



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Oct 10, 2017 – 05:17 PM EDT

PDB ID : 5XXB
EMDB ID: : EMD-6778
Title : Large subunit of Toxoplasma gondii ribosome
Authors : Li, Z.; Guo, Q.; Zheng, L.; Ji, Y.; Xie, Y.; Lai, D.; Lun, Z.; Suo, X.; Gao, N.
Deposited on : unknown
Resolution : 3.17 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.

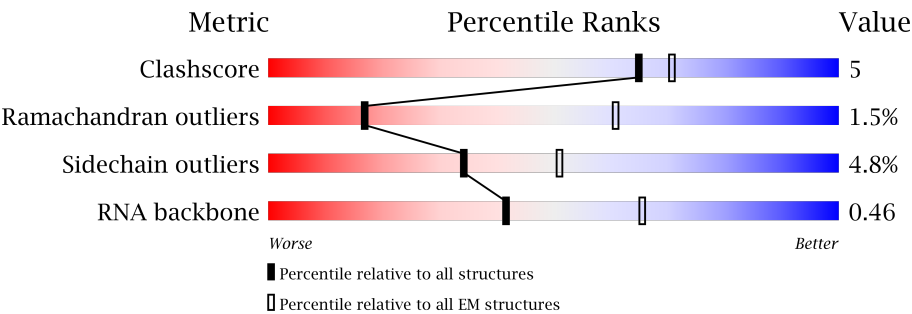
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.17 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	1	3477	64% 23% • 12%
2	3	124	77% 18% 5%
3	4	158	76% 22% ••
4	A	260	88% 6% • 5%
5	B	389	79% 15% • 5%
6	C	416	87% 7% 5%
7	D	310	79% 5% 16%
8	E	193	58% 6% 36%









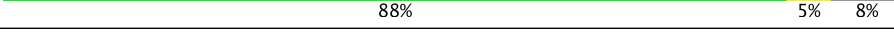
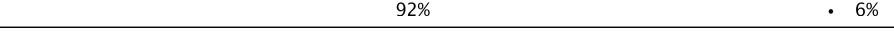
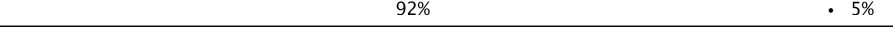
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Mol	Chain	Length	Quality of chain
9	F	258	
10	G	276	
11	H	190	
12	I	221	
13	J	175	
14	K	355	
15	L	134	
16	M	205	
17	N	269	
18	O	195	
19	P	187	
20	Q	187	
21	R	183	
22	S	157	
23	T	133	
24	U	139	
25	V	155	
26	W	167	
27	X	141	
28	Y	146	
29	Z	147	
30	a	54	
31	b	108	
32	c	120	
33	d	134	

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Mol	Chain	Length	Quality of chain
34	e	112	 88%6%6%
35	f	134	 74%6%20%
36	g	123	 91%7%.
37	h	101	 93%. .
38	i	98	 81%8%11%
39	j	84	 82%.14%
40	k	51	 84%10%. .
41	l	129	 38%.60%
42	n	105	 88%5%8%
43	o	96	 92%.6%
44	p	129	 92%.5%

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 121433 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 25S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	3077	Total	C	N	O	P	0	0
			65598	29312	11639	21570	3077		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	118	Total	C	N	O	P	0	0
			2519	1123	452	826	118		

- Molecule 3 is a RNA chain called 5.8S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	157	Total	C	N	O	P	0	0
			3339	1493	586	1103	157		

- Molecule 4 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	246	Total	C	N	O	S	0	0
			1882	1170	379	324	9		

- Molecule 5 is a protein called Ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	369	Total	C	N	O	S	0	0
			2942	1867	561	496	18		

- Molecule 6 is a protein called Ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	394	Total	C	N	O	S	0	0
			3060	1897	621	528	14		

- Molecule 7 is a protein called Ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	261	Total	C	N	O	S	0	0
			2123	1336	406	375	6		

