.42	0.49
25:AC:182:ARG:HG3	25:AC:270:ILE:HD13	1.93	0.49
37:AO:24:TYR:O	37:AO:29:HIS:ND1	2.42	0.49
23:AA:1039:C:C6	30:AH:1:MET:HA	2.47	0.49
23:AA:1137:G:O2'	23:AA:1143:G:O6	2.29	0.49
23:AA:1453:G:H4'	23:AA:1455:U:H3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AA:2333:U:H3	28:AF:40:VAL:CB	2.24	0.49
23:AA:922:G:H2'	23:AA:923:A:C8	2.48	0.49
23:AA:1701:U:OP1	26:AD:149:ARG:CB	2.61	0.49
23:AA:2402:G:N2	23:AA:2405:A:OP2	2.43	0.49
23:AA:2332:U:C1'	28:AF:152:MET:O	2.60	0.49
23:AA:1024:A:OP1	23:AA:1026:C:N4	2.46	0.49
23:AA:1284:A:O2'	27:AE:45:ARG:NH2	2.32	0.48
23:AA:2591:A:OP1	23:AA:2675:G:O2'	2.31	0.48
23:AA:2775:A:H1'	29:AG:67:THR:CG2	2.36	0.48
23:AA:827:A:O2'	25:AC:224:VAL:O	2.29	0.48
23:AA:1312:A:N7	34:AL:12:GLN:HG2	2.28	0.48
23:AA:1764:A:N7	23:AA:1765:A:N6	2.61	0.48
23:AA:616:G:O2'	23:AA:618:A:OP1	2.30	0.48
23:AA:850:G:OP2	32:AJ:41:ARG:HG2	2.14	0.48
24:AB:29:C:O2'	24:AB:51:A:N1	2.41	0.48
23:AA:955:A:H62	33:AK:12:GLN:HA	1.78	0.48
34:AL:102:ARG:HH21	34:AL:122:VAL:HG21	1.78	0.48
23:AA:1067:U:OP2	23:AA:1069:G:O2'	2.31	0.48
23:AA:107:G:H5''	23:AA:108:A:H5''	6.65	0.48
23:AA:504:G:N2	23:AA:505:U:O4	2.45	0.48
23:AA:1845:U:H3'	25:AC:157:SER:N	2.29	0.48
25:AC:129:ALA:HB2	25:AC:191:THR:HG22	1.95	0.48
23:AA:2707:C:H1'	26:AD:200:ASN:HD22	1.78	0.48
23:AA:2312:C:P	49:A1:2:ARG:HH21	2.28	0.48
23:AA:1064:A:N1	23:AA:1185:U:O2'	2.43	0.48
23:AA:1407:C:O2'	23:AA:1838:G:O2'	2.30	0.48
23:AA:2337:A:H2	28:AF:74:ILE:HG22	1.76	0.48
23:AA:18:C:O2'	23:AA:597:U:OP1	2.29	0.48
26:AD:140:PRO:O	26:AD:145:SER:OG	2.29	0.48
26:AD:37:GLN:HB3	26:AD:50:GLN:HG2	1.94	0.48
27:AE:139:PHE:HZ	27:AE:154:VAL:HG11	1.78	0.48
32:AJ:75:ALA:HB3	32:AJ:109:ILE:HG12	1.94	0.48
23:AA:1509:G:N2	23:AA:1593:G:O2'	2.43	0.48
23:AA:346:A:O5'	31:AI:97:ARG:NH1	155.28	0.48
23:AA:489:A:OP1	27:AE:45:ARG:HG3	2.14	0.48
23:AA:576:U:O2	23:AA:605:U:O2'	2.29	0.48
26:AD:56:LYS:HD3	26:AD:86:ARG:HG2	1.96	0.48
23:AA:896:U:H2'	23:AA:897:A:H8	1.79	0.48
27:AE:154:VAL:HA	27:AE:193:VAL:HG23	1.96	0.48
23:AA:1337:A:H4'	23:AA:1338:U:H5''	1.94	0.48
23:AA:1826:G:O6	25:AC:178:SER:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AA:650:U:OP1	27:AE:103:LYS:N	2.47	0.48
23:AA:1215:U:O2'	23:AA:1217:U:OP2	2.22	0.48
23:AA:2007:G:O2'	23:AA:2009:U:OP2	2.29	0.48
27:AE:164:GLU:HA	27:AE:175:VAL:HG21	1.95	0.48
23:AA:1726:A:OP2	23:AA:1743:G:N2	2.46	0.47
23:AA:2815:C:O2'	23:AA:2829:A:N3	2.44	0.47
23:AA:901:G:H2'	23:AA:902:A:C8	2.48	0.47
23:AA:1175:G:N2	23:AA:1176:U:O4	2.43	0.47
23:AA:1825:U:OP2	25:AC:274:ARG:NH2	2.47	0.47
23:AA:675:G:N2	23:AA:678:A:OP2	2.39	0.47
32:AJ:19:VAL:HG13	32:AJ:27:ASN:HB3	1.94	0.47
23:AA:1326:C:OP1	23:AA:1691:G:N1	2.47	0.47
24:AB:4:G:H1	24:AB:111:C:H41	1.62	0.47
52:A4:3:VAL:HG12	52:A4:35:ARG:HG3	1.97	0.47
26:AD:10:ILE:HB	26:AD:27:VAL:HG13	1.96	0.47
23:AA:1737:U:H5''	23:AA:1738:C:H5	1.79	0.47
23:AA:1828:U:OP2	25:AC:150:LYS:NZ	2.44	0.47
23:AA:2642:U:H1'	48:AZ:4:PRO:HB3	1.96	0.47
23:AA:545:G:N1	23:AA:548:A:OP2	2.45	0.47
35:AM:42:ALA:HB2	35:AM:108:LEU:HD21	1.96	0.47
35:AM:14:ARG:HD2	35:AM:98:GLY:O	2.15	0.47
23:AA:1324:A:N7	34:AL:111:GLY:HA3	2.29	0.47
23:AA:201:C:H1'	23:AA:2461:A:H61	1.80	0.47
23:AA:614:U:O2'	38:AP:79:ARG:NH2	2.48	0.47
39:AQ:28:ASN:HA	39:AQ:70:VAL:HA	1.96	0.47
23:AA:1845:U:OP2	25:AC:156:ARG:NE	2.43	0.47
23:AA:809:A:H61	23:AA:1816:A:H8	1.61	0.47
23:AA:2904:U:H5	48:AZ:40:HIS:CD2	2.33	0.47
23:AA:1581:U:C5	23:AA:1584:U:H6	2.32	0.47
23:AA:1796:A:O2'	23:AA:1985:C:OP1	2.33	0.47
23:AA:1862:G:H1	23:AA:1932:C:H5	1.63	0.47
23:AA:926:G:O2'	23:AA:942:C:O2	2.33	0.47
23:AA:1826:G:OP1	25:AC:260:ARG:HD2	2.15	0.47
23:AA:1065:A:H2'	23:AA:1066:G:H4'	1.96	0.47
23:AA:1072:A:N3	23:AA:2513:G:O2'	2.37	0.47
23:AA:1512:U:H2'	23:AA:1513:A:C8	2.49	0.47
23:AA:2686:G:O2'	29:AG:176:THR:HG21	2.15	0.47
23:AA:1533:A:N6	25:AC:100:GLU:N	2.46	0.47
28:AF:36:VAL:HG12	28:AF:154:ILE:HG13	1.97	0.47
31:AI:115:VAL:HG13	31:AI:121:VAL:HG21	1.97	0.47
32:AJ:23:VAL:HG13	38:AP:81:ASN:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AA:2289:U:OP2	43:AU:24:SER:OG	2.17	0.47
23:AA:1055:A:OP1	37:AO:75:SER:HB3	2.15	0.47
23:AA:614:U:H3'	38:AP:79:ARG:HH12	1.79	0.47
46:AX:15:ARG:O	46:AX:20:ARG:NH1	2.48	0.47
23:AA:2443:C:OP1	32:AJ:64:ARG:HB2	2.16	0.46
23:AA:829:U:H5''	25:AC:226:ASN:HD21	1.81	0.46
23:AA:661:U:C5'	27:AE:106:ARG:HD3	2.45	0.46
51:A3:26:ARG:NH1	51:A3:43:GLN:O	2.48	0.46
23:AA:1290:G:H1	37:AO:37:GLN:NE2	2.04	0.46
23:AA:2598:U:O2'	26:AD:159:ASP:HB2	2.15	0.46
23:AA:615:A:OP2	38:AP:79:ARG:NH2	2.49	0.46
23:AA:2231:C:C5'	25:AC:147:LYS:CD	2.94	0.46
26:AD:189:ASP:OD2	26:AD:192:ASN:ND2	2.42	0.46
33:AK:46:GLN:HB3	33:AK:125:LEU:HD13	1.98	0.46
39:AQ:11:ARG:NH1	39:AQ:98:LYS:HG3	2.31	0.46
25:AC:107:PRO:HD2	25:AC:110:LEU:HD22	1.98	0.46
23:AA:2231:C:H5'	25:AC:147:LYS:CD	2.43	0.46
23:AA:700:A:H4'	23:AA:701:G:H5'	1.97	0.46
24:AB:6:U:H4'	35:AM:32:ASN:HD21	1.80	0.46
26:AD:50:GLN:HB3	26:AD:90:GLU:HG2	1.97	0.46
23:AA:1818:A:O3'	25:AC:205:VAL:CG2	2.63	0.46
23:AA:2056:G:N1	23:AA:2060:A:OP2	2.38	0.46
27:AE:7:LEU:HB2	27:AE:126:VAL:HG12	1.98	0.46
23:AA:534:G:H4'	39:AQ:49:LYS:HD2	1.98	0.46
23:AA:378:C:OP2	41:AS:80:ARG:NH1	2.48	0.46
23:AA:1284:A:H4'	27:AE:45:ARG:HH12	1.81	0.46
23:AA:1455:U:N3	23:AA:1468:G:O6	31.73	0.46
23:AA:1482:U:H2'	23:AA:1483:A:H8	1.80	0.46
23:AA:2022:U:H3'	23:AA:2023:C:H2'	1.97	0.46
23:AA:52:A:N7	23:AA:113:U:O2'	16.93	0.46
23:AA:2663:U:H4'	26:AD:90:GLU:OE1	2.16	0.46
41:AS:33:VAL:HG13	41:AS:65:VAL:HG22	1.98	0.46
23:AA:1110:U:N3	23:AA:1114:A:OP2	2.42	0.46
23:AA:1930:G:OP1	25:AC:240:PRO:HB2	2.16	0.46
28:AF:58:GLU:HB3	47:AY:7:PRO:HG2	1.98	0.46
23:AA:1553:A:O2'	23:AA:1555:G:N2	2.48	0.46
23:AA:1184:C:OP1	30:AH:26:LEU:HB3	2.16	0.46
36:AN:114:GLU:HG2	36:AN:115:ILE:HG13	1.98	0.46
23:AA:1475:A:N6	23:AA:1606:C:O2	2.48	0.46
26:AD:122:SER:HB2	26:AD:175:GLY:HA2	1.98	0.46
23:AA:1121:A:O2'	23:AA:1122:U:O4'	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AA:2216:U:H2'	23:AA:2217:G:C8	2.51	0.45
23:AA:329:A:N6	23:AA:396:G:O6	2.49	0.45
23:AA:2333:U:H3	28:AF:40:VAL:HB	1.81	0.45
23:AA:325:A:H2	23:AA:401:U:H1'	1.82	0.45
26:AD:189:ASP:HB3	26:AD:194:VAL:HG22	1.98	0.45
29:AG:121:ILE:HD11	29:AG:140:GLN:HG3	1.98	0.45
34:AL:24:LEU:HD23	34:AL:30:ILE:HG12	1.97	0.45
23:AA:2904:U:C5	48:AZ:40:HIS:ND1	2.84	0.45
23:AA:33:U:O4	23:AA:492:G:O2'	2.34	0.45
23:AA:2648:G:P	26:AD:133:ARG:HH22	2.29	0.45
23:AA:1102:U:H2'	23:AA:1103:G:C8	2.51	0.45
23:AA:1113:A:H2	23:AA:1138:U:H3	1.63	0.45
23:AA:1315:C:H2'	23:AA:1316:G:H8	1.80	0.45
23:AA:1582:U:O5'	23:AA:1583:G:N2	2.50	0.45
23:AA:1847:U:C2	25:AC:201:GLU:HB3	2.52	0.45
23:AA:1944:U:H4'	23:AA:1947:C:H41	1.81	0.45
23:AA:2783:U:OP2	52:A4:19:ARG:NH2	2.49	0.45
23:AA:45:G:N7	23:AA:218:G:O2'	2.38	0.45
32:AJ:77:VAL:HG13	32:AJ:111:ILE:HD13	1.99	0.45
23:AA:1463:A:H2'	23:AA:1465:G:C8	2.51	0.45
23:AA:1482:U:H3	23:AA:1601:U:H5	1.65	0.45
23:AA:2144:A:HO2'	23:AA:2175:G:HO2'	1.59	0.45
23:AA:2331:G:H2'	23:AA:2334:G:H22	1.81	0.45
23:AA:284:C:O2'	23:AA:287:G:N2	2.32	0.45
23:AA:1039:C:C5	30:AH:1:MET:HA	2.51	0.45
23:AA:1095:A:N6	23:AA:1153:C:O2	2.50	0.45
35:AM:40:ILE:HG21	35:AM:73:ALA:HA	1.98	0.45
23:AA:1807:A:H3'	23:AA:1808:U:H2'	1.97	0.45
23:AA:282:A:H2'	23:AA:283:G:H8	1.81	0.45
23:AA:774:G:H5'	23:AA:775:A:H5''	1.99	0.45
32:AJ:77:VAL:HG11	32:AJ:96:LEU:HD21	1.99	0.45
44:AV:19:SER:OG	44:AV:23:ASN:OD1	2.25	0.45
51:A3:11:ALA:O	51:A3:65:LYS:NZ	2.50	0.45
23:AA:2272:U:H5''	23:AA:2273:G:H5'	1.99	0.45
35:AM:19:ARG:NH2	35:AM:47:ASP:OD1	2.45	0.45
23:AA:2711:U:OP1	36:AN:53:ARG:HD3	2.17	0.45
23:AA:606:G:H21	37:AO:37:GLN:NE2	1.92	0.45
23:AA:787:U:H2'	23:AA:788:A:C8	2.52	0.45
23:AA:963:A:H4'	24:AB:94:C:O2	2.16	0.45
23:AA:631:U:H1'	27:AE:90:PHE:HB3	1.98	0.45
23:AA:502:C:N4	40:AR:68:TYR:CG	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AA:1039:C:O2'	37:AO:93:LYS:NZ	2.49	0.45
23:AA:26:G:N2	23:AA:558:A:OP2	2.38	0.45
23:AA:600:U:O2'	30:AH:48:HIS:O	2.31	0.45
23:AA:878:C:OP1	32:AJ:39:LYS:CE	2.65	0.45
35:AM:7:LYS:O	35:AM:11:ARG:HB2	2.16	0.45
23:AA:1038:C:O2'	38:AP:10:LYS:HE2	2.16	0.45
23:AA:1533:A:N7	25:AC:96:TYR:CA	2.73	0.44
23:AA:410:G:O2'	23:AA:411:A:N7	2.50	0.44
23:AA:906:A:N3	24:AB:77:G:O2'	2.50	0.44
33:AK:125:LEU:HB3	33:AK:127:VAL:HG12	2.00	0.44
23:AA:1581:U:P	23:AA:1584:U:C5	3.10	0.44
23:AA:1643:C:OP1	40:AR:35:LYS:N	2.39	0.44
23:AA:1780:G:N1	23:AA:1783:G:OP2	2.45	0.44
23:AA:1819:G:O2'	23:AA:1857:C:OP1	2.34	0.44
23:AA:226:A:O2'	23:AA:466:C:O2	2.33	0.44
23:AA:897:A:H5'	46:AX:45:GLY:HA3	2.00	0.44
