



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 6, 2016 – 01:36 AM EST

PDB ID : 5MGP
EMDB ID: : EMD-3508
Title : Structural basis for ArfA-RF2 mediated translation termination on stop-codon lacking mRNAs
Authors : Huter, P.; Mueller, C.; Beckert, B.; Arenz, S.; Berninghausen, O.; Beckmann, R.; Wilson, N.D.
Deposited on : 2016-11-21
Resolution : 3.10 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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

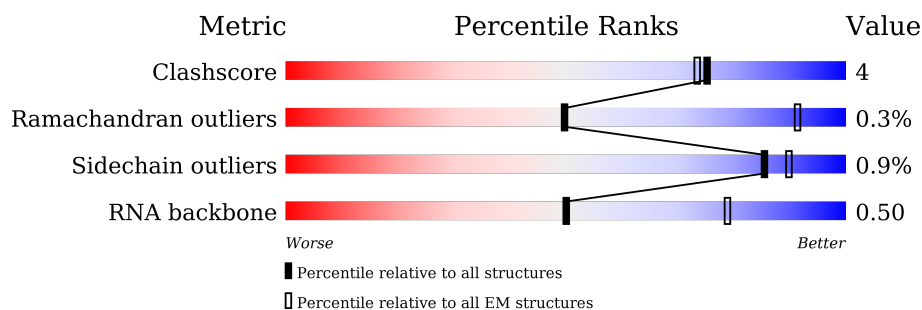
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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





















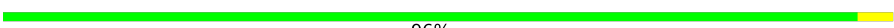






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	A	2903	
2	B	120	
3	C	271	
4	D	209	
5	E	201	
6	F	177	
7	G	176	
8	H	149	

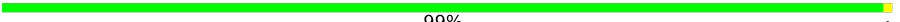
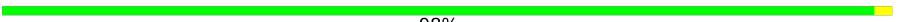
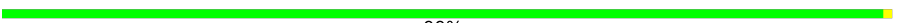












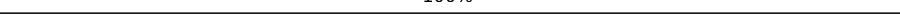
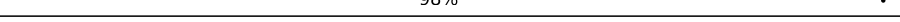
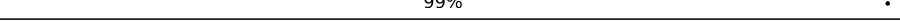
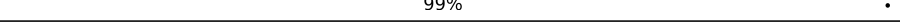
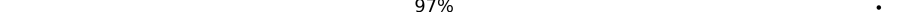
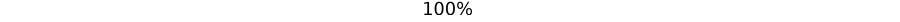


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	J	142	 86% 14%
10	K	122	 86% 14%
11	L	143	 78% 20% .
12	M	136	 82% 16% .
13	N	120	 82% 18% .
14	O	116	 82% 18%
15	P	114	 79% 20% .
16	Q	117	 84% 16%
17	R	103	 88% 12%
18	S	110	 84% 16%
19	T	93	 90% 10%
20	U	102	 90% 10%
21	V	94	 88% 12%
22	W	75	 93% 7%
23	X	77	 88% 12%
24	Y	63	 94% 6%
25	Z	58	 93% 7%
26	0	56	 91% 9%
27	1	50	 96% .
28	2	46	 89% 11%
29	3	64	 73% 25% .
30	4	38	 76% 24%
31	6	66	 91% 9%
32	a	1539	 80% 19% .
33	b	218	 98% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	c	206	 99% .
35	d	205	 98% .
36	e	157	 99% .
37	f	100	 94% 6% .
38	g	151	 99% .
39	h	129	 97% .
40	i	127	 96% .
41	j	98	 98% .
42	k	116	 98% .
43	l	123	 98% .
44	m	114	 98% ..
45	n	101	 99% .
46	o	88	 98% .
47	p	82	 100% .
48	q	80	 100% .
49	r	65	 98% .
50	s	79	 99% .
51	t	85	 99% .
52	u	65	 97% .
53	v	6	 100% .
54	w	45	 80% 18% .
55	x	77	 78% 21% .
56	z	359	 97% .

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 147155 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2900	Total	C	N	O	P	0	0
			62261	27774	11460	20127	2900		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	C	U	conflict	GB 802133627
A	1847	G	A	conflict	GB 802133627
A	2069	A	G	conflict	GB 802133627

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1028480521

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	50	Total	C	N	O	S	0	0
			409	263	75	71			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1539	Total	C	N	O	P	0	0
			33016	14725	6052	10700	1539		

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 45 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 52 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	6	Total	C	N	O	P	0	0
			126	56	22	42	6		

- Molecule 54 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	45	Total	C	N	O	S	0	0
			369	229	76	63	1		

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	x	77	Total	C	N	O	P	0	0
			1646	733	295	541	77		

- Molecule 56 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	359	Total	C	N	O	S	0	0
			2846	1749	500	587	10		

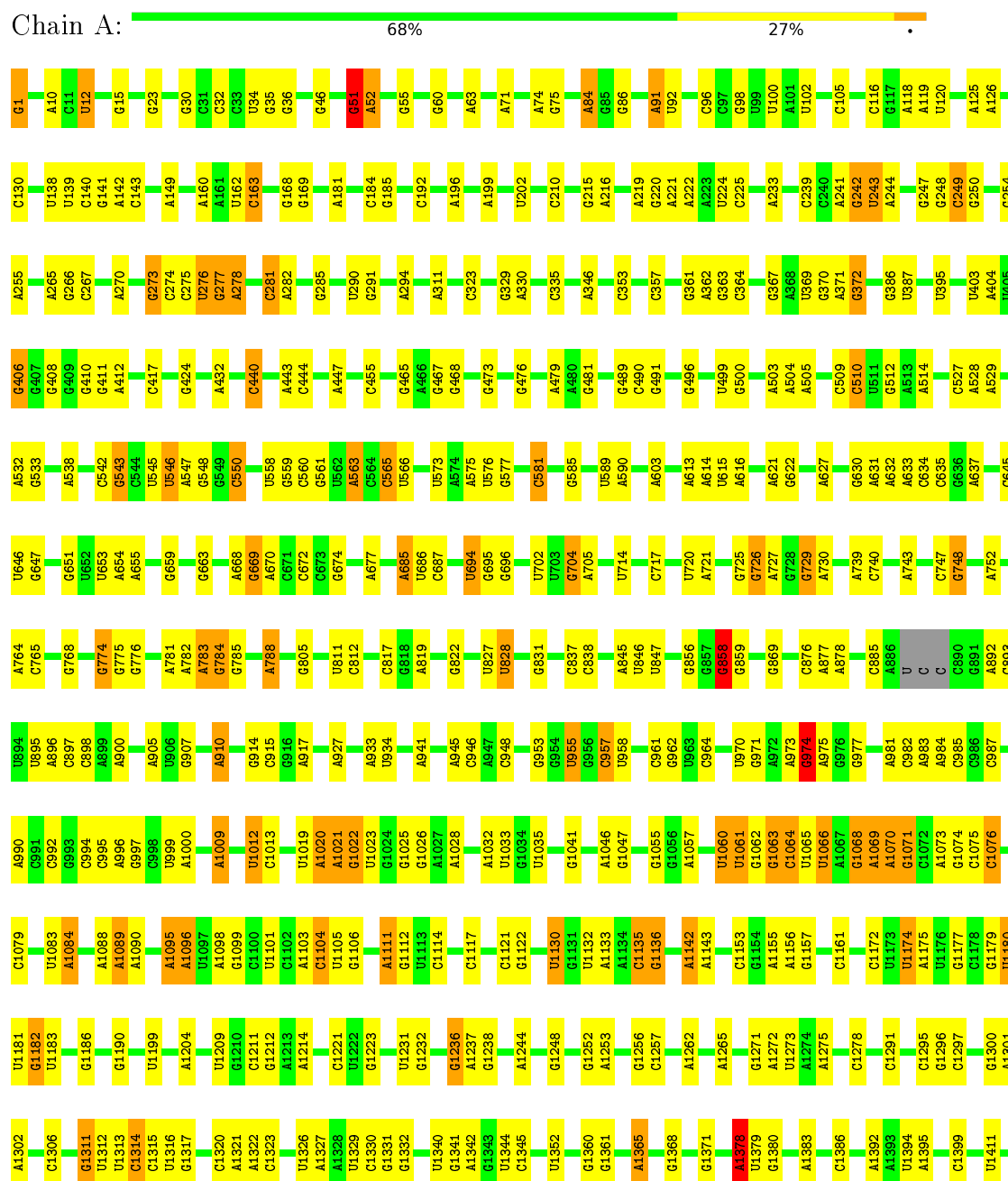
There is a discrepancy between the modelled and reference sequences:

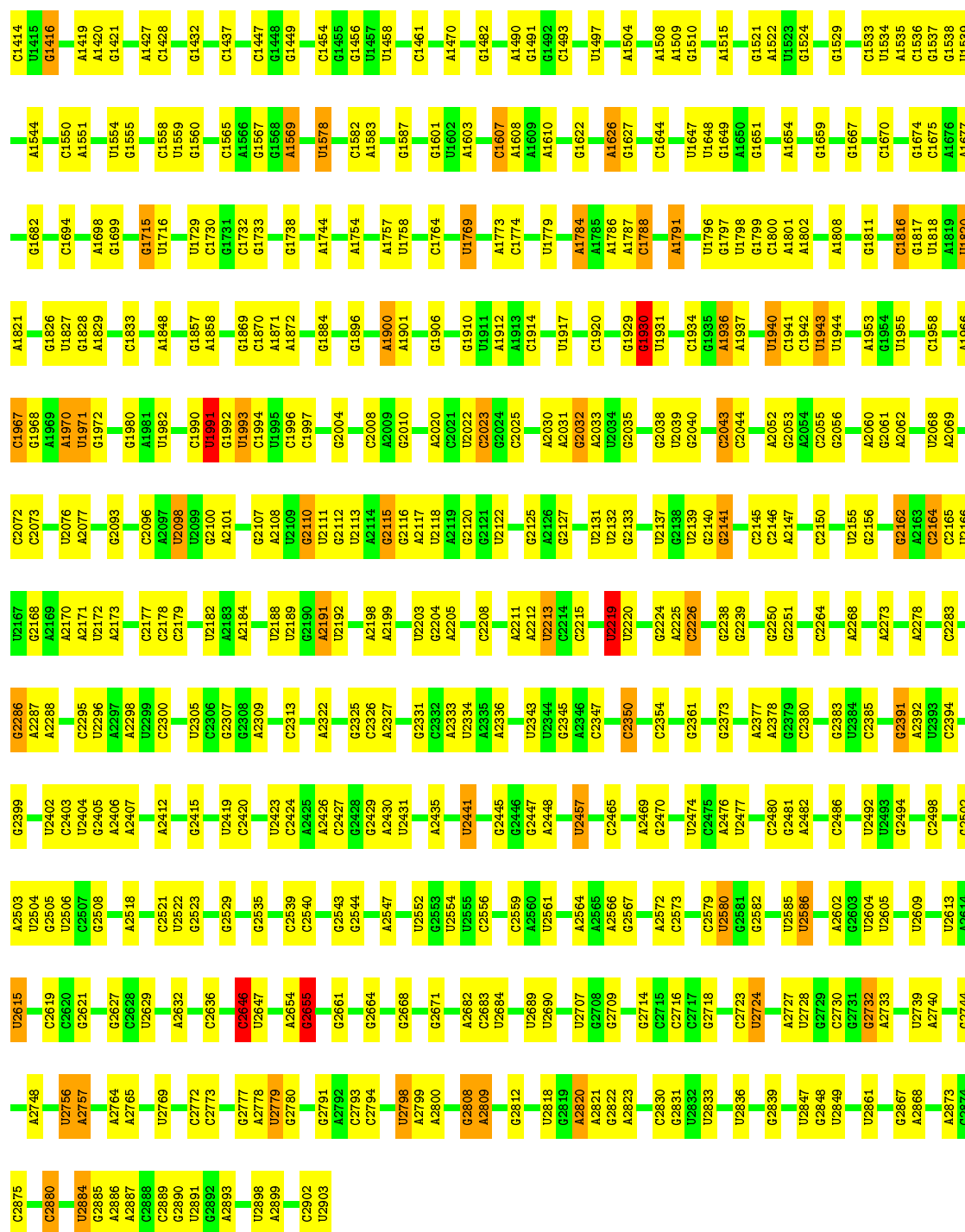
Chain	Residue	Modelled	Actual	Comment	Reference
z	251	ALA	GLY	conflict	UNP P07012

3 Residue-property plots

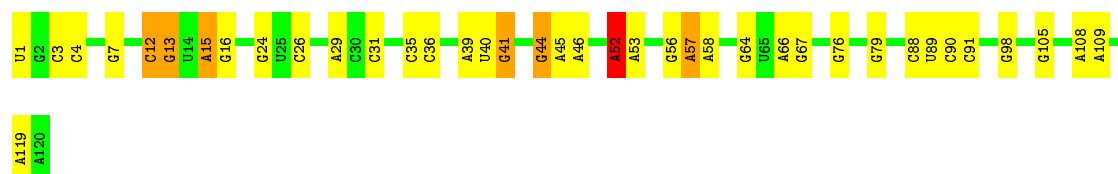
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