- Molecule 8 is a protein called Ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	124	Total	C	N	O	S	0	0
			971	621	177	170	3		

- Molecule 9 is a protein called Ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	250	Total	C	N	O	S	0	0
			2059	1324	389	338	8		

- Molecule 10 is a protein called Ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	233	Total	C	N	O	S	0	0
			1877	1192	357	319	9		

- Molecule 11 is a protein called Ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	187	Total	C	N	O	S	0	0
			1478	938	264	266	10		

- Molecule 12 is a protein called Ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	193	Total	C	N	O	S	0	0
			1540	976	296	258	10		

- Molecule 13 is a protein called Ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	166	Total	C	N	O	S	0	0
			1343	845	258	236	4		

- Molecule 14 is a protein called Ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	199	Total	C	N	O	S	0	0
			1593	1006	321	262	4		

- Molecule 15 is a protein called Ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	131	Total	C	N	O	S	0	0
			1063	674	203	180	6		

- Molecule 16 is a protein called Ribosomal protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	202	Total	C	N	O	S	0	0
			1683	1060	350	268	5		

- Molecule 17 is a protein called Ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	200	Total	C	N	O	S	0	0
			1645	1034	330	272	9		

- Molecule 18 is a protein called Ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	158	Total	C	N	O	S	0	0
			1286	805	249	222	10		

- Molecule 19 is a protein called Ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	186	Total	C	N	O	S	0	0
			1477	918	306	246	7		

- Molecule 20 is a protein called Ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	176	Total	C	N	O	S	0	0
			1473	918	309	236	10		

- Molecule 21 is a protein called Ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	182	Total	C	N	O	S	0	0
			1492	953	282	250	7		

- Molecule 22 is a protein called Ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	154	Total	C	N	O	S	0	0
			1231	775	242	208	6		

- Molecule 23 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	99	Total	C	N	O	S	0	0
			827	531	147	145	4		

- Molecule 24 is a protein called Ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	129	Total	C	N	O	S	0	0
			968	613	178	168	9		

- Molecule 25 is a protein called Ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	63	Total	C	N	O	S	0	0
			533	344	104	82	3		

- Molecule 26 is a protein called Ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	127	Total	C	N	O	S	0	0
			1038	655	194	186	3		

- Molecule 27 is a protein called Ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	124	Total	C	N	O	S	0	0
			1011	629	207	172	3		

- Molecule 28 is a protein called Ribosomal protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	144	Total	C	N	O	S	0	0
			1163	751	214	191	7		

- Molecule 29 is a protein called Ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	145	Total	C	N	O	S	0	0
			1136	724	221	186	5		

- Molecule 30 is a protein called Ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	49	Total	C	N	O	S	0	0
			404	243	93	62	6		

- Molecule 31 is a protein called Ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	96	Total	C	N	O	S	0	0
			725	450	134	134	7		

- Molecule 32 is a protein called Ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	107	Total	C	N	O	S	0	0
			908	573	182	151	2		

- Molecule 33 is a protein called Ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	122	Total	C	N	O	S	0	0
			1011	639	203	165	4		

- Molecule 34 is a protein called Ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	105	Total	C	N	O	S	0	0
			854	546	167	140	1		

- Molecule 35 is a protein called Ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	107	Total	C	N	O	S	0	0
			863	535	191	132	5		

- Molecule 36 is a protein called Ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	121	Total	C	N	O	S	0	0
			981	615	199	165	2		

- Molecule 37 is a protein called Ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	97	Total	C	N	O	S	0	0
			772	481	165	125	1		

- Molecule 38 is a protein called Ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	87	Total	C	N	O	S	0	0
			688	418	152	112	6		

- Molecule 39 is a protein called Ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	72	Total	C	N	O	S	0	0
			591	376	112	102	1		

- Molecule 40 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	49	Total	C	N	O	S	0	0
			419	264	94	59	2		

- Molecule 41 is a protein called Ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	52	Total	C	N	O	S	0	0
			419	263	85	66	5		