29:AG:83:TYR:N	29:AG:135:GLY:O	2.46	0.44
23:AA:1305:U:O2'	35:AM:14:ARG:NH2	123.81	0.44
23:AA:579:U:O2'	37:AO:49:ASP:OD2	2.20	0.44
23:AA:1845:U:H5''	25:AC:157:SER:HB2	1.98	0.44
23:AA:2338:A:C8	28:AF:40:VAL:CG1	2.94	0.44
23:AA:64:A:H61	23:AA:90:A:H62	1.65	0.44
25:AC:132:LEU:HD23	25:AC:135:ILE:HD12	1.98	0.44
23:AA:2521:G:O2'	33:AK:80:GLU:HA	2.17	0.44
23:AA:1658:A:H2	39:AQ:93:ALA:HB2	1.81	0.44
23:AA:1843:U:C5	25:AC:62:TYR:CE2	3.06	0.44
23:AA:59:U:H1'	23:AA:73:A:H2'	2.00	0.44
27:AE:194:ILE:HD12	27:AE:199:ALA:HB2	1.99	0.44
31:AI:87:ILE:HA	31:AI:93:PRO:HA	1.99	0.44
23:AA:1113:A:O2'	23:AA:1141:U:OP1	2.35	0.44
23:AA:1415:A:O2'	23:AA:1417:G:OP2	2.35	0.44
23:AA:43:A:H62	23:AA:482:U:H3	1.64	0.44
23:AA:372:A:N6	41:AS:15:LYS:HG2	2.19	0.44
23:AA:1242:A:O2'	32:AJ:4:HIS:HD2	2.00	0.44
23:AA:144:C:H2'	23:AA:145:A:H8	1.83	0.44
23:AA:582:G:OP1	23:AA:1039:C:N4	2.50	0.44
24:AB:4:G:H22	24:AB:111:C:H5	1.66	0.44
23:AA:1847:U:OP1	25:AC:177:ARG:HG2	2.17	0.44
31:AI:64:ARG:HB2	31:AI:79:PHE:CG	2.53	0.44
39:AQ:17:VAL:HG23	39:AQ:47:ILE:HD11	2.00	0.44
23:AA:1000:G:H2'	23:AA:1001:A:H2'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AA:1482:U:H2'	23:AA:1483:A:C8	2.53	0.44
23:AA:2355:A:H2'	23:AA:2356:A:C8	2.53	0.44
23:AA:2649:U:O2'	23:AA:2845:G:N2	2.51	0.44
52:A4:16:VAL:HG22	52:A4:25:VAL:HG12	1.99	0.44
23:AA:1290:G:N2	37:AO:33:LYS:HB3	2.32	0.44
23:AA:620:G:O2'	23:AA:1292:A:OP1	2.35	0.44
23:AA:1315:C:H2'	23:AA:1316:G:C8	2.53	0.44
23:AA:1500:G:H2'	23:AA:1501:G:H8	1.82	0.44
23:AA:750:A:OP2	23:AA:770:G:N2	2.45	0.44
24:AB:12:U:OP2	24:AB:68:U:O2'	2.32	0.44
25:AC:124:ILE:HD13	25:AC:136:PRO:HG3	1.99	0.44
29:AG:77:GLN:NE2	29:AG:81:GLN:OE1	2.51	0.44
23:AA:1031:C:H5''	46:AX:10:ARG:NH1	2.33	0.43
23:AA:1395:G:N1	23:AA:1408:G:N7	2.66	0.43
23:AA:1615:G:P	25:AC:63:ARG:HH22	2.41	0.43
23:AA:1625:U:H2'	23:AA:1626:A:H8	1.80	0.43
23:AA:1886:A:N6	23:AA:1910:G:O2'	2.51	0.43
25:AC:176:LEU:HD13	25:AC:176:LEU:HA	1.78	0.43
23:AA:2330:G:C4'	28:AF:122:PHE:O	2.66	0.43
23:AA:1521:A:H2'	23:AA:1522:G:H8	1.83	0.43
23:AA:630:G:N7	32:AJ:33:ARG:NH2	2.63	0.43
23:AA:753:U:OP1	23:AA:860:U:O2'	128.29	0.43
23:AA:923:A:H2	23:AA:944:G:H22	1.66	0.43
31:AI:98:ILE:HD12	31:AI:117:LEU:HB2	2.00	0.43
38:AP:20:ILE:HG12	38:AP:97:ILE:HD11	1.99	0.43
40:AR:64:ARG:HG3	40:AR:69:GLN:HA	1.99	0.43
23:AA:125:A:P	50:A2:19:PHE:H	2.42	0.43
23:AA:135:G:H2'	23:AA:136:A:H8	1.84	0.43
23:AA:1875:A:O2'	23:AA:1876:G:O4'	2.35	0.43
23:AA:2505:A:H5'	52:A4:31:LYS:HE3	2.01	0.43
23:AA:1035:C:N3	23:AA:1036:C:N4	3.75	0.43
23:AA:2333:U:N3	28:AF:40:VAL:HG23	2.32	0.43
23:AA:2800:U:OP1	26:AD:179:THR:HG21	2.12	0.43
23:AA:896:U:H2'	23:AA:897:A:C8	2.53	0.43
31:AI:39:ILE:HG12	31:AI:62:ILE:HD11	2.01	0.43
35:AM:33:VAL:HG22	35:AM:108:LEU:HD23	2.00	0.43
23:AA:1091:G:HO2'	23:AA:1155:A:N6	2.16	0.43
23:AA:1293:U:H5''	23:AA:1294:G:H5''	2.00	0.43
23:AA:1362:C:OP1	23:AA:1691:G:O2'	2.26	0.43
23:AA:282:A:H2'	23:AA:283:G:C8	2.54	0.43
23:AA:2903:A:H5'	23:AA:2904:U:H5'	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AA:581:A:OP1	30:AH:1:MET:HE3	1.96	0.43
36:AN:99:LEU:HB3	36:AN:102:LEU:HD13	2.00	0.43
23:AA:1395:G:H8	23:AA:1410:A:H62	1.66	0.43
23:AA:1630:A:H2'	23:AA:1631:G:H2'	2.00	0.43
23:AA:1631:G:OP1	23:AA:1631:G:N2	2.52	0.43
23:AA:2311:U:H3	23:AA:2411:A:H62	1.65	0.43
23:AA:2904:U:H5	48:AZ:40:HIS:CG	2.37	0.43
23:AA:58:G:O6	23:AA:68:A:N6	2.51	0.43
41:AS:3:ILE:HG22	41:AS:70:LEU:HG	1.99	0.43
23:AA:1109:U:N3	23:AA:1114:A:OP1	2.43	0.43
23:AA:2510:C:O2	33:AK:124:LYS:CE	2.67	0.43
23:AA:2613:C:H2'	23:AA:2614:A:C8	2.53	0.43
23:AA:318:A:N6	23:AA:319:G:O6	2.52	0.43
23:AA:513:G:O2'	23:AA:841:C:O3'	2.37	0.43
23:AA:669:C:H2'	23:AA:670:G:H8	1.83	0.43
23:AA:1818:A:H4'	25:AC:207:LYS:H	1.84	0.43
26:AD:2:THR:HA	26:AD:94:VAL:HA	2.01	0.43
33:AK:27:VAL:HG12	33:AK:105:GLU:HG2	2.00	0.43
23:AA:372:A:N6	41:AS:15:LYS:H	2.17	0.43
23:AA:1580:A:OP2	23:AA:1581:U:N3	2.51	0.43
23:AA:2152:G:N2	23:AA:2189:G:O2'	2.52	0.43
33:AK:14:ARG:HD2	33:AK:41:TRP:HH2	1.83	0.43
23:AA:720:A:N3	23:AA:2470:C:O2'	2.47	0.43
30:AH:18:VAL:HG23	30:AH:138:PRO:HB2	2.01	0.43
31:AI:2:ILE:HD13	31:AI:8:LEU:HD21	2.00	0.43
31:AI:96:THR:HA	31:AI:117:LEU:HD13	2.00	0.43
23:AA:1091:G:N2	23:AA:1154:G:O2'	2.51	0.43
23:AA:2783:U:H1'	23:AA:2784:A:H5''	2.00	0.43
23:AA:857:C:OP2	32:AJ:22:GLY:HA2	2.19	0.43
24:AB:54:U:H4'	24:AB:55:A:H5'	2.00	0.42
28:AF:96:MET:O	28:AF:100:LEU:N	2.47	0.42
23:AA:24:G:O2'	39:AQ:78:GLU:O	2.36	0.42
41:AS:92:ARG:NH1	41:AS:100:GLU:OE2	2.52	0.42
42:AT:94:ILE:HG13	42:AT:94:ILE:H	1.64	0.42
23:AA:1449:A:H2'	23:AA:1450:A:C4	2.54	0.42
23:AA:1450:A:H61	23:AA:1635:A:N6	2.16	0.42
23:AA:693:G:H2'	23:AA:694:G:H8	1.84	0.42
25:AC:145:GLU:HB2	25:AC:188:CYS:HB3	2.00	0.42
23:AA:661:U:H5'	27:AE:106:ARG:HD3	2.01	0.42
32:AJ:123:VAL:HG21	32:AJ:136:ILE:HD13	2.02	0.42
23:AA:2277:G:H22	33:AK:84:GLY:HA3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AX:8:LEU:HB2	46:AX:28:LEU:HD13	2.00	0.42
23:AA:1818:A:N6	23:AA:1855:G:O2'	2.42	0.42
23:AA:2144:A:N6	23:AA:2188:C:OP2	2.42	0.42
23:AA:2311:U:OP2	49:A1:2:ARG:HG2	2.19	0.42
23:AA:502:C:H41	40:AR:68:TYR:HB2	1.83	0.42
25:AC:8:PRO:HB3	25:AC:14:ARG:HG3	2.02	0.42
33:AK:46:GLN:HG2	33:AK:126:PRO:HD3	2.01	0.42
23:AA:1423:C:H2'	23:AA:1424:A:C8	2.54	0.42
23:AA:1431:U:H4'	23:AA:1647:A:H4'	2.01	0.42
23:AA:2168:A:H61	23:AA:2176:C:H41	1.67	0.42
23:AA:2716:U:OP2	23:AA:2892:G:N1	2.38	0.42
23:AA:509:G:N2	23:AA:512:A:OP2	2.45	0.42
23:AA:857:C:HO2'	23:AA:1264:A:HO2'	1.63	0.42
23:AA:904:G:O2'	23:AA:961:G:O6	2.28	0.42
23:AA:882:C:H5	23:AA:986:G:H1	1.67	0.42
39:AQ:86:ARG:HA	39:AQ:86:ARG:HD2	1.60	0.42
23:AA:502:C:N4	40:AR:68:TYR:CB	2.82	0.42
23:AA:1110:U:O2'	23:AA:1113:A:N6	2.53	0.42
23:AA:2024:A:O5'	26:AD:138:ARG:NH1	2.44	0.42
23:AA:1918:G:O2'	23:AA:2262:G:O2'	2.34	0.42
23:AA:2309:G:N2	23:AA:2417:U:O2	2.43	0.42
31:AI:113:LYS:HE3	31:AI:117:LEU:HD11	2.01	0.42
23:AA:856:U:H2'	32:AJ:21:ARG:HA	2.01	0.42
33:AK:48:GLU:OE2	33:AK:51:ARG:NH1	2.53	0.42
35:AM:12:LEU:HD23	35:AM:12:LEU:HA	1.60	0.42
23:AA:1111:A:N6	23:AA:1139:A:O3'	2.52	0.42
23:AA:152:C:OP1	23:AA:1396:A:O2'	2.37	0.42
23:AA:1658:A:C2	39:AQ:93:ALA:HB2	2.55	0.42
23:AA:284:C:H2'	23:AA:285:U:C2	2.55	0.42
23:AA:720:A:OP1	27:AE:76:GLY:HA3	2.20	0.42
23:AA:2662:U:O2'	26:AD:90:GLU:OE2	2.28	0.42
27:AE:46:GLN:HG3	27:AE:48:THR:HG22	2.01	0.42
45:AW:14:ILE:HG21	45:AW:57:ALA:HB2	2.02	0.42
23:AA:1847:U:O2	25:AC:201:GLU:CB	2.68	0.42
23:AA:1979:A:N3	23:AA:2587:C:O2'	2.42	0.42
34:AL:17:LEU:HG	34:AL:43:VAL:HG21	2.02	0.42
36:AN:59:GLU:CG	36:AN:78:LEU:HD23	2.48	0.42
41:AS:39:ASN:HD22	41:AS:63:ILE:HG12	1.85	0.42
23:AA:1563:U:H2'	23:AA:1564:G:C8	2.55	0.42
23:AA:2260:A:H2'	23:AA:2261:G:C8	2.55	0.42
23:AA:2382:C:OP1	43:AU:33:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AC:207:LYS:HG2	25:AC:209:GLY:H	1.85	0.42
23:AA:1485:G:H1	23:AA:1598:U:H3	1.68	0.42
23:AA:1713:A:O2'	31:AI:4:GLN:NE2	2.53	0.42
23:AA:150:A:H61	23:AA:179:A:H2	1.68	0.42
23:AA:2642:U:O2	48:AZ:5:LYS:N	2.53	0.42
23:AA:437:A:O2'	23:AA:456:G:OP1	2.36	0.42
24:AB:47:C:H2'	24:AB:48:A:C8	2.55	0.42
28:AF:120:LYS:HB3	28:AF:167:ARG:HH22	1.85	0.42
24:AB:55:A:H1'	28:AF:27:GLU:HB3	2.02	0.42
23:AA:2332:U:O4	28:AF:38:MET:HG2	2.19	0.42
23:AA:1108:C:H3'	23:AA:1109:U:H4'	2.01	0.41
23:AA:124:A:OP2	50:A2:20:ARG:NE	2.41	0.41
23:AA:1477:U:H2'	23:AA:1478:A:C8	2.55	0.41
23:AA:2294:A:H5''	23:AA:2295:A:H5''	2.02	0.41
25:AC:168:GLU:HG3	25:AC:169:GLY:H	1.84	0.41
26:AD:8:ARG:NH2	26:AD:54:GLU:OE1	2.42	0.41
40:AR:13:THR:H	40:AR:16:SER:HB3	1.84	0.41
23:AA:2386:C:O2'	51:A3:54:ASP:OD2	2.31	0.41
23:AA:1250:G:N2	23:AA:1274:G:O2'	2.52	0.41
23:AA:2405:A:C5	23:AA:2406:G:H1'	2.55	0.41
23:AA:2904:U:H5	48:AZ:40:HIS:NE2	2.18	0.41
23:AA:26:G:H1'	23:AA:560:A:H61	1.85	0.41
29:AG:107:VAL:HG11	29:AG:162:ILE:HD11	2.02	0.41
23:AA:2496:A:H4'	33:AK:56:ARG:HD2	2.03	0.41
23:AA:2277:G:C2	33:AK:84:GLY:HA3	2.55	0.41
37:AO:105:ALA:HB1	38:AP:40:PHE:HZ	1.85	0.41
23:AA:1261:G:N2	23:AA:1264:A:OP2	2.46	0.41
23:AA:1479:G:H2'	23:AA:1480:G:H8	1.84	0.41
23:AA:1479:G:H2'	23:AA:1480:G:C8	2.55	0.41
23:AA:1583:G:H5''	23:AA:1584:U:C2	2.55	0.41
23:AA:390:A:H2'	23:AA:391:A:C8	2.55	0.41
23:AA:72:U:OP2	45:AW:54:LYS:NZ	2.53	0.41
23:AA:970:U:H3'	23:AA:971:U:H4'	2.01	0.41
26:AD:34:VAL:HG22	26:AD:85:LYS:HE3	2.02	0.41
27:AE:152:VAL:HG12	27:AE:173:VAL:HG22	2.02	0.41
23:AA:2331:G:C4'	28:AF:129:THR:O	2.45	0.41
23:AA:1278:G:H1'	23:AA:1337:A:H5''	92.85	0.41
23:AA:1771:A:O2'	23:AA:1772:G:N7	2.52	0.41
23:AA:1852:G:OP1	25:AC:230:HIS:HE1	2.02	0.41