• Molecule 1: 23S ribosomal RNA

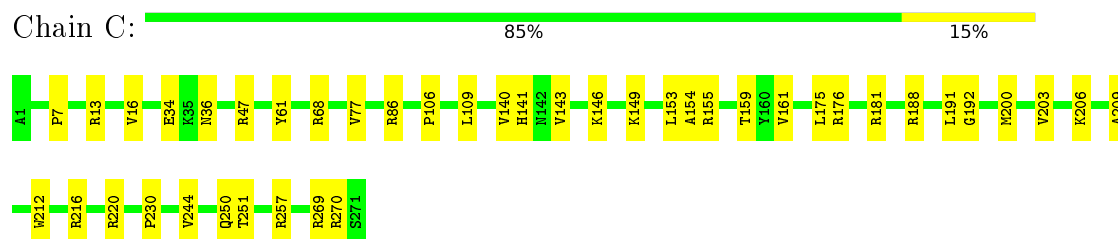




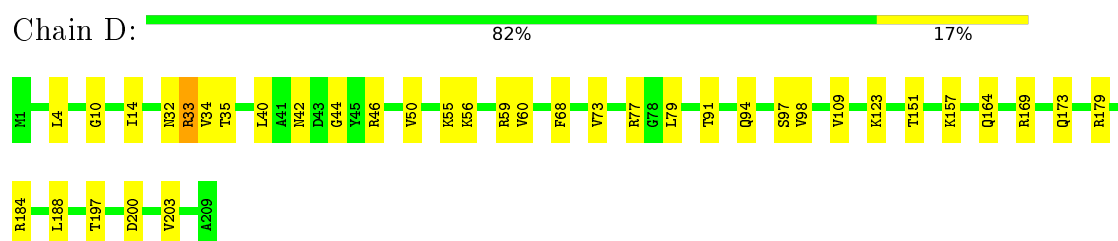
Chain B: 68% 27% 5% •



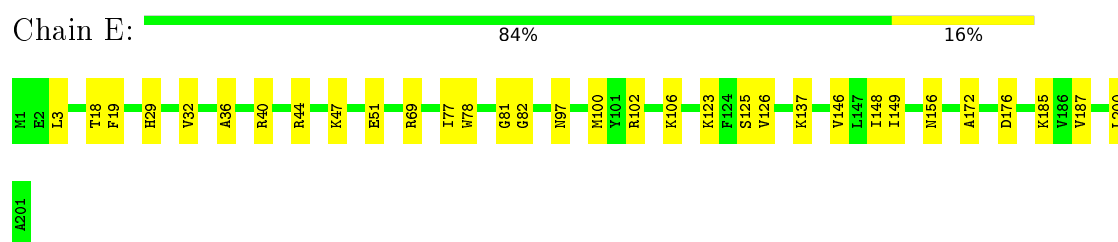
- Molecule 3: 50S ribosomal protein L2



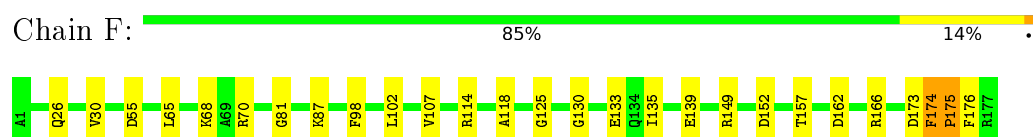
- Molecule 4: 50S ribosomal protein L3



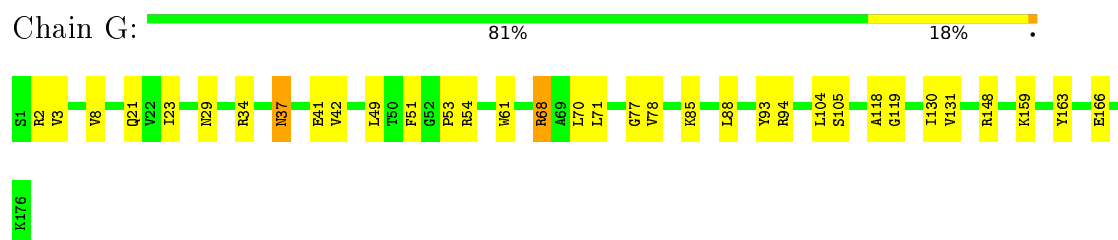
- Molecule 5: 50S ribosomal protein L4



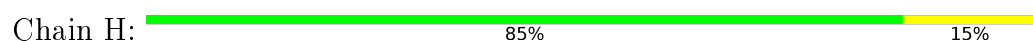
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9





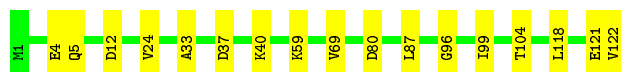
- Molecule 9: 50S ribosomal protein L13

Chain J: 86% 14%



- Molecule 10: 50S ribosomal protein L14

Chain K: 86% 14%



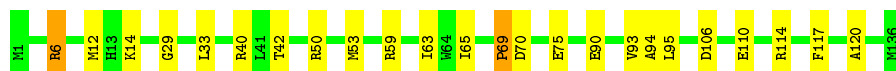
- Molecule 11: 50S ribosomal protein L15

Chain L: 78% 20% .



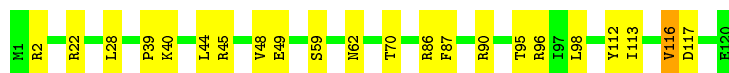
- Molecule 12: 50S ribosomal protein L16

Chain M: 82% 16% .



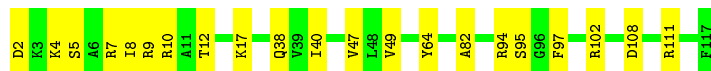
- Molecule 13: 50S ribosomal protein L17

Chain N: 82% 18% .



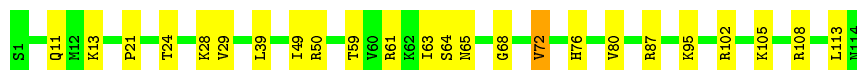
- Molecule 14: 50S ribosomal protein L18

Chain O: 82% 18%




- Molecule 15: 50S ribosomal protein L19

Chain P: 79% 20% .



- Molecule 16: 50S ribosomal protein L20

Chain Q:  84% 16%




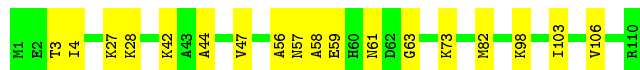
- Molecule 17: 50S ribosomal protein L21

Chain R:  88% 12%



- Molecule 18: 50S ribosomal protein L22

Chain S:  84% 16%



- Molecule 19: 50S ribosomal protein L23

Chain T:  90% 10%



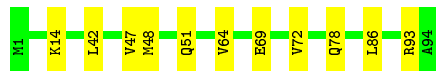
- Molecule 20: 50S ribosomal protein L24

Chain U:  90% 10%



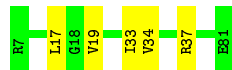
- Molecule 21: 50S ribosomal protein L25

Chain V:  88% 12%




- Molecule 22: 50S ribosomal protein L27

Chain W:  93% 7%



- Molecule 23: 50S ribosomal protein L28

Chain X:  88% 12%



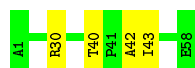
- Molecule 24: 50S ribosomal protein L29

Chain Y:  94% 6%



- Molecule 25: 50S ribosomal protein L30

Chain Z:  93% 7%



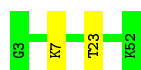
- Molecule 26: 50S ribosomal protein L32

Chain 0:  91% 9%




- Molecule 27: 50S ribosomal protein L33

Chain 1:  96% 4%



- Molecule 28: 50S ribosomal protein L34

Chain 2:  89% 11%




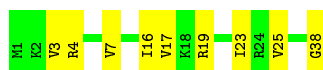
- Molecule 29: 50S ribosomal protein L35

Chain 3:  73% 25% 2%



- Molecule 30: 50S ribosomal protein L36

Chain 4:  76% 24%



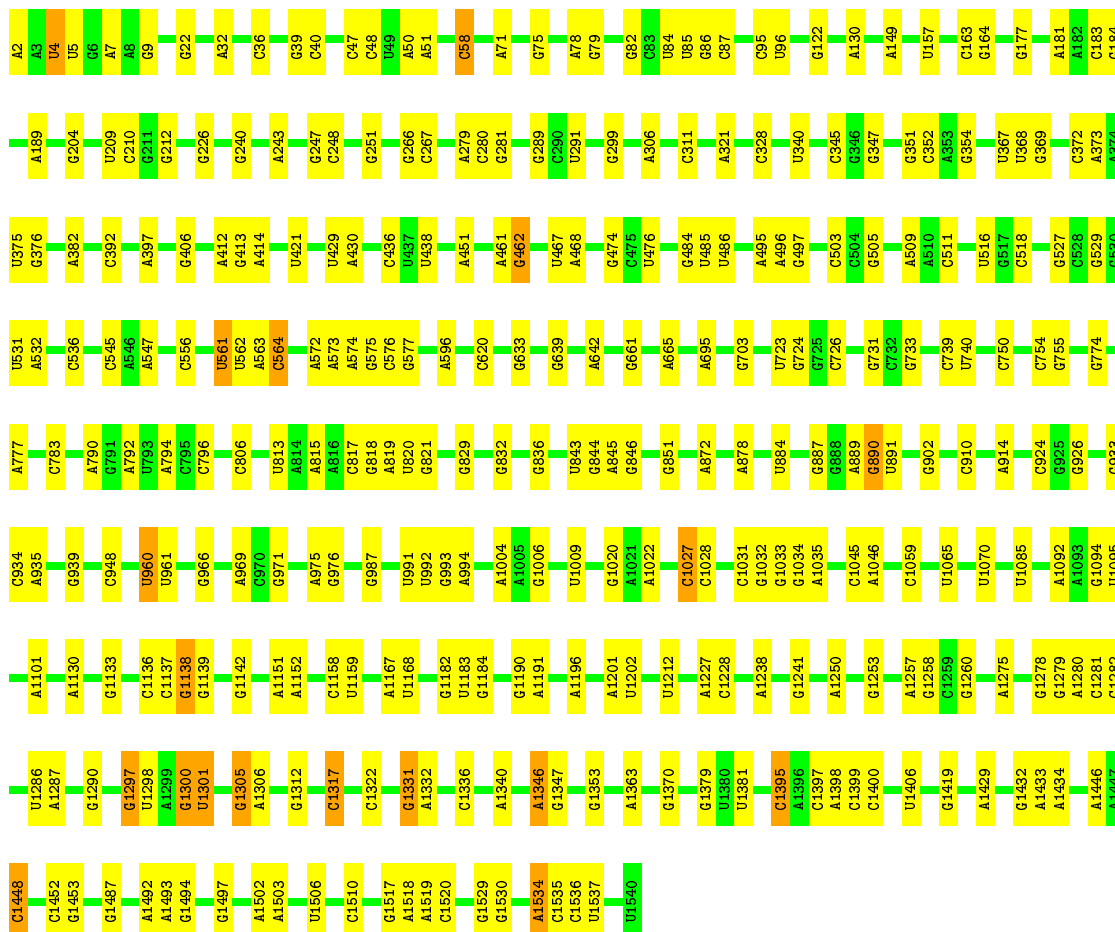
- Molecule 31: 50S ribosomal protein L31

Chain 6: 91% 9%



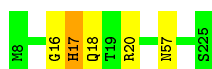
- Molecule 32: 16S ribosomal RNA

Chain a: 80% 19%



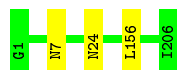
- Molecule 33: 30S ribosomal protein S2

Chain b: 98%



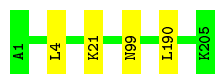
- Molecule 34: 30S ribosomal protein S3

Chain c:  99%



- Molecule 35: 30S ribosomal protein S4

Chain d:  98%



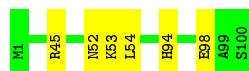
- Molecule 36: 30S ribosomal protein S5

Chain e:  99%



- Molecule 37: 30S ribosomal protein S6

Chain f:  94% 6%



- Molecule 38: 30S ribosomal protein S7

Chain g:  99%



- Molecule 39: 30S ribosomal protein S8

Chain h:  97%



- Molecule 40: 30S ribosomal protein S9

Chain i:  96%



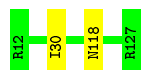
- Molecule 41: 30S ribosomal protein S10

Chain j:  98%



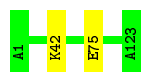
- Molecule 42: 30S ribosomal protein S11

Chain k:  98% .



- Molecule 43: 30S ribosomal protein S12

Chain l:  98% .



- Molecule 44: 30S ribosomal protein S13

Chain m:  98% ..



- Molecule 45: 30S ribosomal protein S14

Chain n:  99% .



- Molecule 46: 30S ribosomal protein S15

Chain o:  98% .



- Molecule 47: 30S ribosomal protein S16

Chain p:  100%

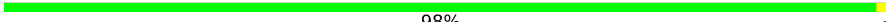
There are no outlier residues recorded for this chain.

- Molecule 48: 30S ribosomal protein S17

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 49: 30S ribosomal protein S18

Chain r:  98% .



- Molecule 50: 30S ribosomal protein S19

Chain s:  99% .



- Molecule 51: 30S ribosomal protein S20

Chain t:  99% .



- Molecule 52: 30S ribosomal protein S21

Chain u:  97% .




- Molecule 53: mRNA

Chain v:  100% .


There are no outlier residues recorded for this chain.

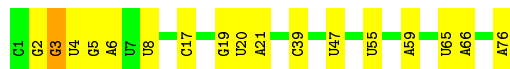
- Molecule 54: Alternative ribosome-rescue factor A

Chain w:  80% 18% .



- Molecule 55: P-site tRNA

Chain x:  78% 21% .



- Molecule 56: Peptide chain release factor 2

Chain z:  97% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	69089	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	302	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	0.75	3/69733 (0.0%)	1.02	184/108786 (0.2%)
10	K	0.41	0/947	0.62	0/1268
11	L	0.37	0/1054	0.67	0/1403
12	M	0.42	0/1093	0.63	2/1460 (0.1%)
13	N	0.39	0/973	0.62	0/1301
14	O	0.38	0/902	0.56	0/1209
15	P	0.41	0/929	0.59	1/1242 (0.1%)
16	Q	0.47	0/960	0.55	0/1278
17	R	0.41	0/829	0.60	0/1107
18	S	0.37	0/864	0.60	0/1156
19	T	0.34	0/744	0.53	0/994
2	B	0.66	1/2876 (0.0%)	1.04	9/4483 (0.2%)
20	U	0.34	0/787	0.57	1/1051 (0.1%)
21	V	0.36	0/766	0.55	0/1025
22	W	0.42	0/582	0.52	0/769
23	X	0.43	0/635	0.54	0/848
24	Y	0.28	0/510	0.54	0/677
25	Z	0.34	0/453	0.57	0/605
26	0	0.41	0/450	0.58	0/599
27	1	0.34	0/416	0.54	0/554
28	2	0.41	0/380	0.54	0/498
29	3	0.39	0/513	0.61	1/676 (0.1%)
3	C	0.44	0/2121	0.62	0/2852
30	4	0.42	0/303	0.54	0/397
31	6	0.31	0/531	0.59	0/709
32	a	0.72	1/36967 (0.0%)	0.99	82/57666 (0.1%)
33	b	0.33	0/1735	0.60	1/2338 (0.0%)
34	c	0.35	0/1651	0.57	1/2225 (0.0%)
35	d	0.36	0/1665	0.63	2/2227 (0.1%)
36	e	0.42	0/1154	0.65	0/1554
37	f	0.36	0/835	0.70	2/1128 (0.2%)
38	g	0.31	0/1195	0.54	0/1602
39	h	0.39	0/989	0.65	1/1326 (0.1%)
4	D	0.43	0/1586	0.58	0/2134

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
40	i	0.35	0/1034	0.62	0/1375
41	j	0.36	0/796	0.62	0/1077
42	k	0.37	0/885	0.57	0/1195
43	l	0.47	0/969	0.66	0/1300
44	m	0.35	0/892	0.65	0/1193
45	n	0.35	0/811	0.59	0/1081
46	o	0.32	0/722	0.60	0/964
47	p	0.40	0/659	0.59	0/884
48	q	0.36	0/657	0.61	0/881
49	r	0.40	0/511	0.58	0/689
5	E	0.38	0/1571	0.57	1/2113 (0.0%)
50	s	0.35	0/652	0.60	0/877
51	t	0.32	0/671	0.53	0/888
52	u	0.35	0/500	0.72	0/668
53	v	0.59	0/139	1.09	0/214
54	w	0.44	0/375	0.80	1/494 (0.2%)
55	x	0.51	0/1839	1.01	7/2866 (0.2%)
56	z	0.35	0/2886	0.56	0/3887
6	F	0.36	0/1434	0.61	0/1926
7	G	0.33	0/1343	0.56	0/1816
8	H	0.31	0/1122	0.55	0/1515
9	J	0.41	0/1152	0.55	0/1551
All	All	0.65	5/159748 (0.0%)	0.92	296/238601 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	M	0	1
13	N	0	1
18	S	0	1
29	3	0	1
33	b	0	1
35	d	0	1
37	f	0	3
40	i	0	2
43	l	0	2
44	m	0	2
49	r	0	1
5	E	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
52	u	0	1
54	w	0	1
56	z	0	2
6	F	0	1
7	G	0	1
9	J	0	1
All	All	0	24