- Molecule 42 is a protein called Ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	97	Total	C	N	O	S	0	0
			790	503	157	125	5		

- Molecule 43 is a protein called Ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	90	Total	C	N	O	S	0	0
			684	428	137	113	6		

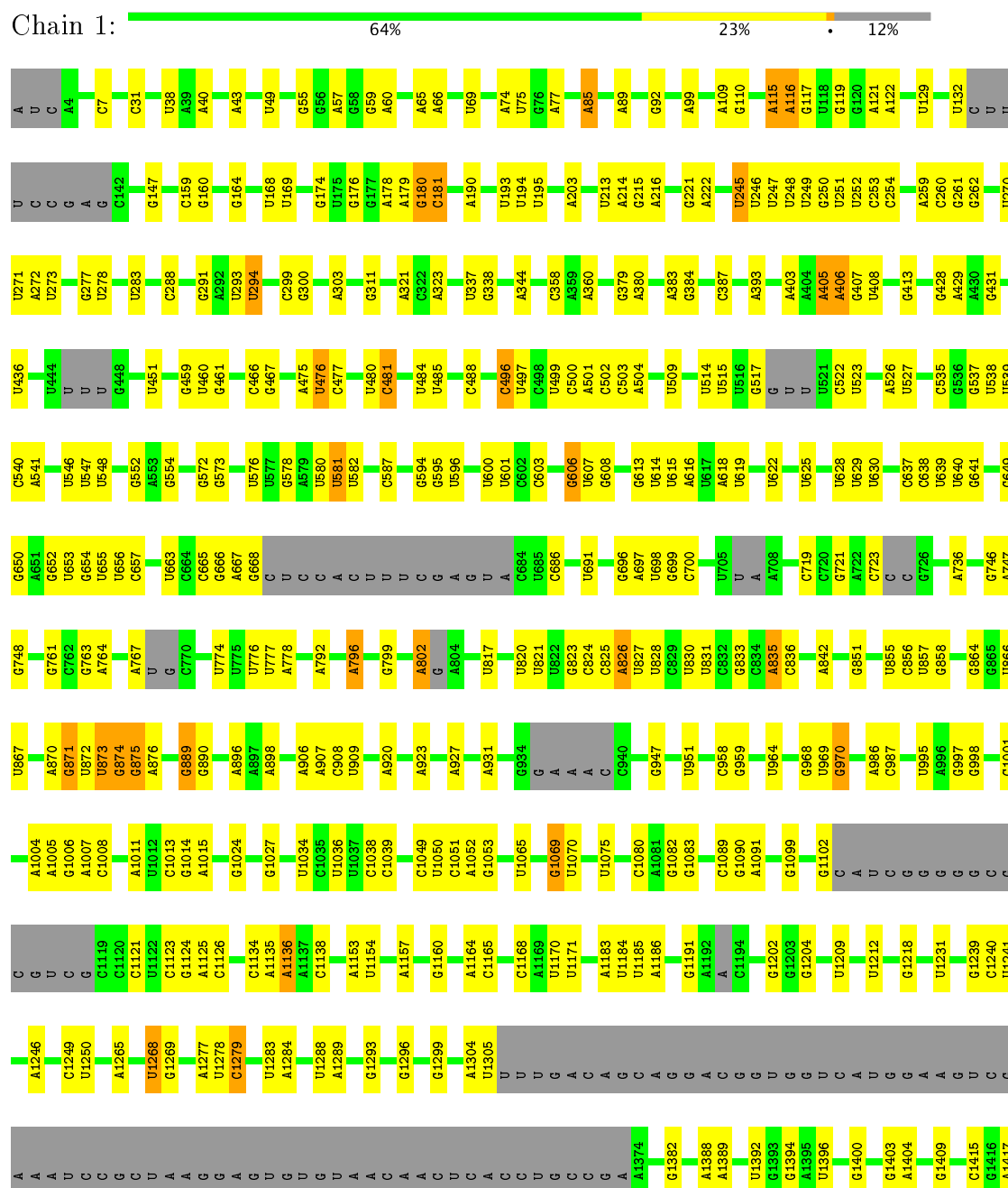
- Molecule 44 is a protein called Ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	122	Total	C	N	O	S	0	0
			974	607	197	161	9		