23:AA:1893:A:C5	23:AA:1894:G:H1'	2.55	0.41
23:AA:2333:U:N3	28:AF:40:VAL:HB	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AA:2392:G:N7	51:A3:39:LYS:NZ	2.57	0.41
23:AA:503:A:N6	23:AA:516:A:H5''	2.36	0.41
23:AA:241:C:O2'	23:AA:651:A:N3	2.48	0.41
23:AA:1533:A:C4	25:AC:97:ALA:O	2.69	0.41
26:AD:156:MET:N	26:AD:156:MET:SD	2.93	0.41
27:AE:19:LEU:HD21	27:AE:199:ALA:HB1	2.02	0.41
23:AA:1177:A:H1'	23:AA:1178:C:H4'	4.56	0.41
23:AA:2850:G:OP1	26:AD:67:LYS:HB3	2.20	0.41
31:AI:11:ALA:HB2	31:AI:83:ALA:HB1	2.03	0.41
23:AA:2566:C:C5'	52:A4:3:VAL:HG21	2.50	0.41
23:AA:1697:G:C6	34:AL:5:LYS:HB2	2.55	0.41
23:AA:2821:U:H5''	23:AA:2823:G:C2	2.56	0.41
27:AE:32:VAL:HG13	27:AE:105:MET:HG2	2.03	0.41
27:AE:80:ALA:HB3	27:AE:83:TRP:CD1	2.55	0.41
47:AY:32:SER:HA	47:AY:44:PRO:HD2	2.01	0.41
49:A1:31:GLU:HB2	49:A1:44:LEU:HD12	2.03	0.41
23:AA:1031:C:O2'	23:AA:1044:A:N3	2.46	0.41
23:AA:1107:G:H22	23:AA:1120:C:H1'	1.86	0.41
23:AA:1388:C:O2'	23:AA:1618:A:N3	2.45	0.41
23:AA:1644:C:OP1	40:AR:76:ARG:NH2	2.54	0.41
26:AD:40:THR:HG22	26:AD:42:GLU:H	1.85	0.41
29:AG:170:ARG:HH12	52:A4:29:ASN:HB3	1.86	0.41
37:AO:31:LEU:HB2	37:AO:34:VAL:HG12	2.03	0.41
39:AQ:69:LEU:HD23	39:AQ:109:ASP:HB3	2.03	0.41
44:AV:14:THR:HG22	44:AV:28:ARG:HD2	2.03	0.41
23:AA:669:C:H2'	23:AA:670:G:C8	2.56	0.41
31:AI:98:ILE:HD13	31:AI:114:ILE:HG23	2.02	0.41
52:A4:29:ASN:HD21	52:A4:32:HIS:CE1	2.39	0.41
23:AA:1520:A:H61	23:AA:1561:G:H2'	1.86	0.41
23:AA:1754:C:H4'	23:AA:2878:U:H3	1.86	0.41
23:AA:1758:A:H1'	23:AA:1772:G:C5	2.56	0.41
23:AA:2048:G:N2	37:AO:25:PHE:CG	2.89	0.41
23:AA:617:A:N6	23:AA:2061:U:OP1	2.54	0.41
23:AA:2156:C:H42	23:AA:2186:G:H1	1.69	0.41
23:AA:1701:U:P	26:AD:149:ARG:HB2	2.60	0.41
33:AK:68:ILE:HA	33:AK:68:ILE:HD13	1.88	0.41
23:AA:23:G:H21	39:AQ:77:ASN:ND2	2.19	0.41
23:AA:2232:A:H5''	25:AC:149:GLY:C	2.41	0.41
23:AA:2593:A:N1	31:AI:28:SER:OG	2.46	0.41
23:AA:2663:U:O2'	26:AD:46:TYR:CZ	2.74	0.41
23:AA:277:C:H2'	23:AA:278:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AA:862:C:H3'	23:AA:863:G:H8	1.86	0.41
23:AA:1847:U:OP1	25:AC:177:ARG:CG	2.69	0.41
28:AF:132:VAL:HB	28:AF:152:MET:HB2	2.02	0.41
33:AK:34:LEU:HB2	33:AK:118:LEU:HD22	2.03	0.41
23:AA:564:U:H5''	39:AQ:25:ARG:HH12	1.86	0.41
47:AY:16:ASP:OD2	47:AY:18:THR:OG1	2.35	0.41
23:AA:1087:C:N4	23:AA:1088:C:H41	2.19	0.41
23:AA:2498:A:N6	23:AA:2503:A:O2'	2.54	0.41
23:AA:2715:G:N1	23:AA:2747:U:OP2	2.32	0.41
23:AA:890:G:O2'	23:AA:892:U:O4	2.33	0.41
25:AC:225:MET:HB3	25:AC:229:ASP:HB2	2.02	0.41
23:AA:2757:U:O2'	26:AD:181:GLN:O	2.33	0.41
23:AA:2422:C:H42	23:AA:2448:G:H1	1.69	0.40
23:AA:828:A:H2'	23:AA:829:U:H4'	2.02	0.40
28:AF:34:ILE:HB	28:AF:91:LEU:HB2	2.03	0.40
31:AI:43:VAL:HG23	31:AI:54:LYS:HA	2.02	0.40
23:AA:1000:G:OP1	33:AK:87:LYS:HG3	2.20	0.40
23:AA:859:C:OP1	38:AP:84:ARG:HA	2.20	0.40
23:AA:1829:A:H2'	23:AA:1830:A:C8	2.56	0.40
23:AA:1985:C:H2'	23:AA:1986:G:H8	1.87	0.40
23:AA:199:A:C2	32:AJ:50:PHE:HZ	2.39	0.40
23:AA:389:A:H3'	23:AA:390:A:H8	1.87	0.40
23:AA:503:A:N1	23:AA:518:A:N6	2.70	0.40
23:AA:588:G:N2	23:AA:589:U:O4	2.40	0.40
23:AA:1378:U:OP2	23:AA:1431:U:O2'	2.31	0.40
23:AA:1490:G:O2'	23:AA:1491:C:O4'	2.37	0.40
27:AE:155:VAL:HB	27:AE:194:ILE:HG22	2.03	0.40
32:AJ:74:TYR:CE2	32:AJ:127:LYS:HE2	2.56	0.40
33:AK:77:LYS:HA	33:AK:78:PRO:HD3	1.93	0.40
23:AA:1110:U:H4'	23:AA:1117:A:C5	2.57	0.40
23:AA:1806:U:H2'	23:AA:1810:A:H62	1.85	0.40
28:AF:43:ALA:HA	28:AF:46:ASN:HB2	2.03	0.40
36:AN:22:PHE:O	36:AN:52:ARG:NH1	2.54	0.40
23:AA:1187:A:OP1	30:AH:28:ARG:NH2	2.50	0.40
23:AA:161:A:N6	23:AA:162:A:H62	2.86	0.40
23:AA:1839:G:O2'	25:AC:44:ASN:HB2	2.22	0.40
30:AH:63:ILE:HG13	30:AH:102:ILE:HD11	2.03	0.40
45:AW:6:ILE:HG22	45:AW:56:VAL:HG21	2.03	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	
2	Ab	224/255 (88%)	213 (95%)	11 (5%)	0	100	100
3	Ac	200/217 (92%)	177 (88%)	23 (12%)	0	100	100
4	Ad	196/200 (98%)	170 (87%)	26 (13%)	0	100	100
5	Ae	154/166 (93%)	147 (96%)	7 (4%)	0	100	100
6	Af	93/98 (95%)	85 (91%)	8 (9%)	0	100	100
7	Ag	150/156 (96%)	144 (96%)	6 (4%)	0	100	100
8	Ah	129/132 (98%)	121 (94%)	8 (6%)	0	100	100
9	Ai	125/132 (95%)	112 (90%)	13 (10%)	0	100	100
10	Aj	95/102 (93%)	88 (93%)	7 (7%)	0	100	100
11	Ak	112/129 (87%)	93 (83%)	19 (17%)	0	100	100
12	Al	133/137 (97%)	118 (89%)	15 (11%)	0	100	100
13	Am	100/121 (83%)	90 (90%)	10 (10%)	0	100	100
14	An	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
15	Ao	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
16	Ap	87/91 (96%)	78 (90%)	9 (10%)	0	100	100
17	Aq	78/87 (90%)	72 (92%)	6 (8%)	0	100	100
18	Ar	52/80 (65%)	51 (98%)	1 (2%)	0	100	100
19	As	78/92 (85%)	69 (88%)	9 (12%)	0	100	100
20	At	79/83 (95%)	77 (98%)	2 (2%)	0	100	100
21	Au	50/58 (86%)	48 (96%)	2 (4%)	0	100	100
22	Av	158/190 (83%)	149 (94%)	9 (6%)	0	100	100
25	AC	272/277 (98%)	257 (94%)	15 (6%)	0	100	100
26	AD	213/220 (97%)	194 (91%)	19 (9%)	0	100	100
27	AE	204/207 (99%)	192 (94%)	12 (6%)	0	100	100
28	AF	173/179 (97%)	142 (82%)	31 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	AG	173/178 (97%)	155 (90%)	18 (10%)	0	100	100
30	AH	143/145 (99%)	131 (92%)	12 (8%)	0	100	100
31	AI	120/122 (98%)	106 (88%)	14 (12%)	0	100	100
32	AJ	144/146 (99%)	135 (94%)	9 (6%)	0	100	100
33	AK	135/144 (94%)	127 (94%)	8 (6%)	0	100	100
34	AL	118/122 (97%)	114 (97%)	4 (3%)	0	100	100
35	AM	117/119 (98%)	103 (88%)	14 (12%)	0	100	100
36	AN	112/116 (97%)	99 (88%)	13 (12%)	0	100	100
37	AO	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
38	AP	100/102 (98%)	93 (93%)	6 (6%)	1 (1%)	18	51
39	AQ	110/117 (94%)	106 (96%)	4 (4%)	0	100	100
40	AR	87/91 (96%)	81 (93%)	6 (7%)	0	100	100
41	AS	101/105 (96%)	89 (88%)	12 (12%)	0	100	100
42	AT	92/217 (42%)	87 (95%)	5 (5%)	0	100	100
43	AU	80/94 (85%)	72 (90%)	8 (10%)	0	100	100
44	AV	56/62 (90%)	53 (95%)	3 (5%)	0	100	100
45	AW	65/73 (89%)	58 (89%)	7 (11%)	0	100	100
46	AX	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
47	AY	57/84 (68%)	45 (79%)	12 (21%)	0	100	100
48	AZ	46/57 (81%)	40 (87%)	6 (13%)	0	100	100
49	A1	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
50	A2	41/45 (91%)	39 (95%)	2 (5%)	0	100	100
51	A3	62/66 (94%)	57 (92%)	5 (8%)	0	100	100
52	A4	35/37 (95%)	35 (100%)	0	0	100	100
All	All	5508/6027 (91%)	5052 (92%)	455 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
38	AP	51	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Ab	196/221 (89%)	196 (100%)	0	100	100
3	Ac	138/175 (79%)	138 (100%)	0	100	100
4	Ad	147/175 (84%)	146 (99%)	1 (1%)	87	97
5	Ae	118/131 (90%)	118 (100%)	0	100	100
6	Af	80/86 (93%)	80 (100%)	0	100	100
7	Ag	118/132 (89%)	118 (100%)	0	100	100
8	Ah	111/113 (98%)	109 (98%)	2 (2%)	64	89
9	Ai	86/109 (79%)	84 (98%)	2 (2%)	56	85
10	Aj	81/91 (89%)	80 (99%)	1 (1%)	75	93
11	Ak	82/104 (79%)	82 (100%)	0	100	100
12	Al	111/119 (93%)	110 (99%)	1 (1%)	82	95
13	Am	62/104 (60%)	61 (98%)	1 (2%)	68	90
14	An	48/53 (91%)	46 (96%)	2 (4%)	34	69
15	Ao	77/81 (95%)	76 (99%)	1 (1%)	73	93
16	Ap	73/77 (95%)	71 (97%)	2 (3%)	50	82
17	Aq	65/82 (79%)	65 (100%)	0	100	100
18	Ar	48/68 (71%)	48 (100%)	0	100	100
19	As	67/80 (84%)	67 (100%)	0	100	100
20	At	61/69 (88%)	61 (100%)	0	100	100
21	Au	40/54 (74%)	40 (100%)	0	100	100
22	Av	147/173 (85%)	143 (97%)	4 (3%)	50	82
25	AC	221/224 (99%)	221 (100%)	0	100	100
26	AD	173/177 (98%)	172 (99%)	1 (1%)	89	97
27	AE	168/169 (99%)	167 (99%)	1 (1%)	89	97
28	AF	141/158 (89%)	139 (99%)	2 (1%)	71	91
29	AG	124/155 (80%)	122 (98%)	2 (2%)	68	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	AH	122/123 (99%)	121 (99%)	1 (1%)	85	96
31	AI	100/100 (100%)	99 (99%)	1 (1%)	80	95
32	AJ	109/112 (97%)	107 (98%)	2 (2%)	64	89
33	AK	108/119 (91%)	107 (99%)	1 (1%)	82	95
34	AL	96/102 (94%)	95 (99%)	1 (1%)	80	95
35	AM	86/95 (90%)	83 (96%)	3 (4%)	41	75
36	AN	93/102 (91%)	92 (99%)	1 (1%)	78	94
37	AO	96/98 (98%)	95 (99%)	1 (1%)	80	95
38	AP	84/86 (98%)	84 (100%)	0	100	100
39	AQ	89/94 (95%)	88 (99%)	1 (1%)	78	94
40	AR	78/82 (95%)	76 (97%)	2 (3%)	51	83
41	AS	81/90 (90%)	80 (99%)	1 (1%)	75	93
42	AT	78/190 (41%)	78 (100%)	0	100	100
43	AU	63/75 (84%)	60 (95%)	3 (5%)	30	64
44	AV	44/52 (85%)	43 (98%)	1 (2%)	56	85
45	AW	58/66 (88%)	58 (100%)	0	100	100
46	AX	52/53 (98%)	52 (100%)	0	100	100
47	AY	23/75 (31%)	23 (100%)	0	100	100
48	AZ	35/50 (70%)	35 (100%)	0	100	100
49	A1	44/47 (94%)	44 (100%)	0	100	100
50	A2	39/40 (98%)	39 (100%)	0	100	100
51	A3	55/57 (96%)	55 (100%)	0	100	100
52	A4	35/35 (100%)	34 (97%)	1 (3%)	48	81
All	All	4451/5123 (87%)	4408 (99%)	43 (1%)	81	95