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	G	OP3-P	-10.84	1.48	1.61
2	B	1	U	OP3-P	-10.63	1.48	1.61
32	a	2	A	OP3-P	-10.52	1.48	1.61
1	A	1142	A	N9-C4	-5.20	1.34	1.37
1	A	528	A	N9-C4	-5.09	1.34	1.37

All (296) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	4	U	N1-C2-O2	11.35	130.74	122.80
32	a	4	U	C2-N1-C1'	10.66	130.49	117.70
32	a	4	U	N3-C2-O2	-10.23	115.04	122.20
1	A	2580	U	N3-C2-O2	-9.91	115.26	122.20
1	A	1914	C	C6-N1-C2	-9.63	116.45	120.30
1	A	1914	C	N3-C2-O2	-9.56	115.21	121.90
1	A	1313	U	C2-N1-C1'	9.41	128.99	117.70
1	A	1914	C	N1-C2-O2	9.36	124.51	118.90
32	a	1158	C	N1-C2-O2	9.31	124.48	118.90
1	A	2580	U	N1-C2-O2	9.00	129.10	122.80
2	B	12	C	C2-N1-C1'	8.90	128.60	118.80
1	A	1313	U	N1-C2-O2	8.87	129.01	122.80
1	A	12	U	N1-C2-O2	8.63	128.84	122.80
2	B	12	C	N1-C2-O2	8.62	124.07	118.90
1	A	2604	U	C2-N1-C1'	8.60	128.02	117.70
32	a	1158	C	C2-N1-C1'	8.50	128.15	118.80
1	A	1917	U	N3-C2-O2	-8.40	116.32	122.20
1	A	12	U	N3-C2-O2	-8.40	116.32	122.20
1	A	955	U	N3-C2-O2	-8.38	116.34	122.20
1	A	12	U	C2-N1-C1'	8.24	127.59	117.70
1	A	2504	U	N3-C2-O2	-8.17	116.48	122.20
1	A	1914	C	C2-N1-C1'	8.16	127.78	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1313	U	N3-C2-O2	-8.14	116.50	122.20
37	f	54	LEU	CA-CB-CG	8.13	134.00	115.30
32	a	1301	U	C2-N1-C1'	7.99	127.28	117.70
1	A	2604	U	N3-C2-O2	-7.92	116.66	122.20
1	A	2884	U	N1-C2-O2	7.87	128.31	122.80
1	A	2605	U	C2-N1-C1'	7.81	127.07	117.70
1	A	1917	U	C2-N1-C1'	7.75	127.00	117.70
1	A	2884	U	N3-C2-O2	-7.63	116.86	122.20
1	A	2162	G	C4-N9-C1'	7.61	136.40	126.50
1	A	2580	U	C2-N1-C1'	7.61	126.83	117.70
1	A	2457	U	N3-C2-O2	-7.51	116.94	122.20
1	A	2504	U	N1-C2-O2	7.49	128.04	122.80
34	c	156	LEU	CA-CB-CG	7.47	132.49	115.30
32	a	1301	U	N1-C2-O2	7.43	128.00	122.80
32	a	516	U	C2-N1-C1'	7.37	126.54	117.70
1	A	2457	U	C2-N1-C1'	7.34	126.51	117.70
1	A	2605	U	N3-C2-O2	-7.27	117.11	122.20
1	A	512	G	O4'-C1'-N9	7.25	114.00	108.20
1	A	2504	U	C2-N1-C1'	7.25	126.40	117.70
1	A	2457	U	N1-C2-O2	7.22	127.85	122.80
1	A	783	A	C8-N9-C4	-7.20	102.92	105.80
32	a	516	U	N3-C2-O2	-7.15	117.19	122.20
32	a	1138	G	N3-C4-C5	-7.13	125.03	128.60
32	a	792	A	O4'-C1'-N9	7.10	113.88	108.20
1	A	974	G	C4-N9-C1'	7.05	135.67	126.50
32	a	754	C	C2-N1-C1'	7.02	126.53	118.80
1	A	1917	U	N1-C2-O2	7.00	127.70	122.80
1	A	1378	A	P-O3'-C3'	6.97	128.06	119.70
32	a	4	U	C6-N1-C1'	-6.97	111.44	121.20
1	A	2043	C	C5-C6-N1	6.95	124.47	121.00
2	B	12	C	N3-C2-O2	-6.93	117.05	121.90
1	A	955	U	C2-N1-C1'	6.89	125.96	117.70
1	A	2162	G	N3-C4-C5	-6.88	125.16	128.60
2	B	12	C	C6-N1-C1'	-6.85	112.58	120.80
2	B	44	G	P-O3'-C3'	6.84	127.91	119.70
32	a	1158	C	N3-C2-O2	-6.81	117.13	121.90
1	A	2884	U	C2-N1-C1'	6.79	125.85	117.70
1	A	1930	G	P-O3'-C3'	6.78	127.84	119.70
1	A	581	C	C6-N1-C2	-6.77	117.59	120.30
32	a	1138	G	N3-C4-N9	6.76	130.06	126.00
1	A	2646	C	C6-N1-C2	-6.74	117.61	120.30
1	A	783	A	N7-C8-N9	6.73	117.16	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	1138	G	C4-N9-C1'	6.72	135.24	126.50
1	A	1920	C	C6-N1-C2	-6.72	117.61	120.30
1	A	1236	G	P-O3'-C3'	6.71	127.76	119.70
32	a	960	U	P-O3'-C3'	6.71	127.75	119.70
32	a	1518	A	O4'-C1'-N9	6.70	113.56	108.20
1	A	1020	A	P-O3'-C3'	6.69	127.73	119.70
1	A	1022	G	P-O3'-C3'	6.68	127.72	119.70
32	a	1305	G	P-O3'-C3'	6.67	127.70	119.70
1	A	1940	U	P-O3'-C3'	6.65	127.68	119.70
1	A	669	G	C4-N9-C1'	6.62	135.10	126.50
32	a	1297	G	P-O3'-C3'	6.59	127.60	119.70
1	A	2162	G	N3-C4-N9	6.58	129.95	126.00
1	A	2579	C	C6-N1-C2	-6.58	117.67	120.30
32	a	813	U	N1-C2-O2	6.54	127.38	122.80
1	A	955	U	N1-C2-O2	6.54	127.38	122.80
32	a	311	C	C6-N1-C2	-6.46	117.71	120.30
32	a	1300	G	P-O3'-C3'	6.46	127.45	119.70
1	A	2162	G	C8-N9-C1'	-6.46	118.61	127.00
55	x	55	U	N3-C2-O2	-6.44	117.69	122.20
1	A	748	G	O4'-C1'-N9	6.44	113.35	108.20
1	A	91	A	P-O3'-C3'	6.44	127.43	119.70
1	A	858	G	P-O3'-C3'	6.43	127.41	119.70
55	x	3	G	P-O3'-C3'	6.42	127.40	119.70
32	a	556	C	C6-N1-C2	-6.39	117.75	120.30
1	A	1626	A	P-O3'-C3'	6.38	127.36	119.70
1	A	1313	U	C6-N1-C1'	-6.38	112.27	121.20
1	A	687	C	N1-C2-O2	6.37	122.72	118.90
32	a	890	G	P-O3'-C3'	6.35	127.31	119.70
1	A	2044	C	C6-N1-C2	-6.34	117.76	120.30
32	a	1432	G	P-O3'-C3'	6.34	127.31	119.70
1	A	242	G	P-O3'-C3'	6.33	127.29	119.70
32	a	1301	U	N3-C2-O2	-6.32	117.78	122.20
32	a	436	C	N1-C2-O2	6.31	122.69	118.90
32	a	1027	C	C6-N1-C2	-6.31	117.78	120.30
32	a	529	G	C5-C6-O6	-6.28	124.83	128.60
54	w	22	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	542	C	N1-C2-O2	6.28	122.67	118.90
1	A	1111	A	P-O3'-C3'	6.27	127.23	119.70
2	B	52	A	P-O3'-C3'	6.25	127.20	119.70
32	a	58	C	C6-N1-C2	-6.25	117.80	120.30
1	A	635	C	C6-N1-C2	-6.23	117.81	120.30
2	B	12	C	O4'-C1'-N1	6.22	113.18	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	1158	C	C6-N1-C1'	-6.22	113.33	120.80
32	a	813	U	N3-C2-O2	-6.20	117.86	122.20
1	A	143	C	N1-C2-O2	6.18	122.61	118.90
1	A	2820	A	OP1-P-O3'	6.16	118.75	105.20
1	A	2798	U	P-O3'-C3'	6.15	127.08	119.70
32	a	1027	C	C5-C6-N1	6.15	124.07	121.00
1	A	2808	G	P-O3'-C3'	6.14	127.07	119.70
35	d	4	LEU	CA-CB-CG	6.13	129.41	115.30
1	A	915	C	C6-N1-C2	-6.11	117.86	120.30
32	a	545	C	N3-C2-O2	-6.08	117.64	121.90
32	a	1182	G	P-O3'-C3'	6.07	126.99	119.70
1	A	2072	C	C5-C6-N1	6.07	124.03	121.00
32	a	924	C	C6-N1-C2	-6.07	117.87	120.30
1	A	1076	C	N1-C2-O2	6.05	122.53	118.90
32	a	545	C	C6-N1-C2	-6.02	117.89	120.30
32	a	754	C	N1-C2-O2	6.02	122.51	118.90
1	A	2723	C	C6-N1-C2	-6.02	117.89	120.30
1	A	992	C	C6-N1-C2	-6.01	117.90	120.30
1	A	669	G	C8-N9-C1'	-6.00	119.20	127.00
55	x	2	G	P-O3'-C3'	5.98	126.88	119.70
32	a	1331	G	P-O3'-C3'	5.98	126.88	119.70
15	P	113	LEU	CA-CB-CG	5.96	129.02	115.30
1	A	2739	U	N3-C2-O2	-5.96	118.03	122.20
55	x	55	U	N1-C2-O2	5.96	126.97	122.80
1	A	1378	A	OP1-P-O3'	5.94	118.28	105.20
1	A	1788	C	C6-N1-C2	-5.91	117.94	120.30
1	A	2604	U	N1-C2-O2	5.91	126.94	122.80
1	A	1161	C	C6-N1-C2	-5.90	117.94	120.30
1	A	417	C	N1-C2-O2	5.89	122.44	118.90
32	a	1190	G	P-O3'-C3'	5.89	126.77	119.70
1	A	163	C	N1-C2-O2	5.89	122.43	118.90
1	A	51	G	P-O3'-C3'	5.88	126.76	119.70
1	A	2072	C	C6-N1-C2	-5.88	117.95	120.30
1	A	974	G	C8-N9-C1'	-5.88	119.36	127.00
1	A	2646	C	C5-C6-N1	5.85	123.93	121.00
1	A	2480	C	C6-N1-C2	-5.84	117.96	120.30
55	x	55	U	C2-N1-C1'	5.82	124.69	117.70
1	A	784	G	P-O3'-C3'	5.82	126.68	119.70
32	a	4	U	C5-C6-N1	5.81	125.61	122.70
1	A	783	A	C5-N7-C8	-5.80	101.00	103.90
32	a	1520	C	N1-C2-O2	5.79	122.38	118.90
1	A	130	C	C6-N1-C2	-5.77	117.99	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	U	C5-C6-N1	5.77	125.58	122.70
1	A	1221	C	C6-N1-C2	-5.77	117.99	120.30
1	A	1291	C	C6-N1-C2	-5.74	118.00	120.30
1	A	565	C	C6-N1-C2	-5.72	118.01	120.30
1	A	2646	C	N1-C2-O2	5.71	122.33	118.90
32	a	1399	C	P-O3'-C3'	5.70	126.54	119.70
1	A	1295	C	C6-N1-C2	-5.70	118.02	120.30
1	A	817	C	C6-N1-C2	-5.70	118.02	120.30
32	a	516	U	N1-C2-O2	5.70	126.79	122.80
1	A	1626	A	OP2-P-O3'	5.69	117.72	105.20
1	A	2604	U	C6-N1-C1'	-5.69	113.24	121.20
1	A	2605	U	N1-C2-O2	5.69	126.78	122.80
1	A	1967	C	N1-C2-O2	5.69	122.31	118.90
32	a	1301	U	C6-N1-C1'	-5.66	113.27	121.20
1	A	2008	C	C6-N1-C2	-5.66	118.03	120.30
32	a	1346	A	O4'-C1'-N9	5.66	112.73	108.20
1	A	974	G	C4-C5-N7	5.66	113.06	110.80
1	A	2354	C	C6-N1-C2	-5.66	118.04	120.30
1	A	1920	C	C5-C6-N1	5.65	123.83	121.00
1	A	2043	C	C6-N1-C2	-5.65	118.04	120.30
1	A	974	G	C6-C5-N7	-5.65	127.01	130.40
32	a	1448	C	N1-C2-O2	5.64	122.29	118.90
32	a	564	C	N1-C2-O2	5.64	122.28	118.90
1	A	2023	C	N1-C2-O2	5.62	122.28	118.90
32	a	503	C	C6-N1-C2	-5.62	118.05	120.30
1	A	546	U	C2-N1-C1'	5.61	124.43	117.70
32	a	878	A	O5'-P-OP1	-5.59	100.67	105.70
32	a	1346	A	C4-N9-C1'	5.59	136.37	126.30
32	a	1138	G	C8-N9-C1'	-5.58	119.75	127.00
1	A	143	C	C6-N1-C2	-5.57	118.07	120.30
1	A	1675	C	N1-C2-O2	5.56	122.23	118.90
1	A	1076	C	C6-N1-C2	-5.56	118.08	120.30
1	A	2739	U	N1-C2-O2	5.54	126.67	122.80
12	M	70	ASP	CB-CG-OD1	5.54	123.28	118.30
55	x	39	C	C6-N1-C2	-5.53	118.09	120.30
2	B	3	C	P-O3'-C3'	5.52	126.32	119.70
1	A	974	G	O4'-C1'-N9	5.52	112.61	108.20
32	a	545	C	N1-C2-O2	5.51	122.21	118.90
1	A	974	G	N7-C8-N9	5.51	115.85	113.10
1	A	1774	C	C6-N1-C2	-5.51	118.10	120.30
1	A	2073	C	N1-C2-O2	5.48	122.19	118.90
1	A	1578	U	N1-C2-O2	5.46	126.62	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	C	N3-C2-O2	-5.44	118.09	121.90
1	A	2098	U	N1-C2-O2	5.44	126.61	122.80
55	x	3	G	OP1-P-O3'	5.44	117.16	105.20
2	B	3	C	OP1-P-O3'	5.43	117.15	105.20
32	a	960	U	N1-C2-O2	5.43	126.60	122.80
1	A	192	C	C6-N1-C2	-5.42	118.13	120.30
1	A	581	C	C5-C6-N1	5.42	123.71	121.00
1	A	1991	U	N1-C2-O2	5.41	126.58	122.80
1	A	2076	U	C2-N1-C1'	5.41	124.19	117.70
32	a	739	C	C6-N1-C2	-5.41	118.14	120.30
35	d	190	LEU	CA-CB-CG	5.38	127.69	115.30
32	a	561	U	P-O3'-C3'	5.37	126.15	119.70
32	a	36	C	C5-C6-N1	5.37	123.68	121.00
1	A	440	C	C6-N1-C2	-5.36	118.16	120.30
1	A	353	C	N1-C2-O2	5.34	122.11	118.90
33	b	16	GLY	N-CA-C	5.34	126.46	113.10
1	A	202	U	N3-C2-O2	-5.34	118.46	122.20
29	3	61	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	1914	C	C5-C6-N1	5.32	123.66	121.00
32	a	1534	A	P-O3'-C3'	5.31	126.07	119.70
1	A	2043	C	N1-C2-O2	5.31	122.08	118.90
32	a	796	C	N1-C2-O2	5.31	122.08	118.90
1	A	546	U	N1-C2-O2	5.30	126.51	122.80
1	A	2457	U	C6-N1-C1'	-5.30	113.78	121.20
1	A	2730	C	C6-N1-C2	-5.30	118.18	120.30
1	A	12	U	C6-N1-C2	-5.30	117.82	121.00
1	A	2076	U	N3-C2-O2	-5.29	118.49	122.20
1	A	1314	C	N1-C2-O2	5.29	122.08	118.90
1	A	702	U	N1-C2-O2	5.29	126.50	122.80
1	A	1675	C	N3-C2-O2	-5.29	118.20	121.90
12	M	6	ARG	CA-CB-CG	5.29	125.03	113.40
1	A	2219	U	N1-C2-O2	5.28	126.50	122.80
1	A	1670	C	C6-N1-C2	-5.27	118.19	120.30
32	a	462	G	C4-N9-C1'	5.27	133.36	126.50
37	f	54	LEU	CB-CG-CD1	-5.27	102.03	111.00
32	a	1059	C	C6-N1-C2	-5.26	118.20	120.30
1	A	1174	U	C5-C6-N1	5.25	125.33	122.70
1	A	1278	C	C6-N1-C2	-5.25	118.20	120.30
1	A	702	U	N3-C2-O2	-5.25	118.53	122.20
1	A	2286	G	P-O3'-C3'	5.24	125.98	119.70
1	A	1135	C	N1-C2-O2	5.23	122.04	118.90
32	a	1317	C	N1-C2-O2	5.23	122.04	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1644	C	C6-N1-C2	-5.23	118.21	120.30
1	A	1021	A	C2-N3-C4	5.23	113.21	110.60
1	A	837	C	C5-C6-N1	5.23	123.61	121.00
1	A	1180	U	N1-C2-O2	5.22	126.46	122.80
1	A	1103	A	OP1-P-O3'	5.22	116.67	105.20
1	A	51	G	OP2-P-O3'	5.21	116.67	105.20
32	a	1518	A	N7-C8-N9	5.21	116.41	113.80
1	A	974	G	N3-C4-N9	5.20	129.12	126.00
32	a	96	U	N1-C2-O2	5.20	126.44	122.80
1	A	2552	U	C2-N1-C1'	5.19	123.93	117.70
1	A	2655	G	O4'-C1'-N9	5.19	112.35	108.20
1	A	1930	G	O4'-C1'-N9	5.18	112.35	108.20
1	A	510	C	N1-C2-O2	5.18	122.01	118.90
1	A	2604	U	O4'-C1'-N1	5.17	112.34	108.20
1	A	163	C	C2-N1-C1'	5.17	124.48	118.80
32	a	740	U	N3-C2-O2	-5.17	118.58	122.20
20	U	51	LEU	CA-CB-CG	5.17	127.18	115.30
32	a	1138	G	C2-N3-C4	5.14	114.47	111.90
1	A	1533	C	N1-C2-O2	5.13	121.98	118.90
1	A	729	G	C4-N9-C1'	5.13	133.17	126.50
32	a	563	A	C4-N9-C1'	5.12	135.52	126.30
1	A	1848	A	N7-C8-N9	5.11	116.36	113.80
1	A	2875	C	C6-N1-C2	-5.09	118.26	120.30
5	E	81	GLY	N-CA-C	-5.09	100.36	113.10
1	A	143	C	C2-N1-C1'	5.09	124.40	118.80
1	A	837	C	C6-N1-C2	-5.09	118.26	120.30
32	a	495	A	P-O3'-C3'	5.08	125.80	119.70
39	h	58	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	1183	U	N3-C2-O2	-5.07	118.65	122.20
32	a	536	C	C6-N1-C2	-5.07	118.27	120.30
32	a	783	C	C6-N1-C2	-5.07	118.27	120.30
1	A	105	C	C6-N1-C2	-5.07	118.27	120.30
1	A	1121	C	C6-N1-C2	-5.07	118.27	120.30
1	A	1330	C	N1-C2-O2	5.07	121.94	118.90
32	a	1395	C	N1-C2-O2	5.07	121.94	118.90
1	A	2504	U	C6-N1-C2	-5.07	117.96	121.00
1	A	2605	U	O4'-C1'-N1	5.07	112.25	108.20
1	A	2769	U	N3-C2-O2	-5.07	118.65	122.20
32	a	754	C	C6-N1-C1'	-5.06	114.72	120.80
32	a	750	C	C6-N1-C2	-5.05	118.28	120.30
1	A	1076	C	N3-C2-O2	-5.05	118.36	121.90
1	A	1990	C	C6-N1-C2	-5.05	118.28	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	910	C	C6-N1-C2	-5.05	118.28	120.30
1	A	1993	U	N1-C2-O2	5.05	126.33	122.80
1	A	417	C	N3-C2-O2	-5.04	118.37	121.90
32	a	1510	C	C6-N1-C2	-5.04	118.28	120.30
1	A	542	C	N3-C2-O2	-5.04	118.37	121.90
1	A	687	C	N3-C2-O2	-5.03	118.38	121.90
1	A	1508	A	O4'-C1'-N9	5.03	112.23	108.20
32	a	36	C	C6-N1-C2	-5.03	118.29	120.30
1	A	1295	C	N3-C2-O2	-5.03	118.38	121.90
1	A	1414	C	C6-N1-C2	-5.03	118.29	120.30
1	A	1940	U	OP2-P-O3'	5.02	116.25	105.20
1	A	915	C	C5-C6-N1	5.02	123.51	121.00
32	a	291	U	N3-C2-O2	-5.02	118.68	122.20
32	a	564	C	N3-C2-O2	-5.02	118.39	121.90
32	a	726	C	C6-N1-C2	-5.02	118.29	120.30
1	A	970	U	C5-C6-N1	5.01	125.21	122.70
32	a	40	C	C6-N1-C2	-5.01	118.30	120.30
1	A	542	C	C6-N1-C2	-5.01	118.30	120.30
1	A	1117	C	N1-C2-O2	5.01	121.90	118.90
32	a	1520	C	C2-N1-C1'	5.01	124.31	118.80
1	A	2636	C	N1-C2-O2	5.00	121.90	118.90
1	A	1994	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	3	30	HIS	Peptide
5	E	82	GLY	Peptide
6	F	173	ASP	Peptide
7	G	118	ALA	Peptide
9	J	81	ILE	Peptide
12	M	59	ARG	Peptide
13	N	116	VAL	Peptide
18	S	63	GLY	Peptide
33	b	17	HIS	Peptide
35	d	21	LYS	Peptide
37	f	52	ASN	Peptide
37	f	94	HIS	Peptide
37	f	98	GLU	Peptide
40	i	124	PRO	Peptide
40	i	56	MET	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
43	l	42	LYS	Peptide
43	l	75	GLU	Peptide
44	m	3	ILE	Peptide
44	m	4	ALA	Mainchain
49	r	18	GLN	Peptide
52	u	8	ASN	Peptide
54	w	44	LYS	Peptide
56	z	119	PHE	Peptide
56	z	311	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62261	0	31314	231	0
2	B	2572	0	1302	11	0
3	C	2082	0	2157	27	0
4	D	1565	0	1616	23	0
5	E	1552	0	1619	20	0
6	F	1410	0	1447	17	0
7	G	1323	0	1374	18	0
8	H	1111	0	1148	13	0
9	J	1129	0	1162	12	0
10	K	938	0	1012	10	0
11	L	1045	0	1117	21	0
12	M	1074	0	1157	14	0
13	N	960	0	1000	13	0
14	O	892	0	923	16	0
15	P	917	0	965	14	0
16	Q	947	0	1022	19	0
17	R	816	0	839	8	0
18	S	857	0	922	11	0
19	T	738	0	807	6	0
20	U	779	0	834	5	0
21	V	753	0	780	8	0
22	W	575	0	592	4	0
23	X	625	0	655	7	0
24	Y	509	0	543	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Z	449	0	491	2	0
26	0	444	0	461	3	0
27	1	409	0	440	2	0
28	2	377	0	418	4	0
29	3	504	0	574	13	0
30	4	302	0	343	6	0
31	6	522	0	522	4	0
32	a	33016	0	16617	0	0
33	b	1704	0	1732	0	0
34	c	1624	0	1699	0	0
35	d	1643	0	1710	0	0
36	e	1141	0	1170	0	0
37	f	817	0	808	0	0
38	g	1181	0	1240	0	0
39	h	979	0	1034	0	0
40	i	1022	0	1070	0	0
41	j	786	0	828	0	0
42	k	869	0	878	0	0
43	l	955	0	1019	0	0
44	m	883	0	944	0	0
45	n	799	0	841	0	0
46	o	714	0	737	0	0
47	p	649	0	666	0	0
48	q	648	0	691	0	0
49	r	504	0	502	0	0
50	s	637	0	665	0	0
51	t	665	0	714	0	0
52	u	495	0	486	0	0
53	v	126	0	67	0	0
54	w	369	0	381	0	0
55	x	1646	0	832	0	0
56	z	2846	0	2744	0	0
All	All	147155	0	99631	465	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 4.