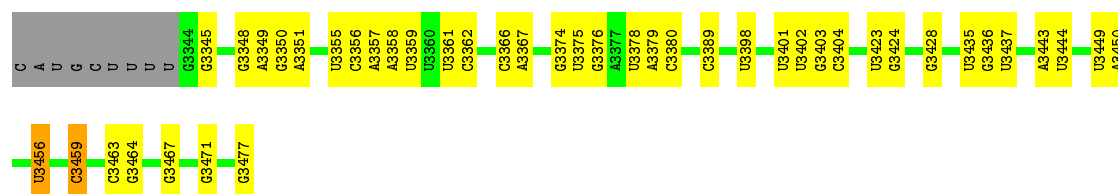
3 Residue-property plots

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: 25S RNA

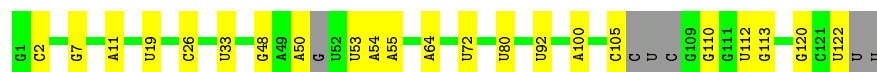




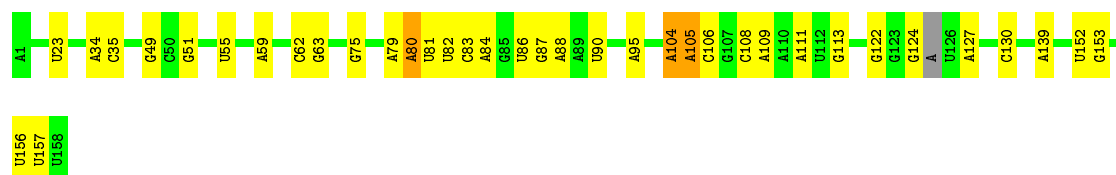
- Molecule 2: 5S RNA

Chain 3: 77% 18% 5%



- Molecule 3: 5.8S RNA

Chain 4: 76% 22% ..