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Ad	115	ASN
8	Ah	56	LYS
8	Ah	105	LEU
9	Ai	20	ARG
9	Ai	115	ARG
10	Aj	102	LEU

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Mol	Chain	Res	Type
12	Al	44	ARG
13	Am	57	ARG
14	An	26	ARG
14	An	45	ARG
15	Ao	54	ARG
16	Ap	9	ARG
16	Ap	32	ARG
22	Av	103	ARG
22	Av	151	LEU
22	Av	164	THR
22	Av	179	ASP
26	AD	131	ILE
27	AE	193	VAL
28	AF	69	LYS
28	AF	125	ARG
29	AG	41	MET
29	AG	175	LYS
30	AH	97	ASN
31	AI	122	LEU
32	AJ	30	THR
32	AJ	114	ASN
33	AK	27	VAL
34	AL	29	ARG
35	AM	22	LEU
35	AM	35	ARG
35	AM	87	LYS
36	AN	11	THR
37	AO	4	VAL
39	AQ	98	LYS
40	AR	47	ASN
40	AR	56	MET
41	AS	8	ASN
43	AU	22	ARG
43	AU	61	ARG
43	AU	75	VAL
44	AV	60	THR
52	A4	35	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
2	Ab	190	ASN

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Mol	Chain	Res	Type
3	Ac	64	ASN
4	Ad	112	GLN
4	Ad	115	ASN
4	Ad	146	GLN
5	Ae	83	HIS
6	Af	70	ASN
7	Ag	67	ASN
9	Ai	33	ASN
9	Ai	77	GLN
11	Ak	22	HIS
11	Ak	40	ASN
11	Ak	101	GLN
12	Al	42	GLN
12	Al	85	HIS
14	An	52	GLN
17	Aq	33	HIS
18	Ar	57	GLN
19	As	22	GLN
20	At	21	ASN
22	Av	82	ASN
22	Av	152	GLN
25	AC	86	ASN
25	AC	133	GLN
25	AC	230	HIS
26	AD	128	GLN
26	AD	148	HIS
26	AD	167	GLN
26	AD	200	ASN
27	AE	75	GLN
28	AF	127	ASN
29	AG	77	GLN
30	AH	48	HIS
30	AH	97	ASN
31	AI	4	GLN
32	AJ	4	HIS
32	AJ	114	ASN
35	AM	43	GLN
36	AN	4	HIS
36	AN	79	HIS
37	AO	37	GLN
37	AO	91	ASN
38	AP	81	ASN