All (465) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2101:A:H61	1:A:2188:U:H3	1.42	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:8:VAL:HB	7:G:49:LEU:HB2	1.79	0.65
1:A:2683:C:OP1	15:P:50:ARG:NH2	2.31	0.64
1:A:2110:G:N2	1:A:2179:C:N3	2.46	0.64
18:S:27:LYS:HG2	18:S:28:LYS:HG2	8.95	0.63
1:A:1858:A:N6	1:A:1884:G:O2'	2.30	0.63
1:A:585:G:N7	16:Q:5:ARG:NH1	2.46	0.63
1:A:2523:G:HO2'	1:A:2764:A:HO2'	1.43	0.62
17:R:34:GLU:HG2	17:R:60:LYS:HG2	1.81	0.62
9:J:35:ARG:HB2	9:J:54:ILE:HD11	1.81	0.62
22:W:17:LEU:HD21	22:W:37:ARG:HH21	1.65	0.62
1:A:254:G:N7	29:3:4:LYS:NZ	2.47	0.61
1:A:1223:G:OP1	17:R:68:ARG:NH2	2.33	0.61
1:A:249:C:O2	29:3:11:LYS:NZ	2.33	0.61
1:A:2682:A:H61	1:A:2728:U:H1'	1.66	0.61
14:O:4:LYS:HE3	14:O:8:ILE:HD11	1.83	0.61
23:X:36:ARG:HG2	23:X:45:PHE:HB3	1.82	0.61
20:U:14:THR:OG1	20:U:68:ASN:ND2	2.34	0.60
1:A:2098:U:H3	1:A:2191:A:H61	1.48	0.60
6:F:114:ARG:NH2	31:6:46:GLY:O	2.35	0.60
20:U:33:VAL:HG13	20:U:66:VAL:HG22	1.84	0.59
1:A:243:U:OP1	29:3:7:ARG:NH1	2.34	0.59
1:A:1817:G:OP2	3:C:155:ARG:NH2	2.35	0.59
1:A:2032:G:N2	4:D:151:THR:OG1	2.34	0.59
7:G:85:LYS:HG3	7:G:131:VAL:HG22	1.84	0.59
11:L:109:LYS:HE3	11:L:128:THR:HG22	1.85	0.59
1:A:910:A:H62	12:M:12:MET:HA	1.67	0.59
12:M:69:PRO:HA	12:M:94:ALA:HB2	1.85	0.59
21:V:64:VAL:HG22	21:V:69:GLU:HG2	1.83	0.59
3:C:143:VAL:HB	3:C:153:LEU:HB2	1.83	0.59
11:L:95:LEU:HD22	11:L:100:ILE:HD11	1.85	0.59
1:A:224:U:OP2	1:A:408:G:N2	2.36	0.59
1:A:685:A:H5''	1:A:788:A:H62	1.67	0.58
10:K:121:GLU:HG2	10:K:122:VAL:HG23	1.84	0.58
8:H:66:ASN:HD22	8:H:135:HIS:HD2	1.52	0.58
6:F:55:ASP:OD2	6:F:149:ARG:NH2	2.35	0.58
1:A:2139:U:H2'	1:A:2140:G:H8	1.67	0.58
1:A:781:A:OP1	3:C:216:ARG:NH2	2.37	0.58
1:A:1153:C:OP1	16:Q:91:ARG:NH2	2.36	0.58
23:X:5:GLN:O	23:X:73:ARG:NH2	2.37	0.58
3:C:153:LEU:HD13	3:C:175:LEU:HD21	1.84	0.58
26:0:37:HIS:ND1	26:0:38:LEU:O	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1365:A:OP1	23:X:2:ARG:NH1	2.36	0.58
1:A:2116:G:O6	1:A:2165:C:N4	2.37	0.57
1:A:994:C:OP1	16:Q:52:ARG:NH2	2.37	0.57
7:G:94:ARG:HB2	7:G:105:SER:HB2	1.86	0.57
1:A:1416:G:O2'	1:A:1587:G:N2	2.37	0.57
18:S:57:ASN:OD1	18:S:61:ASN:ND2	2.37	0.57
6:F:133:GLU:HB3	6:F:135:ILE:HG13	1.87	0.57
2:B:39:A:O2'	2:B:46:A:N1	2.38	0.57
1:A:1:G:N2	1:A:2903:U:O2'	2.38	0.57
25:Z:40:THR:HG23	25:Z:42:ALA:H	1.69	0.57
1:A:1063:G:H1	1:A:1075:C:H42	1.51	0.56
6:F:68:LYS:HB3	6:F:81:GLY:HA2	1.87	0.56
1:A:468:G:OP2	28:2:37:LYS:NZ	2.37	0.56
1:A:877:A:O2'	1:A:900:A:N6	2.37	0.56
15:P:105:LYS:O	15:P:108:ARG:NH2	2.39	0.56
1:A:958:U:OP2	12:M:14:LYS:NZ	2.38	0.56
11:L:78:ARG:NH2	11:L:80:SER:OG	2.39	0.56
11:L:128:THR:OG1	11:L:129:LYS:N	2.37	0.56
12:M:110:GLU:OE2	12:M:114:ARG:NH1	2.39	0.56
1:A:2296:U:OP2	14:O:9:ARG:NH2	2.38	0.56
18:S:82:MET:HB2	18:S:98:LYS:HB2	1.88	0.56
1:A:1064:C:N4	1:A:1066:U:O2'	2.37	0.56
7:G:23:ILE:HD11	7:G:42:VAL:HG11	1.88	0.56
1:A:443:A:N6	5:E:36:ALA:O	2.39	0.55
15:P:59:THR:HA	15:P:72:VAL:HA	1.88	0.55
1:A:2313:C:H5''	6:F:87:LYS:HD2	1.89	0.55
7:G:148:ARG:NH2	7:G:166:GLU:OE2	2.39	0.55
8:H:94:ILE:HG23	8:H:98:ASP:HB3	1.89	0.55
1:A:2220:U:O2'	8:H:97:ARG:NH2	2.40	0.55
1:A:2199:A:OP1	23:X:36:ARG:NH2	2.39	0.55
5:E:47:LYS:HB2	5:E:51:GLU:HB2	1.89	0.55
7:G:3:VAL:HG12	7:G:68:ARG:HD2	1.89	0.55
1:A:2655:G:O2'	1:A:2664:G:N1	2.38	0.54
1:A:2780:G:N1	9:J:102:GLU:OE2	2.40	0.54
2:B:76:G:N3	21:V:78:GLN:NE2	2.51	0.54
1:A:561:G:HO2'	16:Q:44:TYR:HH	1.56	0.54
1:A:948:C:O2	1:A:984:A:O2'	2.23	0.54
3:C:154:ALA:HB2	3:C:161:VAL:HG23	1.89	0.54
6:F:118:ALA:O	6:F:166:ARG:NH1	2.41	0.54
1:A:2391:G:H2'	1:A:2424:C:H41	1.73	0.54
1:A:1817:G:OP1	3:C:86:ARG:NH2	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:A:H5''	11:L:67:THR:HG21	1.90	0.54
1:A:2831:G:N2	1:A:2884:U:OP2	2.38	0.54
1:A:2521:C:O2'	1:A:2564:A:N3	2.40	0.53
4:D:77:ARG:NH2	4:D:200:ASP:OD1	2.40	0.53
1:A:1297:C:O2'	1:A:1302:A:N1	2.40	0.53
5:E:123:LYS:HE3	5:E:125:SER:HB2	1.88	0.53
19:T:6:ARG:NH1	19:T:42:GLU:OE1	2.42	0.53
3:C:141:HIS:ND1	3:C:192:GLY:O	2.38	0.53
22:W:33:ILE:HG22	22:W:34:VAL:HG23	1.90	0.53
1:A:1651:G:OP2	13:N:40:LYS:NZ	2.41	0.53
21:V:72:VAL:HG12	21:V:93:ARG:HA	1.91	0.53
1:A:2540:C:O2'	1:A:2740:A:N3	2.41	0.53
9:J:36:LEU:HD22	9:J:121:LYS:HB2	1.91	0.53
4:D:14:ILE:HA	15:P:11:GLN:HE22	1.74	0.53
5:E:149:ILE:HD11	5:E:172:ALA:HA	1.89	0.53
9:J:17:VAL:HG23	9:J:137:PRO:HB2	1.91	0.53
12:M:75:GLU:HB2	12:M:90:GLU:HG3	1.91	0.53
1:A:1715:G:N2	1:A:1716:U:O4	2.41	0.53
1:A:2773:C:OP1	4:D:169:ARG:NH2	2.43	0.53
2:B:57:A:H4'	6:F:26:GLN:HE21	1.72	0.53
29:3:32:LEU:HD23	29:3:35:LYS:HD2	1.90	0.52
1:A:1315:C:O2'	1:A:1392:A:N3	2.38	0.52
1:A:1601:G:OP1	19:T:64:LYS:NZ	2.37	0.52
1:A:1779:U:OP2	1:A:1784:A:N6	2.41	0.52
14:O:94:ARG:NH2	14:O:97:PHE:O	2.39	0.52
1:A:1032:A:H1'	30:4:23:ILE:HD13	1.90	0.52
4:D:179:ARG:HB3	4:D:188:LEU:HD12	1.91	0.52
15:P:29:VAL:HG22	15:P:80:VAL:HG12	1.92	0.52
19:T:13:ALA:HB3	19:T:33:LYS:HD3	1.90	0.52
7:G:29:ASN:HB2	7:G:78:VAL:HA	1.92	0.52
1:A:499:U:H5''	20:U:42:LYS:HE3	1.91	0.52
4:D:35:THR:HG22	4:D:73:VAL:HG21	1.92	0.52
13:N:44:LEU:HD23	13:N:113:ILE:HD13	1.91	0.52
1:A:1992:G:N2	1:A:1996:C:O2'	2.43	0.51
1:A:2205:A:H61	1:A:2219:U:H3	1.57	0.51
4:D:109:VAL:HG22	4:D:203:VAL:HG22	1.92	0.51
21:V:42:LEU:HD13	21:V:47:VAL:HG21	1.93	0.51
20:U:3:LYS:O	20:U:93:ARG:NH2	2.40	0.51
1:A:2508:G:H1	1:A:2580:U:H5	1.59	0.51
10:K:80:ASP:OD2	15:P:61:ARG:NH1	2.40	0.51
5:E:77:ILE:HG13	5:E:78:TRP:HD1	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1071:G:H1'	1:A:1089:A:H2'	1.91	0.51
1:A:1798:U:OP2	3:C:270:ARG:NH2	2.41	0.51
31:6:11:GLU:HA	31:6:25:ARG:HA	1.93	0.51
1:A:1012:U:OP2	16:Q:69:ARG:NH1	2.39	0.51
5:E:176:ASP:OD1	5:E:176:ASP:N	2.44	0.51
14:O:8:ILE:O	14:O:12:THR:OG1	2.29	0.51
12:M:50:ARG:HD3	12:M:65:ILE:HD11	1.92	0.51
1:A:274:C:H42	1:A:363:G:H1	1.57	0.51
1:A:1607:C:N4	1:A:1622:G:OP2	2.41	0.51
1:A:2847:U:OP1	15:P:95:LYS:NZ	2.36	0.51
7:G:93:TYR:OH	7:G:159:LYS:NZ	2.41	0.51
1:A:1041:G:H1	1:A:1114:C:H42	1.59	0.50
1:A:560:C:O2'	16:Q:47:ARG:NH2	2.43	0.50
15:P:63:ILE:HA	15:P:68:GLY:HA2	1.92	0.50
1:A:2212:A:H4'	1:A:2213:U:H5	1.76	0.50
1:A:910:A:N3	1:A:2264:C:O2'	2.39	0.50
8:H:51:ARG:HG3	8:H:55:GLU:HB2	1.93	0.50
11:L:111:ILE:HD12	11:L:111:ILE:H	1.76	0.50
1:A:1799:G:N2	1:A:1818:U:O2'	2.45	0.50
1:A:981:A:OP2	1:A:982:C:N4	2.37	0.50
1:A:2772:C:H5'	4:D:173:GLN:HE21	1.76	0.50
22:W:17:LEU:HD11	22:W:37:ARG:HE	1.76	0.50
11:L:76:GLU:HB2	11:L:111:ILE:HD13	1.92	0.50
5:E:125:SER:O	5:E:137:LYS:NZ	2.41	0.50
16:Q:109:VAL:HG12	16:Q:113:LYS:HE2	1.94	0.50
1:A:1248:G:OP1	5:E:44:ARG:NH1	2.44	0.50
1:A:1826:G:O2'	1:A:1971:U:OP2	2.30	0.50
1:A:51:G:H4'	1:A:52:A:H5'	1.93	0.50
16:Q:78:PHE:HE2	16:Q:94:LEU:HD21	1.77	0.50
1:A:210:C:OP1	28:2:29:GLN:NE2	2.40	0.49
7:G:34:ARG:HH12	7:G:70:LEU:HD22	1.77	0.49
1:A:1155:A:H5''	16:Q:54:ARG:HH11	1.77	0.49
1:A:2141:G:H1	1:A:2150:C:H42	1.58	0.49
1:A:1068:G:O6	1:A:1069:A:N6	2.45	0.49
1:A:1667:G:O2'	1:A:1991:U:O4	2.27	0.49
1:A:2115:G:OP1	1:A:2166:U:O2'	2.29	0.49
1:A:630:G:N2	1:A:633:A:OP2	2.40	0.49
1:A:828:U:O4	1:A:858:G:N2	40.69	0.49
1:A:1816:C:N4	3:C:34:GLU:OE2	2.32	0.49
19:T:8:LEU:HD11	24:Y:22:LEU:HD12	1.94	0.49
1:A:2880:C:O3'	13:N:90:ARG:NH2	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:106:PRO:HG2	3:C:109:LEU:HB2	1.95	0.49
28:2:24:THR:HG23	28:2:27:GLY:H	1.77	0.49
11:L:57:LEU:HD22	29:3:53:ASP:HB3	1.94	0.49
1:A:1326:U:H2'	1:A:1327:A:H8	1.78	0.49
3:C:106:PRO:HD2	3:C:109:LEU:HD22	1.94	0.49
1:A:406:G:H5'	4:D:4:LEU:HD22	165.71	0.49
2:B:7:G:O2'	14:O:38:GLN:NE2	2.45	0.49
1:A:500:G:N1	1:A:503:A:OP2	2.46	0.49
4:D:10:GLY:H	4:D:197:THR:HG23	1.78	0.49
11:L:20:GLY:HA2	11:L:28:GLY:HA2	1.94	0.49
13:N:86:ARG:NE	13:N:117:ASP:OD2	2.45	0.49
30:4:7:VAL:HG22	30:4:38:GLY:HA3	1.95	0.48
1:A:273:G:O6	1:A:364:C:N4	2.36	0.48
1:A:563:A:N3	16:Q:36:GLN:NE2	2.61	0.48
4:D:55:LYS:HD2	4:D:60:VAL:HB	1.94	0.48
1:A:2830:C:OP1	4:D:56:LYS:NZ	2.41	0.48
2:B:52:A:N7	14:O:64:TYR:OH	2.33	0.48
8:H:125:THR:HG21	8:H:148:ALA:HB2	1.94	0.48
10:K:69:VAL:HG21	10:K:104:THR:HG21	1.96	0.48
18:S:3:THR:HG21	18:S:58:ALA:HB2	1.96	0.48
1:A:1342:A:O2'	1:A:1344:U:OP2	2.26	0.48
1:A:1361:G:HO2'	1:A:2215:C:HO2'	1.61	0.48
1:A:476:G:N1	1:A:479:A:OP2	2.43	0.48
1:A:704:G:H2'	1:A:726:G:H22	1.78	0.48
17:R:49:ILE:HG22	17:R:54:VAL:HA	1.94	0.48
1:A:2539:C:H5'	30:4:3:VAL:HG21	1.96	0.48
1:A:647:G:N2	1:A:2350:C:O2'	2.44	0.48
1:A:729:G:OP2	3:C:206:LYS:NZ	2.37	0.48
15:P:28:LYS:HG2	15:P:39:LEU:HG	1.96	0.48
1:A:2646:C:OP2	1:A:2732:G:O2'	2.27	0.48
7:G:163:TYR:HB2	7:G:166:GLU:HB2	1.95	0.48
18:S:73:LYS:HB2	18:S:106:VAL:HB	1.94	0.48
19:T:3:ARG:HH12	19:T:7:LEU:HD21	1.78	0.48
1:A:651:G:H5'	29:3:18:LYS:HG3	1.96	0.48
1:A:2343:U:O2'	1:A:2373:G:O2'	2.26	0.48
1:A:2441:U:OP2	1:A:2586:U:O2'	2.31	0.48
1:A:514:A:N3	1:A:581:C:O2'	2.46	0.48
1:A:1791:A:N6	1:A:1828:G:O2'	2.42	0.48
1:A:2457:U:H5	1:A:2494:G:H1	1.61	0.47
3:C:68:ARG:O	3:C:188:ARG:NH1	2.47	0.47
10:K:99:ILE:HD12	10:K:118:LEU:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:36:GLU:HA	20:U:61:GLU:HG2	1.95	0.47
1:A:2522:U:O2'	1:A:2647:U:OP1	2.25	0.47
12:M:42:THR:HG22	12:M:93:VAL:HG12	1.96	0.47
1:A:538:A:H5''	9:J:7:LYS:HE3	1.96	0.47
1:A:1796:U:H2'	1:A:1797:G:H8	1.79	0.47
12:M:29:GLY:HA2	12:M:106:ASP:HB2	1.96	0.47
24:Y:49:ASP:OD1	24:Y:52:ARG:NH2	2.47	0.47
1:A:1323:C:OP1	18:S:98:LYS:NZ	2.43	0.47
9:J:11:VAL:HG11	9:J:50:THR:HA	1.96	0.47
16:Q:43:GLN:HE21	17:R:77:PHE:HB3	1.78	0.47
26:O:27:LEU:HD23	26:O:36:LYS:HB3	1.96	0.47
1:A:2615:U:C2	26:O:3:GLN:HA	2.49	0.47
1:A:1061:U:H4'	1:A:1070:A:C4	2.49	0.47
1:A:558:U:H2'	1:A:559:G:H8	1.79	0.47
7:G:104:LEU:HD21	7:G:130:ILE:HD11	1.96	0.47
11:L:19:LEU:HA	11:L:27:LEU:HD13	1.95	0.47
29:3:14:LYS:HB3	29:3:22:LYS:HE2	1.97	0.47
1:A:362:A:H3'	1:A:363:G:H8	1.79	0.47
1:A:2394:C:H5''	11:L:63:LYS:HE3	1.95	0.47
14:O:40:ILE:HG12	14:O:47:VAL:HG12	1.97	0.47
15:P:21:PRO:HD3	15:P:49:ILE:HD12	1.95	0.47
27:1:7:LYS:HA	27:1:23:THR:HA	1.97	0.47
1:A:1069:A:OP1	1:A:1096:A:O2'	2.33	0.47
1:A:1509:A:H2'	1:A:1510:G:H8	1.79	0.47
3:C:209:ALA:HA	3:C:212:TRP:CE2	2.50	0.47
3:C:250:GLN:NE2	3:C:251:THR:O	2.47	0.47
16:Q:108:LEU:HA	17:R:48:LYS:HE3	1.97	0.47
6:F:125:GLY:O	6:F:157:THR:OG1	2.32	0.47
15:P:24:THR:HB	15:P:87:ARG:HB3	1.97	0.47
1:A:1136:G:O2'	1:A:2038:G:O2'	2.23	0.46
1:A:2010:G:H5''	18:S:42:LYS:HB2	1.96	0.46
5:E:126:VAL:O	5:E:156:ASN:ND2	2.47	0.46
13:N:59:SER:OG	13:N:62:ASN:OD1	2.33	0.46
1:A:1788:C:OP1	3:C:220:ARG:NH2	2.48	0.46
5:E:29:HIS:HA	5:E:32:VAL:HG12	1.98	0.46
8:H:83:LYS:HA	8:H:149:GLU:HB3	1.97	0.46
14:O:7:ARG:NH1	14:O:95:SER:O	2.46	0.46
1:A:1340:U:OP1	19:T:19:LYS:NZ	2.38	0.46
1:A:1378:A:O2'	1:A:1380:G:OP2	2.33	0.46
1:A:2561:U:O3'	10:K:40:LYS:NZ	2.48	0.46
3:C:140:VAL:HG12	3:C:191:LEU:HD23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:2:ASP:OD2	14:O:5:SER:N	2.40	0.46
1:A:1416:G:N2	1:A:1582:C:O2	2.46	0.46
1:A:2809:A:OP2	1:A:2890:G:N1	2.45	0.46
1:A:971:G:OP1	1:A:974:G:O2'	2.28	0.46
8:H:67:ALA:HA	8:H:138:VAL:HG11	1.97	0.46
1:A:1068:G:N2	1:A:1095:A:O3'	2.49	0.46
1:A:1682:G:OP2	1:A:1699:G:N2	2.42	0.46
1:A:1930:G:O2'	1:A:1968:G:N1	2.48	0.46
1:A:276:U:O2'	1:A:278:A:N6	2.47	0.46
1:A:465:G:OP1	28:2:12:ARG:NH1	2.48	0.46
1:A:764:A:O2'	1:A:781:A:N6	2.49	0.46
11:L:95:LEU:HD11	11:L:125:LEU:HD21	1.98	0.46
13:N:28:LEU:HD23	13:N:48:VAL:HG11	1.98	0.46
1:A:1900:A:H1'	1:A:1970:A:H2'	1.98	0.46
7:G:88:LEU:HD21	7:G:104:LEU:HD22	1.98	0.46
1:A:1509:A:H2'	1:A:1510:G:C8	2.50	0.46
1:A:84:A:N1	1:A:98:G:O2'	2.41	0.46
5:E:148:ILE:HA	5:E:187:VAL:HG13	1.98	0.46