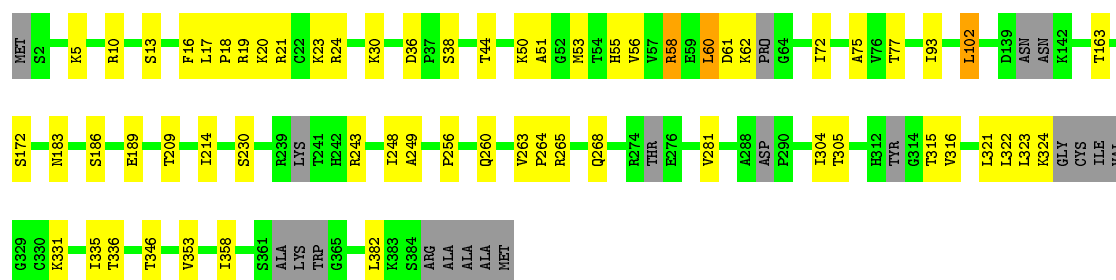
- Molecule 4: Ribosomal protein uL2

Chain A: 88% 6% • 5%



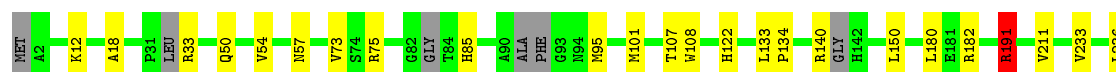
- Molecule 5: Ribosomal protein uL3

Chain B: 79% 15% • 5%

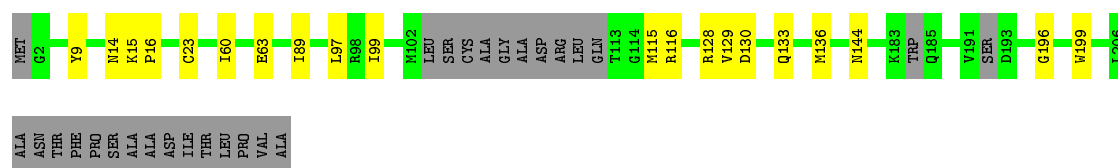


- Molecule 6: Ribosomal protein uL4

Chain C: 87% 7% 5%







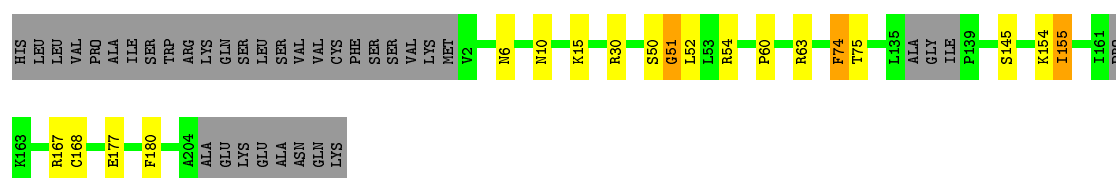
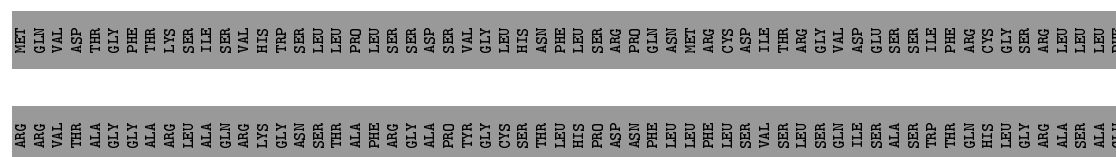
- Molecule 13: Ribosomal protein uL5