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Mol	Chain	Res	Type
39	AQ	77	ASN
40	AR	47	ASN
41	AS	8	ASN
41	AS	39	ASN
41	AS	44	HIS
43	AU	20	ASN
44	AV	16	ASN
48	AZ	19	HIS
48	AZ	40	HIS
49	A1	26	ASN
49	A1	45	HIS
50	A2	17	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Aa	1537/1555 (98%)	461 (29%)	0
23	AA	2895/2923 (99%)	794 (27%)	28 (0%)
24	AB	113/115 (98%)	16 (14%)	0
All	All	4545/4593 (98%)	1271 (27%)	28 (0%)

All (1271) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Aa	6	U
1	Aa	8	G
1	Aa	9	A
1	Aa	10	G
1	Aa	23	G
1	Aa	30	A
1	Aa	33	A
1	Aa	40	G
1	Aa	41	C
1	Aa	45	G
1	Aa	48	C
1	Aa	49	C
1	Aa	50	U
1	Aa	51	A
1	Aa	52	A
1	Aa	59	C
1	Aa	60	A

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Mol	Chain	Res	Type
1	Aa	61	A
1	Aa	62	G
1	Aa	66	A
1	Aa	68	C
1	Aa	69	G
1	Aa	70	A
1	Aa	71	A
1	Aa	75	A
1	Aa	76	C
1	Aa	78	A
1	Aa	82	G
1	Aa	83	C
1	Aa	84	U
1	Aa	85	U
1	Aa	88	U
1	Aa	89	U
1	Aa	92	C
1	Aa	94	G
1	Aa	99	U
1	Aa	100	A
1	Aa	107	G
1	Aa	120	C
1	Aa	129	A
1	Aa	140	A
1	Aa	150	U
1	Aa	162	A
1	Aa	163	C
1	Aa	165	G
1	Aa	183	U
1	Aa	184	A
1	Aa	185	U
1	Aa	186	U
1	Aa	187	U
1	Aa	188	U
1	Aa	191	A
1	Aa	193	C
1	Aa	194	G
1	Aa	197	U
1	Aa	199	G
1	Aa	200	U
1	Aa	201	U
1	Aa	203	A

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Mol	Chain	Res	Type
1	Aa	204	A
1	Aa	206	A
1	Aa	208	U
1	Aa	209	G
1	Aa	210	A
1	Aa	211	A
1	Aa	213	G
1	Aa	219	C
1	Aa	220	U
1	Aa	221	U
1	Aa	222	G
1	Aa	224	U
1	Aa	228	A
1	Aa	230	U
1	Aa	231	U
1	Aa	234	A
1	Aa	252	U
1	Aa	253	U
1	Aa	255	G
1	Aa	256	C
1	Aa	257	U
1	Aa	258	A
1	Aa	259	G
1	Aa	264	U
1	Aa	267	G
1	Aa	269	U
1	Aa	274	G
1	Aa	275	C
1	Aa	279	C
1	Aa	289	G
1	Aa	291	U
1	Aa	297	G
1	Aa	301	A
1	Aa	309	G
1	Aa	335	A
1	Aa	336	C
1	Aa	337	A
1	Aa	339	G
1	Aa	352	A
1	Aa	354	G
1	Aa	355	G
1	Aa	356	G