13:N:45:ARG:HG2	13:N:95:THR:HG21	1.98	0.46
1:A:1394:U:H4'	1:A:1603:A:H4'	1.98	0.46
1:A:1869:G:N2	1:A:1872:A:OP2	2.46	0.46
1:A:1953:A:O2'	1:A:2559:C:O2	2.32	0.45
6:F:107:VAL:HG11	6:F:175:PRO:HG2	1.98	0.45
1:A:1754:A:O3'	15:P:102:ARG:NH2	2.49	0.45
18:S:47:VAL:HG23	18:S:103:ILE:HG21	1.96	0.45
22:W:19:VAL:HG22	22:W:34:VAL:HG22	1.98	0.45
1:A:1019:U:OP1	1:A:1035:U:O2'	2.25	0.45
1:A:2107:G:N2	1:A:2182:U:O2	2.33	0.45
5:E:106:LYS:HG3	5:E:200:LEU:HD23	1.97	0.45
9:J:44:TYR:O	16:Q:63:ARG:NE	2.46	0.45
18:S:4:ILE:O	18:S:57:ASN:ND2	2.50	0.45
1:A:184:C:H2'	1:A:185:G:C8	2.51	0.45
1:A:2469:A:N6	1:A:2481:G:O2'	2.49	0.45
7:G:29:ASN:ND2	7:G:77:GLY:O	2.41	0.45
1:A:116:C:O2'	1:A:126:A:N3	2.45	0.45
4:D:97:SER:OG	4:D:98:VAL:N	2.50	0.45
8:H:62:LEU:HA	8:H:65:ALA:HB3	1.98	0.45
1:A:1796:U:H2'	1:A:1797:G:C8	2.52	0.45
1:A:1769:U:O2'	1:A:1958:C:OP1	2.34	0.45
4:D:34:VAL:HG22	4:D:50:VAL:HG12	1.98	0.45
12:M:40:ARG:HD2	12:M:93:VAL:HG21	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1156:A:C8	16:Q:50:ARG:HG2	2.52	0.45
1:A:1360:G:N7	1:A:1371:G:N2	2.65	0.45
1:A:2477:U:O2	30:4:4:ARG:NH2	2.50	0.45
1:A:674:G:H1'	5:E:69:ARG:HE	1.82	0.45
5:E:18:THR:HA	5:E:106:LYS:HE3	1.99	0.45
8:H:3:VAL:HA	8:H:38:PRO:HA	1.99	0.45
15:P:13:LYS:HE3	15:P:76:HIS:HA	1.98	0.45
31:6:20:ASN:ND2	31:6:37:CYS:SG	2.83	0.45
1:A:974:G:H8	1:A:990:A:H62	1.64	0.45
2:B:79:G:N7	21:V:14:LYS:NZ	2.65	0.45
3:C:77:VAL:HG21	3:C:109:LEU:HD11	1.99	0.45
1:A:290:U:H2'	1:A:291:G:H8	1.81	0.45
1:A:543:G:O6	1:A:550:C:N4	2.41	0.45
9:J:4:PHE:O	16:Q:63:ARG:NH2	2.39	0.45
1:A:964:C:O2'	1:A:2273:A:N3	2.40	0.44
1:A:410:G:N2	1:A:432:A:N7	40.79	0.44
6:F:174:PHE:O	6:F:176:PHE:N	2.50	0.44
1:A:1084:A:N3	1:A:1105:U:O2'	2.46	0.44
5:E:97:ASN:ND2	5:E:100:MET:SD	2.90	0.44
1:A:2543:G:H2'	1:A:2544:G:C8	2.53	0.44
1:A:160:A:N3	1:A:2208:C:O2'	2.47	0.44
1:A:672:C:OP2	11:L:42:SER:OG	2.32	0.44
1:A:705:A:OP2	1:A:725:G:N1	2.42	0.44
9:J:56:VAL:HB	9:J:124:VAL:HG12	1.98	0.44
10:K:4:GLU:HG2	10:K:5:GLN:HG2	2.00	0.44
1:A:30:G:O2'	1:A:1214:A:N3	2.46	0.44
5:E:102:ARG:NH1	5:E:200:LEU:O	2.49	0.44
16:Q:27:ARG:HG2	16:Q:33:VAL:HG12	2.00	0.44
1:A:917:A:H5''	1:A:2268:A:H61	1.83	0.44
1:A:694:U:H3	1:A:768:G:H1	1.66	0.44
7:G:21:GLN:NE2	7:G:37:ASN:O	2.50	0.44
6:F:139:GLU:HG2	31:6:27:THR:HG23	1.99	0.44
1:A:1231:U:H2'	1:A:1232:G:H8	1.83	0.44
4:D:33:ARG:HG3	4:D:73:VAL:HB	2.00	0.44
10:K:12:ASP:HB2	10:K:96:GLY:HA3	1.99	0.44
1:A:2627:G:N2	1:A:2777:G:OP2	2.48	0.44
17:R:5:PHE:HE1	17:R:14:VAL:HG11	1.83	0.44
23:X:13:THR:HG22	23:X:27:ARG:HG2	1.99	0.44
1:A:1936:A:H2	1:A:1943:U:H3	1.66	0.43
1:A:32:C:N4	1:A:447:A:OP2	2.50	0.43
11:L:49:GLY:HA3	11:L:58:TYR:HE1	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:94:THR:HA	11:L:97:ALA:HB3	2.00	0.43
1:A:1651:G:H4'	13:N:39:PRO:HG2	1.99	0.43
1:A:102:U:H1'	24:Y:2:LYS:HE2	2.00	0.43
1:A:1028:A:N3	1:A:2486:C:O2'	2.44	0.43
1:A:1060:U:H4'	1:A:1061:U:H5'	2.00	0.43
1:A:957:C:H5'	12:M:75:GLU:HG2	2.00	0.43
8:H:93:SER:OG	8:H:121:VAL:O	2.34	0.43
14:O:49:VAL:HG21	14:O:82:ALA:HA	2.00	0.43
15:P:64:SER:OG	15:P:65:ASN:N	2.50	0.43
1:A:2039:U:H2'	1:A:2040:G:C8	2.53	0.43
1:A:2724:U:OP1	4:D:123:LYS:NZ	2.47	0.43
3:C:159:THR:HG23	3:C:176:ARG:HG2	2.00	0.43
2:B:29:A:O2'	2:B:58:A:N1	2.43	0.43
3:C:230:PRO:HB2	3:C:244:VAL:HG21	2.00	0.43
1:A:2295:C:OP1	14:O:10:ARG:NH1	2.40	0.43
1:A:1055:G:H1	1:A:1104:C:H42	1.67	0.43
2:B:15:A:H3'	2:B:16:G:H8	1.83	0.43
3:C:7:PRO:HB3	3:C:13:ARG:HG3	2.00	0.43
3:C:16:VAL:HB	3:C:203:VAL:HG22	2.01	0.43
10:K:24:VAL:HG13	10:K:33:ALA:HB2	2.00	0.43
1:A:631:A:N3	1:A:2415:G:O2'	2.42	0.43
1:A:1032:A:H2	1:A:1122:G:H22	1.67	0.43
1:A:1199:U:H1'	16:Q:3:VAL:HG22	2.00	0.43
14:O:108:ASP:OD1	14:O:111:ARG:NH1	2.52	0.43
6:F:98:PHE:O	6:F:102:LEU:N	2.48	0.43
10:K:59:LYS:HB2	10:K:87:LEU:HB2	2.00	0.43
1:A:2117:A:H61	1:A:2166:U:H3	1.67	0.42
7:G:2:ARG:HA	7:G:2:ARG:HD3	4.71	0.42
10:K:33:ALA:HB1	10:K:37:ASP:HB2	2.01	0.42
17:R:77:PHE:HD1	17:R:84:ARG:HB3	1.84	0.42
2:B:98:G:H1	21:V:14:LYS:HB2	1.84	0.42
1:A:2116:G:H1	1:A:2164:C:H42	1.67	0.42
1:A:589:U:H2'	1:A:590:A:C8	2.54	0.42
1:A:1009:A:N3	1:A:1153:C:O2'	2.46	0.42
1:A:1365:A:O5'	23:X:27:ARG:NH2	2.46	0.42
1:A:739:A:H1'	1:A:740:C:H5	1.84	0.42
1:A:774:G:H5''	3:C:47:ARG:HH21	1.84	0.42
1:A:1470:A:N6	1:A:1521:G:O2'	2.52	0.42
1:A:270:A:N1	1:A:369:U:O2'	2.39	0.42
3:C:36:ASN:HB2	3:C:61:TYR:HB2	2.02	0.42
1:A:2822:G:H5''	4:D:164:GLN:HE22	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:32:LEU:HD22	9:J:54:ILE:HG21	2.01	0.42
11:L:62:PRO:HB2	29:3:29:ARG:HH11	1.84	0.42
11:L:85:VAL:HG21	11:L:90:VAL:HG22	2.00	0.42
11:L:61:LEU:HD23	29:3:26:ALA:HB2	2.01	0.42
1:A:168:G:H2'	1:A:169:G:H8	1.85	0.42
1:A:1980:G:O2'	1:A:1982:U:OP2	2.31	0.42
4:D:40:LEU:HA	4:D:44:GLY:H	1.84	0.42
13:N:87:PHE:HD1	13:N:90:ARG:HD3	1.84	0.42
29:3:15:LYS:HE2	29:3:19:GLY:HA2	2.02	0.42
1:A:2420:C:H5''	27:1:7:LYS:HD2	2.01	0.42
5:E:146:VAL:HG12	5:E:185:LYS:HB2	2.01	0.42
2:B:41:G:H21	6:F:65:LEU:HD11	1.84	0.42
7:G:41:GLU:HA	7:G:54:ARG:HH21	1.83	0.42
21:V:51:GLN:HE22	21:V:86:LEU:HD21	1.85	0.42
29:3:31:ILE:O	29:3:35:LYS:NZ	2.51	0.42
1:A:277:G:H4'	1:A:278:A:C5	2.55	0.42
1:A:558:U:H2'	1:A:559:G:C8	2.54	0.42
12:M:40:ARG:HG2	12:M:95:LEU:HD23	2.02	0.42
13:N:96:ARG:HH22	13:N:116:VAL:HG13	1.85	0.42
1:A:2756:U:H1'	1:A:2757:A:H5''	2.01	0.42
1:A:2839:G:O2'	13:N:49:GLU:OE1	2.37	0.42
1:A:955:U:H5	1:A:962:G:H1	1.67	0.42
8:H:55:GLU:HG2	8:H:58:LEU:HD12	2.01	0.42
1:A:2220:U:H4'	8:H:97:ARG:HH21	1.84	0.42
1:A:1296:G:OP1	1:A:2709:G:O2'	2.26	0.42
1:A:527:C:N4	1:A:2779:U:OP2	2.42	0.42
1:A:2848:G:O2'	1:A:2868:A:N6	2.53	0.42
9:J:37:ARG:NH2	9:J:110:PRO:HG3	2.35	0.42
17:R:40:MET:HG3	17:R:48:LYS:HA	2.00	0.42
1:A:987:C:O2'	1:A:1000:A:N3	2.48	0.42
1:A:2224:G:H4'	1:A:2226:C:C2	2.55	0.42
1:A:2831:G:OP2	4:D:59:ARG:NH1	2.52	0.42
3:C:257:ARG:HG2	3:C:269:ARG:HH12	1.85	0.42
6:F:30:VAL:HA	6:F:157:THR:HA	2.01	0.42
9:J:99:ARG:HA	9:J:102:GLU:HB3	2.02	0.41
12:M:33:LEU:HB2	12:M:117:PHE:CD1	2.56	0.41
12:M:53:MET:HE2	12:M:63:ILE:HG12	2.02	0.41
1:A:1550:C:H2'	1:A:1551:A:C8	2.55	0.41
1:A:2405:G:O2'	1:A:2412:A:N6	2.53	0.41
1:A:247:G:OP2	1:A:249:C:N4	2.53	0.41
4:D:68:PHE:HE1	4:D:79:LEU:HD21	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:A:O2'	1:A:2404:U:OP1	2.36	0.41
1:A:243:U:OP2	1:A:254:G:N1	2.44	0.41
1:A:576:U:H2'	1:A:577:G:C8	2.55	0.41
1:A:1820:U:C2	3:C:200:MET:HB2	2.55	0.41
8:H:12:LEU:HB2	8:H:19:VAL:HG11	2.01	0.41
1:A:2380:C:H5'	14:O:17:LYS:HZ1	1.86	0.41
18:S:56:ALA:HA	18:S:59:GLU:HG2	2.02	0.41
29:3:31:ILE:HG13	29:3:31:ILE:H	1.71	0.41
1:A:1447:C:O2'	1:A:1544:A:N3	2.43	0.41
1:A:444:C:OP1	5:E:40:ARG:NH2	2.54	0.41
1:A:720:U:H2'	1:A:721:A:C8	2.55	0.41
12:M:53:MET:HB2	12:M:120:ALA:HB2	2.03	0.41
1:A:372:G:C4	23:X:60:LYS:HD2	2.55	0.41
1:A:2481:G:HO2'	1:A:2482:A:H8	1.68	0.41
1:A:281:C:H2'	1:A:282:A:H8	1.85	0.41
1:A:704:G:H1'	1:A:727:A:H61	1.85	0.41
16:Q:78:PHE:HE1	16:Q:109:VAL:HA	1.85	0.41
1:A:1361:G:O2'	1:A:2215:C:O2'	2.29	0.41
1:A:2377:A:H2'	1:A:2378:A:C8	2.55	0.41
4:D:4:LEU:HD23	4:D:32:ASN:HD22	1.85	0.41
11:L:55:MET:HA	11:L:56:PRO:HD3	1.96	0.41
25:Z:40:THR:HG22	25:Z:43:ILE:HG12	2.03	0.41
1:A:1130:U:N3	1:A:2025:C:OP1	2.38	0.41
1:A:2619:C:H5''	4:D:157:LYS:HA	2.03	0.41
6:F:125:GLY:HA2	6:F:162:ASP:HA	2.03	0.41
6:F:130:GLY:HA2	6:F:152:ASP:HA	2.02	0.41
1:A:2419:U:OP1	29:3:40:LYS:NZ	2.51	0.41
5:E:3:LEU:HD21	5:E:19:PHE:HE2	1.85	0.41
1:A:663:G:H5''	11:L:17:LYS:HD3	2.02	0.41
1:A:743:A:O2'	1:A:1659:G:OP1	2.31	0.41
5:E:69:ARG:HD3	5:E:69:ARG:HH11	1.73	0.41
7:G:51:PHE:HZ	7:G:71:LEU:HD22	1.85	0.41
13:N:22:ARG:HG3	13:N:70:THR:HA	2.03	0.41
13:N:98:LEU:O	13:N:112:TYR:N	2.49	0.41
21:V:48:MET:SD	21:V:51:GLN:NE2	2.94	0.41
1:A:1311:G:H21	1:A:1603:A:H62	1.69	0.41
1:A:1316:U:H2'	1:A:1317:G:C8	2.56	0.41
1:A:1827:U:O2'	1:A:1970:A:N3	2.41	0.41
1:A:2298:A:OP1	6:F:70:ARG:NH2	2.54	0.40
18:S:44:ALA:HA	18:S:47:VAL:HG12	2.04	0.40
30:4:17:VAL:HG12	30:4:19:ARG:HG3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1181:U:H2'	1:A:1182:G:C8	2.56	0.40
1:A:694:U:H5'	1:A:1569:A:C5	2.56	0.40
2:B:13:G:N2	2:B:16:G:N3	2.68	0.40
3:C:146:LYS:HB2	3:C:149:LYS:HB2	2.04	0.40
14:O:10:ARG:HH21	14:O:10:ARG:HD2	1.76	0.40
14:O:102:ARG:HH21	14:O:102:ARG:HD2	1.74	0.40
1:A:977:G:H5'	16:Q:54:ARG:HH12	1.86	0.40
1:A:1316:U:H2'	1:A:1317:G:H8	1.87	0.40
4:D:91:THR:HG22	4:D:94:GLN:HB2	2.03	0.40
7:G:53:PRO:HG3	7:G:61:TRP:CE2	2.57	0.40
11:L:131:ALA:HA	11:L:134:ALA:HB3	2.03	0.40
30:4:16:ILE:HD13	30:4:25:VAL:HG22	2.02	0.40
14:O:5:SER:HA	14:O:8:ILE:HD12	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	
3	C	269/271 (99%)	252 (94%)	17 (6%)	0	100	100
4	D	207/209 (99%)	194 (94%)	13 (6%)	0	100	100
5	E	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
6	F	175/177 (99%)	160 (91%)	13 (7%)	2 (1%)	17	55
7	G	174/176 (99%)	161 (92%)	12 (7%)	1 (1%)	30	68
8	H	147/149 (99%)	131 (89%)	16 (11%)	0	100	100
9	J	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
10	K	120/122 (98%)	106 (88%)	14 (12%)	0	100	100
11	L	141/143 (99%)	123 (87%)	17 (12%)	1 (1%)	26	65
12	M	134/136 (98%)	127 (95%)	6 (4%)	1 (1%)	26	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	N	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
14	O	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
15	P	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
16	Q	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
17	R	101/103 (98%)	88 (87%)	13 (13%)	0	100	100
18	S	108/110 (98%)	98 (91%)	10 (9%)	0	100	100
19	T	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
20	U	100/102 (98%)	90 (90%)	10 (10%)	0	100	100
21	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
22	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
23	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
24	Y	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
25	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
26	0	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
27	1	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
28	2	44/46 (96%)	44 (100%)	0	0	100	100
29	3	62/64 (97%)	52 (84%)	9 (14%)	1 (2%)	12	44
30	4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
31	6	64/66 (97%)	57 (89%)	7 (11%)	0	100	100
33	b	216/218 (99%)	189 (88%)	24 (11%)	3 (1%)	14	48
34	c	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
35	d	203/205 (99%)	179 (88%)	24 (12%)	0	100	100
36	e	155/157 (99%)	129 (83%)	26 (17%)	0	100	100
37	f	98/100 (98%)	83 (85%)	14 (14%)	1 (1%)	19	58
38	g	149/151 (99%)	137 (92%)	12 (8%)	0	100	100
39	h	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
40	i	125/127 (98%)	103 (82%)	22 (18%)	0	100	100
41	j	96/98 (98%)	83 (86%)	12 (12%)	1 (1%)	19	58
42	k	114/116 (98%)	93 (82%)	21 (18%)	0	100	100
43	l	121/123 (98%)	97 (80%)	24 (20%)	0	100	100
44	m	112/114 (98%)	99 (88%)	12 (11%)	1 (1%)	21	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	n	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
46	o	86/88 (98%)	78 (91%)	7 (8%)	1 (1%)	16	52
47	p	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
48	q	78/80 (98%)	67 (86%)	11 (14%)	0	100	100
49	r	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
50	s	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
51	t	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
52	u	63/65 (97%)	41 (65%)	21 (33%)	1 (2%)	12	44
54	w	43/45 (96%)	28 (65%)	11 (26%)	4 (9%)	1	4
56	z	357/359 (99%)	334 (94%)	22 (6%)	1 (0%)	46	80
All	All	5979/6081 (98%)	5420 (91%)	540 (9%)	19 (0%)	50	80