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Mol	Chain	Res	Type
1	Aa	358	G
1	Aa	359	G
1	Aa	360	C
1	Aa	362	G
1	Aa	364	A
1	Aa	375	U
1	Aa	376	U
1	Aa	380	C
1	Aa	381	A
1	Aa	389	A
1	Aa	392	G
1	Aa	395	U
1	Aa	406	C
1	Aa	411	C
1	Aa	412	G
1	Aa	413	U
1	Aa	414	G
1	Aa	415	A
1	Aa	416	G
1	Aa	417	U
1	Aa	418	G
1	Aa	419	A
1	Aa	420	U
1	Aa	421	G
1	Aa	422	A
1	Aa	423	A
1	Aa	424	G
1	Aa	425	G
1	Aa	426	U
1	Aa	430	C
1	Aa	431	G
1	Aa	432	G
1	Aa	434	U
1	Aa	437	U
1	Aa	438	A
1	Aa	440	A
1	Aa	441	A
1	Aa	442	C
1	Aa	449	A
1	Aa	450	U
1	Aa	451	U
1	Aa	452	A

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Mol	Chain	Res	Type
1	Aa	456	A
1	Aa	458	G
1	Aa	460	A
1	Aa	461	C
1	Aa	464	A
1	Aa	465	U
1	Aa	484	A
1	Aa	485	U
1	Aa	486	C
1	Aa	487	U
1	Aa	488	U
1	Aa	492	G
1	Aa	499	A
1	Aa	503	A
1	Aa	504	G
1	Aa	505	A
1	Aa	506	A
1	Aa	507	A
1	Aa	513	G
1	Aa	514	G
1	Aa	516	U
1	Aa	517	A
1	Aa	519	C
1	Aa	522	C
1	Aa	526	C
1	Aa	529	G
1	Aa	532	G
1	Aa	535	G
1	Aa	539	U
1	Aa	541	A
1	Aa	542	U
1	Aa	543	A
1	Aa	548	G
1	Aa	554	A
1	Aa	555	A
1	Aa	567	A
1	Aa	570	U
1	Aa	571	A
1	Aa	580	A
1	Aa	581	A
1	Aa	584	C
1	Aa	585	G

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Mol	Chain	Res	Type
1	Aa	596	G
1	Aa	603	A
1	Aa	610	A
1	Aa	619	C
1	Aa	628	C
1	Aa	638	G
1	Aa	639	G
1	Aa	640	G
1	Aa	641	U
1	Aa	642	C
1	Aa	647	G
1	Aa	649	A
1	Aa	650	A
1	Aa	657	A
1	Aa	661	U
1	Aa	666	G
1	Aa	670	A
1	Aa	673	A
1	Aa	674	G
1	Aa	695	A
1	Aa	696	G
1	Aa	702	A
1	Aa	703	A
1	Aa	711	G
1	Aa	712	A
1	Aa	724	A
1	Aa	729	A
1	Aa	731	U
1	Aa	739	G
1	Aa	756	A
1	Aa	763	G
1	Aa	772	C
1	Aa	781	G
1	Aa	798	A
1	Aa	801	U
1	Aa	813	C
1	Aa	818	C
1	Aa	823	A
1	Aa	825	C
1	Aa	826	G
1	Aa	827	A
1	Aa	829	G

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Mol	Chain	Res	Type
1	Aa	835	U
1	Aa	836	A
1	Aa	840	G
1	Aa	847	G
1	Aa	850	U
1	Aa	852	C
1	Aa	853	C
1	Aa	854	G
1	Aa	881	A
1	Aa	894	G
1	Aa	898	A
1	Aa	910	A
1	Aa	911	G
1	Aa	923	A
1	Aa	924	A
1	Aa	935	G
1	Aa	943	C
1	Aa	944	A
1	Aa	949	C
1	Aa	950	G
1	Aa	953	G
1	Aa	954	G
1	Aa	955	A
1	Aa	956	G
1	Aa	958	A
1	Aa	959	U
1	Aa	961	U
1	Aa	969	U
1	Aa	970	U
1	Aa	972	G
1	Aa	973	A
1	Aa	974	A
1	Aa	975	G
1	Aa	977	A
1	Aa	978	A
1	Aa	980	G
1	Aa	983	A
1	Aa	984	A
1	Aa	985	G
1	Aa	986	A
1	Aa	991	U
1	Aa	1001	U

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Mol	Chain	Res	Type
1	Aa	1002	G
1	Aa	1003	A
1	Aa	1007	C
1	Aa	1008	C
1	Aa	1011	U
1	Aa	1012	G
1	Aa	1013	A
1	Aa	1015	A
1	Aa	1016	A
1	Aa	1017	C
1	Aa	1022	G
1	Aa	1023	A
1	Aa	1026	U
1	Aa	1032	C
1	Aa	1033	U
1	Aa	1035	C
1	Aa	1036	C
1	Aa	1038	C
1	Aa	1039	U
1	Aa	1041	C
1	Aa	1042	G
1	Aa	1043	G
1	Aa	1047	A
1	Aa	1048	C
1	Aa	1052	G
1	Aa	1055	A
1	Aa	1056	C
1	Aa	1057	A
1	Aa	1064	G
1	Aa	1065	C
1	Aa	1066	A
1	Aa	1076	U
1	Aa	1077	C
1	Aa	1091	A
1	Aa	1092	G
1	Aa	1094	U
1	Aa	1096	U
1	Aa	1101	U
1	Aa	1105	G
1	Aa	1106	U
1	Aa	1109	C
1	Aa	1112	A

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Mol	Chain	Res	Type
1	Aa	1113	A
1	Aa	1115	G
1	Aa	1119	G
1	Aa	1123	C
1	Aa	1130	G
1	Aa	1135	G
1	Aa	1136	U
1	Aa	1137	U
1	Aa	1138	G
1	Aa	1141	A
1	Aa	1142	U
1	Aa	1143	C
1	Aa	1146	U
1	Aa	1148	A
1	Aa	1149	G
1	Aa	1150	U
1	Aa	1151	U
1	Aa	1154	G
1	Aa	1156	A
1	Aa	1157	C
1	Aa	1165	U
1	Aa	1167	A
1	Aa	1168	C
1	Aa	1169	U
1	Aa	1172	C
1	Aa	1173	G
1	Aa	1174	G
1	Aa	1175	U
1	Aa	1177	A
1	Aa	1178	C
1	Aa	1179	A
1	Aa	1181	A
1	Aa	1187	G
1	Aa	1188	G
1	Aa	1189	A
1	Aa	1190	A
1	Aa	1191	G
1	Aa	1194	G
1	Aa	1202	C
1	Aa	1203	G
1	Aa	1206	A
1	Aa	1207	A

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Mol	Chain	Res	Type
1	Aa	1208	A
1	Aa	1209	U
1	Aa	1210	C
1	Aa	1211	A
1	Aa	1216	G
1	Aa	1222	U
1	Aa	1224	U
1	Aa	1225	G
1	Aa	1226	A
1	Aa	1228	U
1	Aa	1230	G
1	Aa	1234	U
1	Aa	1235	A
1	Aa	1236	C
1	Aa	1238	C
1	Aa	1243	G
1	Aa	1246	A
1	Aa	1248	A
1	Aa	1250	U
1	Aa	1251	G
1	Aa	1256	A
1	Aa	1260	A
1	Aa	1266	C
1	Aa	1267	A
1	Aa	1268	G
1	Aa	1270	G
1	Aa	1274	C
1	Aa	1275	C
1	Aa	1280	G
1	Aa	1281	G
1	Aa	1282	U
1	Aa	1283	C
1	Aa	1286	G
1	Aa	1287	C
1	Aa	1288	A
1	Aa	1289	A
1	Aa	1290	A
1	Aa	1291	U
1	Aa	1292	C
1	Aa	1296	U
1	Aa	1297	A
1	Aa	1300	G

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Mol	Chain	Res	Type
1	Aa	1305	U
1	Aa	1307	U
1	Aa	1308	C
1	Aa	1309	A
1	Aa	1310	G
1	Aa	1311	U
1	Aa	1312	U
1	Aa	1313	C
1	Aa	1314	G
1	Aa	1315	G
1	Aa	1319	G
1	Aa	1320	U
1	Aa	1322	G
1	Aa	1327	C
1	Aa	1329	A
1	Aa	1332	C
1	Aa	1333	G
1	Aa	1335	C
1	Aa	1336	U
1	Aa	1337	A
1	Aa	1338	C
1	Aa	1339	A
1	Aa	1341	G
1	Aa	1345	C
1	Aa	1347	G
1	Aa	1348	G
1	Aa	1356	A
1	Aa	1357	G
1	Aa	1361	U
1	Aa	1363	G
1	Aa	1368	U
1	Aa	1371	G
1	Aa	1373	A
1	Aa	1378	A
1	Aa	1380	G
1	Aa	1387	A
1	Aa	1391	U
1	Aa	1392	C
1	Aa	1393	C
1	Aa	1404	A
1	Aa	1408	A
1	Aa	1419	C

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Mol	Chain	Res	Type
1	Aa	1421	C
1	Aa	1428	A
1	Aa	1429	G
1	Aa	1438	A
1	Aa	1448	G
1	Aa	1451	G
1	Aa	1456	A
1	Aa	1461	U
1	Aa	1462	U
1	Aa	1463	U
1	Aa	1464	A
1	Aa	1466	G
1	Aa	1468	G
1	Aa	1476	U
1	Aa	1483	U
1	Aa	1495	U
1	Aa	1505	G
1	Aa	1508	G
1	Aa	1510	A
1	Aa	1514	A
1	Aa	1515	G
1	Aa	1540	G
1	Aa	1541	G
1	Aa	1543	U
23	AA	11	U
23	AA	15	G
23	AA	27	G
23	AA	28	A
23	AA	34	U
23	AA	36	G
23	AA	43	A
23	AA	51	G
23	AA	52	A
23	AA	53	A
23	AA	55	G
23	AA	63	U
23	AA	70	G
23	AA	71	A
23	AA	74	U
23	AA	75	G
23	AA	83	G
23	AA	84	A