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	b	18	GLN
44	m	4	ALA
46	o	46	LYS
54	w	13	ASP
54	w	33	LYS
54	w	36	LYS
29	3	31	ILE
52	u	37	TYR
6	F	175	PRO
7	G	119	GLY
56	z	322	GLN
33	b	17	HIS
37	f	53	LYS
6	F	174	PHE
33	b	20	ARG
54	w	12	LYS
12	M	69	PRO
11	L	111	ILE
41	j	42	LEU

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	
3	C	216/216 (100%)	215 (100%)	1 (0%)	92	96
4	D	164/164 (100%)	160 (98%)	4 (2%)	57	84
5	E	165/165 (100%)	165 (100%)	0	100	100
6	F	148/148 (100%)	148 (100%)	0	100	100
7	G	137/137 (100%)	135 (98%)	2 (2%)	72	90
8	H	114/114 (100%)	114 (100%)	0	100	100
9	J	116/116 (100%)	115 (99%)	1 (1%)	84	94
10	K	103/103 (100%)	103 (100%)	0	100	100
11	L	102/102 (100%)	101 (99%)	1 (1%)	82	93
12	M	109/109 (100%)	108 (99%)	1 (1%)	84	94
13	N	100/100 (100%)	99 (99%)	1 (1%)	82	93
14	O	86/86 (100%)	86 (100%)	0	100	100
15	P	99/99 (100%)	98 (99%)	1 (1%)	82	93
16	Q	89/89 (100%)	89 (100%)	0	100	100
17	R	84/84 (100%)	83 (99%)	1 (1%)	78	92
18	S	93/93 (100%)	93 (100%)	0	100	100
19	T	80/80 (100%)	80 (100%)	0	100	100
20	U	83/83 (100%)	83 (100%)	0	100	100
21	V	78/78 (100%)	78 (100%)	0	100	100
22	W	57/57 (100%)	57 (100%)	0	100	100
23	X	67/67 (100%)	66 (98%)	1 (2%)	72	90
24	Y	55/55 (100%)	55 (100%)	0	100	100
25	Z	48/48 (100%)	47 (98%)	1 (2%)	61	86
26	0	47/47 (100%)	47 (100%)	0	100	100
27	1	45/45 (100%)	45 (100%)	0	100	100
28	2	38/38 (100%)	38 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	3	51/51 (100%)	51 (100%)	0	100	100
30	4	34/34 (100%)	34 (100%)	0	100	100
31	6	59/59 (100%)	59 (100%)	0	100	100
33	b	180/180 (100%)	179 (99%)	1 (1%)	90	95
34	c	170/170 (100%)	168 (99%)	2 (1%)	78	92
35	d	172/172 (100%)	171 (99%)	1 (1%)	90	95
36	e	114/119 (96%)	112 (98%)	2 (2%)	66	88
37	f	87/87 (100%)	86 (99%)	1 (1%)	80	93
38	g	124/124 (100%)	123 (99%)	1 (1%)	86	94
39	h	104/104 (100%)	101 (97%)	3 (3%)	50	81
40	i	105/105 (100%)	102 (97%)	3 (3%)	50	81
41	j	86/86 (100%)	85 (99%)	1 (1%)	78	92
42	k	89/89 (100%)	87 (98%)	2 (2%)	60	85
43	l	103/103 (100%)	103 (100%)	0	100	100
44	m	92/92 (100%)	92 (100%)	0	100	100
45	n	79/83 (95%)	78 (99%)	1 (1%)	76	91
46	o	76/76 (100%)	75 (99%)	1 (1%)	76	91
47	p	65/65 (100%)	65 (100%)	0	100	100
48	q	74/74 (100%)	74 (100%)	0	100	100
49	r	48/56 (86%)	48 (100%)	0	100	100
50	s	70/70 (100%)	69 (99%)	1 (1%)	74	90
51	t	65/65 (100%)	64 (98%)	1 (2%)	72	90
52	u	44/55 (80%)	44 (100%)	0	100	100
54	w	38/38 (100%)	34 (90%)	4 (10%)	8	31
56	z	305/305 (100%)	299 (98%)	6 (2%)	63	86
All	All	4957/4985 (99%)	4911 (99%)	46 (1%)	85	94

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	181	ARG
4	D	33	ARG
4	D	42	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	46	ARG
4	D	184	ARG
7	G	37	ASN
7	G	68	ARG
9	J	123	LYS
11	L	27	LEU
12	M	6	ARG
13	N	2	ARG
15	P	72	VAL
17	R	43	ASN
23	X	26	ARG
25	Z	30	ARG
33	b	57	ASN
34	c	7	ASN
34	c	24	ASN
35	d	99	ASN
36	e	145	ASN
36	e	156	ARG
37	f	45	ARG
38	g	147	ASN
39	h	2	MET
39	h	37	ASN
39	h	79	ARG
40	i	3	ASN
40	i	17	ARG
40	i	105	ARG
41	j	16	ARG
42	k	30	ILE
42	k	118	ASN
45	n	85	ARG
46	o	86	LEU
50	s	2	ARG
51	t	20	ASN
54	w	14	ASN
54	w	16	ILE
54	w	33	LYS
54	w	34	LYS
56	z	8	ASN
56	z	200	ARG
56	z	245	ARG
56	z	255	ASN
56	z	276	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	z	337	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	32	ASN
4	D	42	ASN
4	D	150	GLN
4	D	164	GLN
7	G	37	ASN
7	G	138	GLN
8	H	66	ASN
9	J	40	HIS
14	O	38	GLN
15	P	2	ASN
15	P	11	GLN
16	Q	43	GLN
17	R	6	GLN
17	R	18	GLN
17	R	43	ASN
17	R	91	GLN
18	S	7	HIS
18	S	9	HIS
19	T	15	HIS
20	U	68	ASN
22	W	8	ASN
33	b	18	GLN
33	b	57	ASN
33	b	119	GLN
34	c	7	ASN
34	c	24	ASN
34	c	189	HIS
35	d	151	GLN
36	e	145	ASN
37	f	55	HIS
37	f	63	ASN
38	g	147	ASN
39	h	3	GLN
39	h	37	ASN
39	h	66	GLN
39	h	75	GLN
40	i	3	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	i	4	GLN
40	i	30	ASN
40	i	49	GLN
42	k	118	ASN
44	m	7	ASN
45	n	60	GLN
47	p	18	GLN
47	p	63	GLN
47	p	79	ASN
48	q	30	HIS
49	r	51	GLN
50	s	51	HIS
51	t	2	ASN
51	t	20	ASN
54	w	5	GLN
54	w	21	HIS
54	w	32	ASN
56	z	8	ASN
56	z	38	ASN
56	z	199	HIS
56	z	252	GLN
56	z	276	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2898/2903 (99%)	588 (20%)	29 (1%)
2	B	119/120 (99%)	27 (22%)	2 (1%)
32	a	1538/1539 (99%)	272 (17%)	0
53	v	5/6 (83%)	0	0
55	x	76/77 (98%)	14 (18%)	0
All	All	4636/4645 (99%)	901 (19%)	31 (0%)