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Mol	Chain	Res	Type
23	AA	90	A
23	AA	92	G
23	AA	93	U
23	AA	96	G
23	AA	101	G
23	AA	102	A
23	AA	104	C
23	AA	117	A
23	AA	119	U
23	AA	124	A
23	AA	141	U
23	AA	148	U
23	AA	149	U
23	AA	152	C
23	AA	156	A
23	AA	157	U
23	AA	158	G
23	AA	161	A
23	AA	164	A
23	AA	167	U
23	AA	168	A
23	AA	170	C
23	AA	172	U
23	AA	173	A
23	AA	177	G
23	AA	178	A
23	AA	180	G
23	AA	184	C
23	AA	185	A
23	AA	199	A
23	AA	202	A
23	AA	213	C
23	AA	215	G
23	AA	216	A
23	AA	218	G
23	AA	219	A
23	AA	224	A
23	AA	225	A
23	AA	233	U
23	AA	246	U
23	AA	251	G
23	AA	255	G

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Mol	Chain	Res	Type
23	AA	268	A
23	AA	269	G
23	AA	270	C
23	AA	279	A
23	AA	280	C
23	AA	285	U
23	AA	286	U
23	AA	287	G
23	AA	292	U
23	AA	293	U
23	AA	298	U
23	AA	299	U
23	AA	300	G
23	AA	301	U
23	AA	302	A
23	AA	307	A
23	AA	309	U
23	AA	310	C
23	AA	311	U
23	AA	312	A
23	AA	316	G
23	AA	320	U
23	AA	321	U
23	AA	327	G
23	AA	328	G
23	AA	333	C
23	AA	335	U
23	AA	345	C
23	AA	353	A
23	AA	365	A
23	AA	366	G
23	AA	373	A
23	AA	388	A
23	AA	389	A
23	AA	392	U
23	AA	394	U
23	AA	397	U
23	AA	402	C
23	AA	404	U
23	AA	406	A
23	AA	410	G
23	AA	411	A

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Mol	Chain	Res	Type
23	AA	417	A
23	AA	432	G
23	AA	435	A
23	AA	444	C
23	AA	447	A
23	AA	449	U
23	AA	451	U
23	AA	452	G
23	AA	458	A
23	AA	460	C
23	AA	481	C
23	AA	482	U
23	AA	486	G
23	AA	490	C
23	AA	492	G
23	AA	493	A
23	AA	501	C
23	AA	502	C
23	AA	503	A
23	AA	504	G
23	AA	506	A
23	AA	512	A
23	AA	513	G
23	AA	518	A
23	AA	523	A
23	AA	527	G
23	AA	535	G
23	AA	538	G
23	AA	539	G
23	AA	550	A
23	AA	553	A
23	AA	554	C
23	AA	557	G
23	AA	558	A
23	AA	559	A
23	AA	563	G
23	AA	566	U
23	AA	572	C
23	AA	574	A
23	AA	576	U
23	AA	577	A
23	AA	578	G

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Mol	Chain	Res	Type
23	AA	580	C
23	AA	591	A
23	AA	592	A
23	AA	594	G
23	AA	606	G
23	AA	611	U
23	AA	616	G
23	AA	617	A
23	AA	618	A
23	AA	639	U
23	AA	644	C
23	AA	645	A
23	AA	646	A
23	AA	647	G
23	AA	659	A
23	AA	672	A
23	AA	679	G
23	AA	682	A
23	AA	689	A
23	AA	690	U
23	AA	698	U
23	AA	699	U
23	AA	702	U
23	AA	713	A
23	AA	715	A
23	AA	720	A
23	AA	722	A
23	AA	730	A
23	AA	731	U
23	AA	735	C
23	AA	750	A
23	AA	754	U
23	AA	755	C
23	AA	759	U
23	AA	760	A
23	AA	761	A
23	AA	762	C
23	AA	763	A
23	AA	765	U
23	AA	766	G
23	AA	768	A
23	AA	771	G

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Mol	Chain	Res	Type
23	AA	775	A
23	AA	792	U
23	AA	793	G
23	AA	797	A
23	AA	802	G
23	AA	809	A
23	AA	810	A
23	AA	816	G
23	AA	820	G
23	AA	822	G
23	AA	827	A
23	AA	829	U
23	AA	830	U
23	AA	834	A
23	AA	835	U
23	AA	836	C
23	AA	837	G
23	AA	840	C
23	AA	841	C
23	AA	842	U
23	AA	850	G
23	AA	856	U
23	AA	857	C
23	AA	868	A
23	AA	870	C
23	AA	872	U
23	AA	891	A
23	AA	892	U
23	AA	904	G
23	AA	911	A
23	AA	914	G
23	AA	918	G
23	AA	920	A
23	AA	926	G
23	AA	928	C
23	AA	940	U
23	AA	943	C
23	AA	949	C
23	AA	952	A
23	AA	955	A
23	AA	957	C
23	AA	960	C

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Mol	Chain	Res	Type
23	AA	964	U
23	AA	968	A
23	AA	969	A
23	AA	970	U
23	AA	971	U
23	AA	972	A
23	AA	973	A
23	AA	975	U
23	AA	977	A
23	AA	985	A
23	AA	986	G
23	AA	988	C
23	AA	989	A
23	AA	990	G
23	AA	992	A
23	AA	997	G
23	AA	1003	A
23	AA	1005	G
23	AA	1012	G
23	AA	1018	A
23	AA	1019	A
23	AA	1024	A
23	AA	1025	A
23	AA	1027	A
23	AA	1034	A
23	AA	1040	A
23	AA	1043	U
23	AA	1047	G
23	AA	1049	C
23	AA	1056	U
23	AA	1057	A
23	AA	1066	G
23	AA	1067	U
23	AA	1069	G
23	AA	1070	A
23	AA	1076	A
23	AA	1077	U
23	AA	1078	G
23	AA	1086	G
23	AA	1087	C
23	AA	1088	C
23	AA	1089	C

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Mol	Chain	Res	Type
23	AA	1091	G
23	AA	1092	A
23	AA	1093	C
23	AA	1094	A
23	AA	1095	A
23	AA	1100	G
23	AA	1102	U
23	AA	1105	U
23	AA	1106	G
23	AA	1109	U
23	AA	1111	A
23	AA	1113	A
23	AA	1114	A
23	AA	1115	G
23	AA	1116	C
23	AA	1117	A
23	AA	1118	G
23	AA	1119	C
23	AA	1120	C
23	AA	1122	U
23	AA	1126	U
23	AA	1127	U
23	AA	1128	A
23	AA	1132	A
23	AA	1133	G
23	AA	1137	G
23	AA	1138	U
23	AA	1139	A
23	AA	1140	A
23	AA	1143	G
23	AA	1145	U
23	AA	1148	C
23	AA	1150	A
23	AA	1151	G
23	AA	1155	A
23	AA	1156	G
23	AA	1158	G
23	AA	1160	C
23	AA	1161	A
23	AA	1162	C
23	AA	1163	U
23	AA	1174	U

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Mol	Chain	Res	Type
23	AA	1176	U
23	AA	1178	C
23	AA	1179	C
23	AA	1186	A
23	AA	1200	A
23	AA	1201	G
23	AA	1208	A
23	AA	1214	C
23	AA	1215	U
23	AA	1216	U
23	AA	1217	U
23	AA	1218	G
23	AA	1225	G
23	AA	1245	G
23	AA	1250	G
23	AA	1258	A
23	AA	1265	G
23	AA	1267	A
23	AA	1274	G
23	AA	1275	A
23	AA	1276	G
23	AA	1284	A
23	AA	1285	A
23	AA	1286	G
23	AA	1290	G
23	AA	1291	A
23	AA	1294	G
23	AA	1298	G
23	AA	1300	G
23	AA	1304	G
23	AA	1309	G
23	AA	1310	A
23	AA	1320	G
23	AA	1326	C
23	AA	1337	A
23	AA	1338	U
23	AA	1339	U
23	AA	1340	G
23	AA	1342	C
23	AA	1344	A
23	AA	1348	U
23	AA	1349	U

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Mol	Chain	Res	Type
23	AA	1351	C
23	AA	1354	G
23	AA	1358	A
23	AA	1367	C
23	AA	1370	C
23	AA	1386	U
23	AA	1387	C
23	AA	1389	U
23	AA	1392	G
23	AA	1394	U
23	AA	1402	A
23	AA	1405	G
23	AA	1415	A
23	AA	1416	U
23	AA	1417	G
23	AA	1420	U
23	AA	1422	A
23	AA	1423	C
23	AA	1432	A
23	AA	1440	A
23	AA	1443	A
23	AA	1445	C
23	AA	1447	A
23	AA	1450	A
23	AA	1451	U
23	AA	1453	G
23	AA	1454	U
23	AA	1455	U
23	AA	1457	U
23	AA	1459	A
23	AA	1463	A
23	AA	1464	U
23	AA	1471	A
23	AA	1472	C
23	AA	1481	A
23	AA	1489	A
23	AA	1490	G
23	AA	1491	C
23	AA	1494	G
23	AA	1495	C
23	AA	1496	G
23	AA	1497	A

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Mol	Chain	Res	Type
23	AA	1498	U
23	AA	1499	U
23	AA	1503	U
23	AA	1504	U
23	AA	1510	U
23	AA	1516	C
23	AA	1518	G
23	AA	1519	U
23	AA	1520	A
23	AA	1521	A
23	AA	1525	U
23	AA	1526	G
23	AA	1527	A
23	AA	1532	U
23	AA	1533	A
23	AA	1534	G
23	AA	1536	C
23	AA	1537	A
23	AA	1540	U
23	AA	1550	G
23	AA	1551	U
23	AA	1552	U
23	AA	1553	A
23	AA	1554	A
23	AA	1555	G
23	AA	1556	G
23	AA	1559	G
23	AA	1561	G
23	AA	1569	G
23	AA	1570	G
23	AA	1575	A
23	AA	1576	A
23	AA	1578	A
23	AA	1579	C
23	AA	1580	A
23	AA	1581	U
23	AA	1582	U
23	AA	1583	G
23	AA	1584	U
23	AA	1586	U
23	AA	1587	C
23	AA	1591	G