All (901) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	15	G
1	A	23	G
1	A	34	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	35	G
1	A	36	G
1	A	46	G
1	A	51	G
1	A	52	A
1	A	55	G
1	A	60	G
1	A	63	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	92	U
1	A	96	C
1	A	100	U
1	A	118	A
1	A	119	A
1	A	120	U
1	A	125	A
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	149	A
1	A	162	U
1	A	163	C
1	A	181	A
1	A	196	A
1	A	199	A
1	A	215	G
1	A	216	A
1	A	219	A
1	A	220	G
1	A	221	A
1	A	222	A
1	A	225	C
1	A	233	A
1	A	239	C
1	A	241	A
1	A	242	G
1	A	243	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	248	G
1	A	249	C
1	A	250	G
1	A	255	A
1	A	265	A
1	A	266	G
1	A	267	C
1	A	273	G
1	A	275	C
1	A	276	U
1	A	277	G
1	A	278	A
1	A	281	C
1	A	285	G
1	A	294	A
1	A	311	A
1	A	323	C
1	A	329	G
1	A	330	A
1	A	335	C
1	A	346	A
1	A	357	C
1	A	361	G
1	A	367	G
1	A	370	G
1	A	371	A
1	A	372	G
1	A	386	G
1	A	387	U
1	A	395	U
1	A	403	U
1	A	404	A
1	A	406	G
1	A	411	G
1	A	412	A
1	A	424	G
1	A	440	C
1	A	455	C
1	A	467	G
1	A	473	G
1	A	481	G
1	A	489	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	490	C
1	A	491	G
1	A	496	G
1	A	504	A
1	A	505	A
1	A	509	C
1	A	510	C
1	A	529	A
1	A	532	A
1	A	533	G
1	A	543	G
1	A	545	U
1	A	547	A
1	A	548	G
1	A	550	C
1	A	563	A
1	A	565	C
1	A	566	U
1	A	573	U
1	A	575	A
1	A	603	A
1	A	613	A
1	A	614	A
1	A	615	U
1	A	616	A
1	A	621	A
1	A	622	G
1	A	627	A
1	A	632	A
1	A	634	C
1	A	637	A
1	A	645	C
1	A	646	U
1	A	653	U
1	A	654	A
1	A	655	A
1	A	659	G
1	A	668	A
1	A	669	G
1	A	670	A
1	A	677	A
1	A	685	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	686	U
1	A	694	U
1	A	695	G
1	A	696	G
1	A	704	G
1	A	714	U
1	A	717	C
1	A	726	G
1	A	730	A
1	A	747	C
1	A	748	G
1	A	752	A
1	A	765	C
1	A	775	G
1	A	776	G
1	A	782	A
1	A	783	A
1	A	784	G
1	A	785	G
1	A	788	A
1	A	805	G
1	A	811	U
1	A	812	C
1	A	819	A
1	A	822	G
1	A	827	U
1	A	828	U
1	A	831	G
1	A	838	C
1	A	845	A
1	A	846	U
1	A	847	U
1	A	856	G
1	A	858	G
1	A	859	G
1	A	869	G
1	A	876	C
1	A	878	A
1	A	885	C
1	A	892	A
1	A	893	C
1	A	895	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	896	A
1	A	897	C
1	A	898	C
1	A	905	A
1	A	907	G
1	A	910	A
1	A	914	G
1	A	927	A
1	A	933	A
1	A	934	U
1	A	941	A
1	A	945	A
1	A	946	C
1	A	953	G
1	A	957	C
1	A	961	C
1	A	973	A
1	A	974	G
1	A	975	A
1	A	983	A
1	A	985	C
1	A	995	C
1	A	996	A
1	A	997	G
1	A	999	U
1	A	1009	A
1	A	1012	U
1	A	1013	C
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1025	G
1	A	1026	G
1	A	1033	U
1	A	1046	A
1	A	1047	G
1	A	1057	A
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1063	G
1	A	1064	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1065	U
1	A	1066	U
1	A	1068	G
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1073	A
1	A	1074	G
1	A	1076	C
1	A	1079	C
1	A	1083	U
1	A	1084	A
1	A	1088	A
1	A	1089	A
1	A	1090	A
1	A	1095	A
1	A	1096	A
1	A	1098	A
1	A	1099	G
1	A	1101	U
1	A	1104	C
1	A	1106	G
1	A	1111	A
1	A	1112	G
1	A	1130	U
1	A	1132	U
1	A	1133	A
1	A	1135	C
1	A	1136	G
1	A	1142	A
1	A	1143	A
1	A	1157	G
1	A	1172	C
1	A	1174	U
1	A	1175	A
1	A	1177	G
1	A	1179	G
1	A	1180	U
1	A	1186	G
1	A	1204	A
1	A	1209	U
1	A	1211	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1212	G
1	A	1236	G
1	A	1237	A
1	A	1238	G
1	A	1244	A
1	A	1252	G
1	A	1253	A
1	A	1256	G
1	A	1257	C
1	A	1262	A
1	A	1265	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1275	A
1	A	1300	G
1	A	1301	A
1	A	1306	C
1	A	1311	G
1	A	1312	U
1	A	1314	C
1	A	1320	C
1	A	1321	A
1	A	1322	A
1	A	1329	U
1	A	1332	G
1	A	1341	G
1	A	1345	C
1	A	1352	U
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1386	C
1	A	1395	A
1	A	1411	U
1	A	1416	G
1	A	1419	A
1	A	1420	A
1	A	1421	G
1	A	1427	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1428	C
1	A	1437	C
1	A	1449	G
1	A	1454	C
1	A	1456	G
1	A	1458	U
1	A	1461	C
1	A	1482	G
1	A	1490	A
1	A	1491	G
1	A	1493	C
1	A	1497	U
1	A	1504	A
1	A	1515	A
1	A	1522	A
1	A	1524	G
1	A	1529	G
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1538	G
1	A	1539	U
1	A	1554	U
1	A	1555	G
1	A	1558	C
1	A	1559	U
1	A	1560	G
1	A	1565	C
1	A	1567	G
1	A	1569	A
1	A	1578	U
1	A	1583	A
1	A	1607	C
1	A	1608	A
1	A	1610	A
1	A	1627	G
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1654	A
1	A	1674	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1677	A
1	A	1694	C
1	A	1698	A
1	A	1715	G
1	A	1729	U
1	A	1730	C
1	A	1732	C
1	A	1733	G
1	A	1738	G
1	A	1744	A
1	A	1757	A
1	A	1758	U
1	A	1764	C
1	A	1769	U
1	A	1773	A
1	A	1784	A
1	A	1786	A
1	A	1787	A
1	A	1791	A
1	A	1800	C
1	A	1801	A
1	A	1802	A
1	A	1808	A
1	A	1811	G
1	A	1816	C
1	A	1820	U
1	A	1821	A
1	A	1829	A
1	A	1833	C
1	A	1857	G
1	A	1870	C
1	A	1871	A
1	A	1896	G
1	A	1900	A
1	A	1901	A
1	A	1906	G
1	A	1910	G
1	A	1912	A
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1934	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1936	A
1	A	1937	A
1	A	1940	U
1	A	1941	C
1	A	1942	C
1	A	1943	U
1	A	1944	U
1	A	1955	U
1	A	1966	A
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1991	U
1	A	1993	U
1	A	1997	C
1	A	2004	G
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2030	A
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2035	G
1	A	2043	C
1	A	2052	A
1	A	2053	G
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2068	U
1	A	2069	A
1	A	2077	A
1	A	2093	G
1	A	2096	C
1	A	2100	G
1	A	2108	A
1	A	2110	G
1	A	2111	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2112	G
1	A	2113	U
1	A	2115	G
1	A	2118	U
1	A	2120	G
1	A	2122	U
1	A	2125	G
1	A	2127	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2137	U
1	A	2141	G
1	A	2145	C
1	A	2146	C
1	A	2147	A
1	A	2155	U
1	A	2156	G
1	A	2162	G
1	A	2164	C
1	A	2168	G
1	A	2170	A
1	A	2171	A
1	A	2172	U
1	A	2173	A
1	A	2177	C
1	A	2178	C
1	A	2184	A
1	A	2189	U
1	A	2191	A
1	A	2192	U
1	A	2198	A
1	A	2203	U
1	A	2204	G
1	A	2211	A
1	A	2213	U
1	A	2219	U
1	A	2225	A
1	A	2226	C
1	A	2238	G
1	A	2239	G
1	A	2250	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2251	G
1	A	2278	A
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2300	C
1	A	2305	U
1	A	2307	G
1	A	2309	A
1	A	2322	A
1	A	2325	G
1	A	2327	A
1	A	2331	G
1	A	2333	A
1	A	2334	U
1	A	2336	A
1	A	2345	G
1	A	2347	C
1	A	2350	C
1	A	2361	G
1	A	2383	G
1	A	2385	C
1	A	2391	G
1	A	2392	A
1	A	2399	G
1	A	2402	U
1	A	2403	C
1	A	2406	A
1	A	2407	A
1	A	2423	U
1	A	2426	A
1	A	2427	C
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2435	A
1	A	2441	U
1	A	2445	G
1	A	2447	G
1	A	2448	A
1	A	2465	C
1	A	2470	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2474	U
1	A	2476	A
1	A	2492	U
1	A	2498	C
1	A	2502	G
1	A	2503	A
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2529	G
1	A	2535	G
1	A	2547	A
1	A	2554	U
1	A	2556	C
1	A	2566	A
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2582	G
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2609	U
1	A	2613	U
1	A	2615	U
1	A	2621	G
1	A	2629	U
1	A	2632	A
1	A	2646	C
1	A	2654	A
1	A	2655	G
1	A	2661	G
1	A	2668	G
1	A	2671	G
1	A	2684	U
1	A	2689	U
1	A	2690	U
1	A	2707	U
1	A	2714	G
1	A	2716	C
1	A	2718	G
1	A	2724	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2727	A
1	A	2732	G
1	A	2733	A
1	A	2744	G
1	A	2748	A
1	A	2757	A
1	A	2765	A
1	A	2778	A
1	A	2779	U
1	A	2791	G
1	A	2793	C
1	A	2794	C
1	A	2799	A
1	A	2800	A
1	A	2808	G
1	A	2809	A
1	A	2812	G
1	A	2818	U
1	A	2820	A
1	A	2821	A
1	A	2823	A
1	A	2833	U
1	A	2836	U
1	A	2849	U
1	A	2861	U
1	A	2867	G
1	A	2873	A
1	A	2880	C
1	A	2885	G
1	A	2886	A
1	A	2887	A
1	A	2889	C
1	A	2891	U
1	A	2893	A
1	A	2898	U
1	A	2899	A
1	A	2902	C
2	B	4	C
2	B	12	C
2	B	13	G
2	B	15	A
2	B	24	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	26	C
2	B	31	C
2	B	35	C
2	B	36	C
2	B	40	U
2	B	41	G
2	B	44	G
2	B	45	A
2	B	53	A
2	B	56	G
2	B	57	A
2	B	64	G
2	B	66	A
2	B	67	G
2	B	88	C
2	B	89	U
2	B	90	C
2	B	91	C
2	B	105	G
2	B	108	A
2	B	109	A
2	B	119	A
32	a	4	U
32	a	5	U
32	a	7	A
32	a	9	G
32	a	22	G
32	a	32	A
32	a	39	G
32	a	47	C
32	a	48	C
32	a	50	A
32	a	51	A
32	a	58	C
32	a	71	A
32	a	75	G
32	a	78	A
32	a	79	G
32	a	82	G
32	a	84	U
32	a	85	U
32	a	86	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	87	C
32	a	95	C
32	a	122	G
32	a	130	A
32	a	149	A
32	a	157	U
32	a	163	C
32	a	164	G
32	a	177	G
32	a	181	A
32	a	183	C
32	a	184	G
32	a	189	A
32	a	204	G
32	a	209	U
32	a	210	C
32	a	212	G
32	a	226	G
32	a	240	G
32	a	243	A
32	a	247	G
32	a	248	C
32	a	251	G
32	a	266	G
32	a	267	C
32	a	279	A
32	a	280	C
32	a	281	G
32	a	289	G
32	a	299	G
32	a	306	A
32	a	321	A
32	a	328	C
32	a	340	U
32	a	345	C
32	a	347	G
32	a	351	G
32	a	352	C
32	a	354	G
32	a	367	U
32	a	368	U
32	a	369	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	372	C
32	a	373	A
32	a	375	U
32	a	376	G
32	a	382	A
32	a	392	C
32	a	397	A
32	a	406	G
32	a	412	A
32	a	413	G
32	a	414	A
32	a	421	U
32	a	429	U
32	a	430	A
32	a	438	U
32	a	451	A
32	a	461	A
32	a	462	G
32	a	467	U
32	a	468	A
32	a	474	G
32	a	476	U
32	a	484	G
32	a	485	U
32	a	486	U
32	a	496	A
32	a	497	G
32	a	505	G
32	a	509	A
32	a	511	C
32	a	518	C
32	a	527	G
32	a	531	U
32	a	532	A
32	a	547	A
32	a	561	U
32	a	562	U
32	a	564	C
32	a	572	A
32	a	573	A
32	a	574	A
32	a	575	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	576	C
32	a	577	G
32	a	596	A
32	a	620	C
32	a	633	G
32	a	639	G
32	a	642	A
32	a	661	G
32	a	665	A
32	a	695	A
32	a	703	G
32	a	723	U
32	a	724	G
32	a	731	G
32	a	733	G
32	a	755	G
32	a	774	G
32	a	777	A
32	a	790	A
32	a	794	A
32	a	806	C
32	a	815	A
32	a	817	C
32	a	818	G
32	a	819	A
32	a	820	U
32	a	821	G
32	a	829	G
32	a	832	G
32	a	836	G
32	a	843	U
32	a	844	G
32	a	845	A
32	a	846	G
32	a	851	G
32	a	872	A
32	a	884	U
32	a	887	G
32	a	889	A
32	a	890	G
32	a	891	U
32	a	902	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	914	A
32	a	926	G
32	a	933	G
32	a	934	C
32	a	935	A
32	a	939	G
32	a	948	C
32	a	960	U
32	a	961	U
32	a	966	G
32	a	969	A
32	a	971	G
32	a	975	A
32	a	976	G
32	a	987	G
32	a	991	U
32	a	992	U
32	a	993	G
32	a	994	A
32	a	1004	A
32	a	1006	G
32	a	1009	U
32	a	1020	G
32	a	1022	A
32	a	1027	C
32	a	1028	C
32	a	1031	C
32	a	1032	G
32	a	1033	G
32	a	1034	G
32	a	1035	A
32	a	1045	C
32	a	1046	A
32	a	1065	U
32	a	1070	U
32	a	1085	U
32	a	1092	A
32	a	1094	G
32	a	1095	U
32	a	1101	A
32	a	1130	A
32	a	1133	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	1136	C
32	a	1137	C
32	a	1138	G
32	a	1139	G
32	a	1142	G
32	a	1151	A
32	a	1152	A
32	a	1159	U
32	a	1167	A
32	a	1168	U
32	a	1183	U
32	a	1184	G
32	a	1191	A
32	a	1196	A
32	a	1201	A
32	a	1202	U
32	a	1212	U
32	a	1227	A
32	a	1228	C
32	a	1238	A
32	a	1241	G
32	a	1250	A
32	a	1253	G
32	a	1257	A
32	a	1258	G
32	a	1260	G
32	a	1275	A
32	a	1278	G
32	a	1279	G
32	a	1280	A
32	a	1281	C
32	a	1282	C
32	a	1286	U
32	a	1287	A
32	a	1290	G
32	a	1297	G
32	a	1298	U
32	a	1300	G
32	a	1301	U
32	a	1305	G
32	a	1306	A
32	a	1312	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	1317	C
32	a	1322	C
32	a	1331	G
32	a	1332	A
32	a	1336	C
32	a	1340	A
32	a	1346	A
32	a	1347	G
32	a	1353	G
32	a	1363	A
32	a	1370	G
32	a	1379	G
32	a	1381	U
32	a	1395	C
32	a	1397	C
32	a	1398	A
32	a	1400	C
32	a	1406	U
32	a	1419	G
32	a	1429	A
32	a	1433	A
32	a	1434	A
32	a	1446	A
32	a	1448	C
32	a	1452	C
32	a	1453	G
32	a	1487	G
32	a	1492	A
32	a	1493	A
32	a	1494	G
32	a	1497	G
32	a	1502	A
32	a	1503	A
32	a	1506	U
32	a	1517	G
32	a	1519	A
32	a	1529	G
32	a	1530	G
32	a	1534	A
32	a	1535	C
32	a	1536	C
32	a	1537	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	x	3	G
55	x	4	U
55	x	5	G
55	x	6	A
55	x	8	U
55	x	17	C
55	x	19	G
55	x	20	U
55	x	21	A
55	x	47	U
55	x	59	A
55	x	65	U
55	x	66	A
55	x	76	A

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	86	G
1	A	91	A
1	A	242	G
1	A	546	U
1	A	774	G
1	A	784	G
1	A	858	G
1	A	1020	A
1	A	1022	G
1	A	1111	A
1	A	1182	G
1	A	1190	G
1	A	1236	G
1	A	1300	G
1	A	1331	G
1	A	1378	A
1	A	1399	C
1	A	1432	G
1	A	1490	A
1	A	1626	A
1	A	1930	G
1	A	1940	U
1	A	2286	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2326	C
1	A	2391	G
1	A	2756	U
1	A	2798	U
1	A	2808	G
2	B	44	G
2	B	52	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.