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Mol	Chain	Res	Type
23	AA	1594	U
23	AA	1605	A
23	AA	1606	C
23	AA	1613	G
23	AA	1616	A
23	AA	1625	U
23	AA	1627	G
23	AA	1629	U
23	AA	1630	A
23	AA	1631	G
23	AA	1632	A
23	AA	1633	A
23	AA	1634	A
23	AA	1635	A
23	AA	1636	U
23	AA	1639	G
23	AA	1652	A
23	AA	1653	A
23	AA	1654	A
23	AA	1661	C
23	AA	1666	A
23	AA	1675	G
23	AA	1679	A
23	AA	1683	U
23	AA	1684	A
23	AA	1690	A
23	AA	1691	G
23	AA	1692	C
23	AA	1693	G
23	AA	1718	G
23	AA	1719	C
23	AA	1732	U
23	AA	1737	U
23	AA	1738	C
23	AA	1740	G
23	AA	1745	A
23	AA	1747	G
23	AA	1757	U
23	AA	1758	A
23	AA	1759	G
23	AA	1760	G
23	AA	1761	G

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Mol	Chain	Res	Type
23	AA	1762	U
23	AA	1765	A
23	AA	1768	C
23	AA	1771	A
23	AA	1772	G
23	AA	1790	G
23	AA	1791	G
23	AA	1797	G
23	AA	1800	A
23	AA	1806	U
23	AA	1808	U
23	AA	1809	C
23	AA	1811	A
23	AA	1813	A
23	AA	1814	A
23	AA	1818	A
23	AA	1826	G
23	AA	1827	C
23	AA	1828	U
23	AA	1829	A
23	AA	1830	A
23	AA	1835	U
23	AA	1843	U
23	AA	1846	A
23	AA	1856	A
23	AA	1860	C
23	AA	1878	U
23	AA	1879	U
23	AA	1880	A
23	AA	1885	G
23	AA	1889	G
23	AA	1895	C
23	AA	1897	U
23	AA	1898	C
23	AA	1899	U
23	AA	1900	G
23	AA	1901	C
23	AA	1902	G
23	AA	1903	A
23	AA	1904	A
23	AA	1907	U
23	AA	1909	C

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Mol	Chain	Res	Type
23	AA	1911	A
23	AA	1912	A
23	AA	1914	C
23	AA	1918	G
23	AA	1933	G
23	AA	1935	C
23	AA	1937	G
23	AA	1938	U
23	AA	1945	A
23	AA	1950	U
23	AA	1956	G
23	AA	1958	U
23	AA	1963	A
23	AA	1964	A
23	AA	1965	A
23	AA	1966	U
23	AA	1971	U
23	AA	1982	U
23	AA	1989	C
23	AA	1990	C
23	AA	1992	C
23	AA	1994	C
23	AA	1996	A
23	AA	1997	A
23	AA	1998	A
23	AA	1999	G
23	AA	2009	U
23	AA	2018	U
23	AA	2019	G
23	AA	2020	U
23	AA	2023	C
23	AA	2024	A
23	AA	2029	G
23	AA	2030	A
23	AA	2047	A
23	AA	2057	A
23	AA	2058	A
23	AA	2059	G
23	AA	2060	A
23	AA	2062	G
23	AA	2070	C
23	AA	2073	G

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Mol	Chain	Res	Type
23	AA	2075	G
23	AA	2076	A
23	AA	2082	C
23	AA	2083	G
23	AA	2085	A
23	AA	2087	A
23	AA	2088	G
23	AA	2089	A
23	AA	2096	G
23	AA	2097	G
23	AA	2103	U
23	AA	2107	G
23	AA	2109	A
23	AA	2110	G
23	AA	2111	C
23	AA	2115	A
23	AA	2117	A
23	AA	2118	U
23	AA	2119	U
23	AA	2120	G
23	AA	2126	C
23	AA	2129	C
23	AA	2139	A
23	AA	2140	C
23	AA	2143	G
23	AA	2145	U
23	AA	2147	G
23	AA	2153	A
23	AA	2155	C
23	AA	2157	U
23	AA	2158	U
23	AA	2160	G
23	AA	2161	A
23	AA	2164	C
23	AA	2172	C
23	AA	2173	U
23	AA	2174	A
23	AA	2175	G
23	AA	2176	C
23	AA	2183	G
23	AA	2185	A
23	AA	2186	G

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Mol	Chain	Res	Type
23	AA	2188	C
23	AA	2190	C
23	AA	2193	G
23	AA	2194	U
23	AA	2195	G
23	AA	2198	A
23	AA	2204	C
23	AA	2215	U
23	AA	2224	U
23	AA	2225	A
23	AA	2229	C
23	AA	2230	G
23	AA	2231	C
23	AA	2232	A
23	AA	2238	U
23	AA	2240	U
23	AA	2241	C
23	AA	2243	U
23	AA	2252	A
23	AA	2261	G
23	AA	2262	G
23	AA	2263	C
23	AA	2265	G
23	AA	2266	G
23	AA	2290	C
23	AA	2295	A
23	AA	2305	A
23	AA	2306	G
23	AA	2310	C
23	AA	2314	A
23	AA	2316	G
23	AA	2321	C
23	AA	2328	A
23	AA	2329	U
23	AA	2330	G
23	AA	2331	G
23	AA	2332	U
23	AA	2333	U
23	AA	2334	G
23	AA	2335	G
23	AA	2336	A
23	AA	2337	A

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Mol	Chain	Res	Type
23	AA	2345	A
23	AA	2346	U
23	AA	2347	A
23	AA	2352	G
23	AA	2353	U
23	AA	2358	G
23	AA	2361	U
23	AA	2362	A
23	AA	2370	U
23	AA	2374	C
23	AA	2377	C
23	AA	2385	A
23	AA	2388	A
23	AA	2396	A
23	AA	2409	G
23	AA	2410	G
23	AA	2411	A
23	AA	2412	C
23	AA	2429	U
23	AA	2433	C
23	AA	2434	A
23	AA	2441	G
23	AA	2449	C
23	AA	2450	U
23	AA	2451	C
23	AA	2455	G
23	AA	2456	G
23	AA	2457	A
23	AA	2458	U
23	AA	2459	A
23	AA	2460	A
23	AA	2461	A
23	AA	2462	A
23	AA	2463	G
23	AA	2468	C
23	AA	2472	G
23	AA	2474	G
23	AA	2475	A
23	AA	2485	U
23	AA	2486	A
23	AA	2503	A
23	AA	2511	G

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Mol	Chain	Res	Type
23	AA	2521	G
23	AA	2525	C
23	AA	2529	G
23	AA	2530	A
23	AA	2531	U
23	AA	2532	G
23	AA	2540	A
23	AA	2544	C
23	AA	2545	A
23	AA	2547	C
23	AA	2556	G
23	AA	2561	C
23	AA	2562	G
23	AA	2568	A
23	AA	2569	A
23	AA	2570	G
23	AA	2581	U
23	AA	2589	U
23	AA	2592	A
23	AA	2593	A
23	AA	2594	G
23	AA	2599	A
23	AA	2600	C
23	AA	2604	A
23	AA	2605	G
23	AA	2613	C
23	AA	2626	G
23	AA	2629	A
23	AA	2630	G
23	AA	2636	U
23	AA	2640	U
23	AA	2642	U
23	AA	2646	U
23	AA	2648	G
23	AA	2650	G
23	AA	2656	A
23	AA	2657	G
23	AA	2672	G
23	AA	2679	U
23	AA	2681	A
23	AA	2687	A
23	AA	2692	A

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Mol	Chain	Res	Type
23	AA	2695	G
23	AA	2696	G
23	AA	2697	G
23	AA	2699	U
23	AA	2700	G
23	AA	2712	G
23	AA	2716	U
23	AA	2741	G
23	AA	2745	G
23	AA	2750	C
23	AA	2753	U
23	AA	2756	G
23	AA	2757	U
23	AA	2759	G
23	AA	2760	A
23	AA	2761	C
23	AA	2764	G
23	AA	2769	G
23	AA	2771	G
23	AA	2775	A
23	AA	2778	G
23	AA	2784	A
23	AA	2788	A
23	AA	2793	G
23	AA	2794	C
23	AA	2796	C
23	AA	2798	C
23	AA	2800	U
23	AA	2801	C
23	AA	2803	A
23	AA	2804	G
23	AA	2805	A
23	AA	2806	U
23	AA	2808	A
23	AA	2817	A
23	AA	2820	U
23	AA	2821	U
23	AA	2822	C
23	AA	2823	G
23	AA	2824	G
23	AA	2827	A
23	AA	2828	U

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Mol	Chain	Res	Type
23	AA	2829	A
23	AA	2831	G
23	AA	2832	A
23	AA	2838	C
23	AA	2840	A
23	AA	2843	A
23	AA	2850	G
23	AA	2853	U
23	AA	2854	A
23	AA	2855	A
23	AA	2879	G
23	AA	2887	G
23	AA	2888	A
23	AA	2892	G
23	AA	2899	A
23	AA	2900	C
23	AA	2903	A
23	AA	2913	G
23	AA	2914	A
23	AA	2919	A
24	AB	10	U
24	AB	22	G
24	AB	23	U
24	AB	24	C
24	AB	33	U
24	AB	39	G
24	AB	40	C
24	AB	43	A
24	AB	51	A
24	AB	55	A
24	AB	64	A
24	AB	87	C
24	AB	88	G
24	AB	106	G
24	AB	111	C
24	AB	113	G

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	AA	99	U
23	AA	160	G

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Mol	Chain	Res	Type
23	AA	267	G
23	AA	268	A
23	AA	291	G
23	AA	451	U
23	AA	487	U
23	AA	513	G
23	AA	576	U
23	AA	577	A
23	AA	688	A
23	AA	697	U
23	AA	711	G
23	AA	840	C
23	AA	987	U
23	AA	1024	A
23	AA	1075	G
23	AA	1190	A
23	AA	1267	A
23	AA	1372	C
23	AA	1385	G
23	AA	1731	G
23	AA	1845	U
23	AA	2117	A
23	AA	2450	U
23	AA	2568	A
23	AA	2749	G
23	AA	2783	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 205 ligands modelled in this entry, 205 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	AA	6
24	AB	1
1	Aa	1
13	Am	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	2207:U	O3'	2208:A	P	9.06
1	AA	2132:A	O3'	2133:G	P	8.44
1	AA	1096:C	O3'	1097:U	P	6.77
1	Aa	465:U	O3'	466:G	P	3.97
1	AA	1153:C	O3'	1154:G	P	3.61
1	AA	1448:U	O3'	1449:A	P	3.51
1	AB	114:G	O3'	115:C	P	3.40
1	AA	2217:G	O3'	2218:G	P	3.39
1	Am	93:ARG	C	94:GLY	N	3.26