Chain J: 81% 13% 5%



- Molecule 14: Ribosomal protein eL13

Chain K: 51% 5% 44%



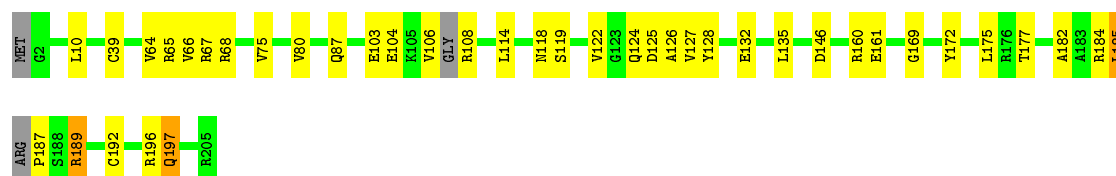
- Molecule 15: Ribosomal protein eL14

Chain L: 82% 12% 6%



- Molecule 16: Ribosomal protein eL15

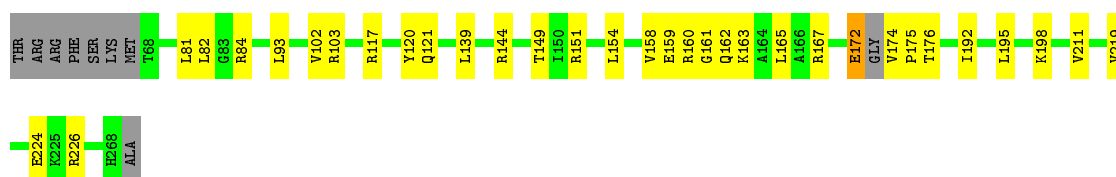
Chain M: 79% 18% 3%



- Molecule 17: Ribosomal protein uL13

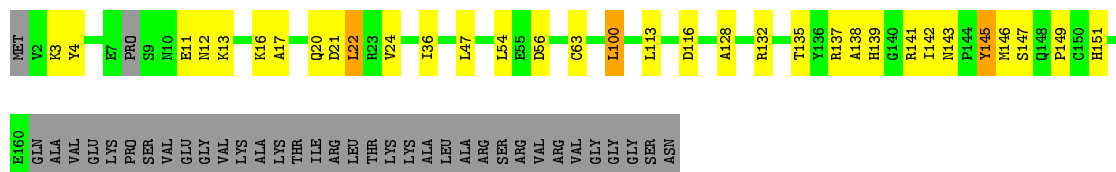
Chain N: 62% 12% 26%





• Molecule 18: Ribosomal protein uL22

Chain O: 64% 15% 19%



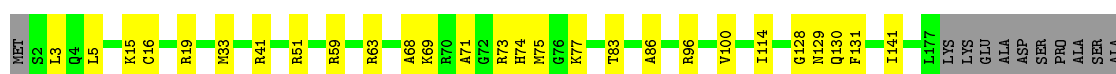
• Molecule 19: Ribosomal protein eL18

Chain P: 83% 14% 3%



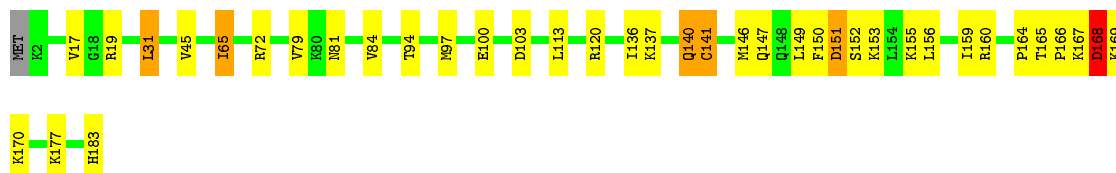
• Molecule 20: Ribosomal protein eL19

Chain Q: 80% 14% 6%



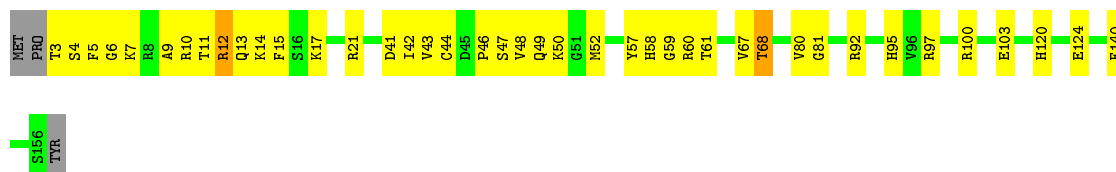
• Molecule 21: Ribosomal protein eL20

Chain R: 78% 18% 4%



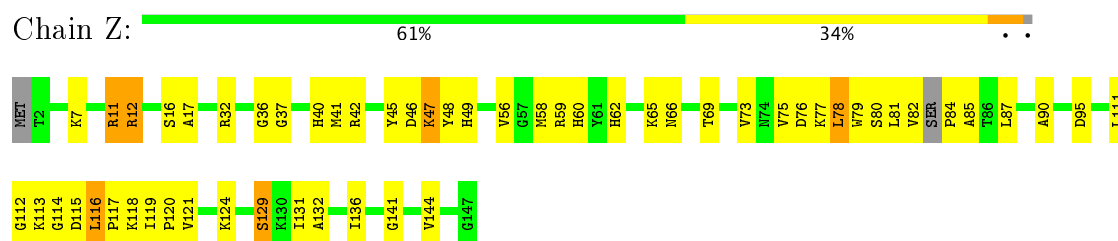
• Molecule 22: Ribosomal protein eL21

Chain S: 72% 25% 3%

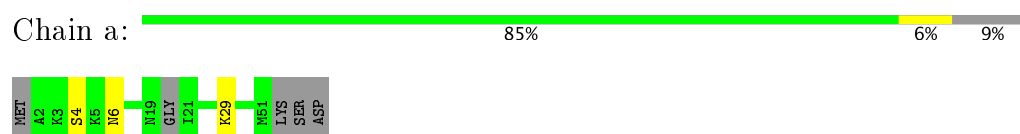


• Molecule 23: Ribosomal protein eL22

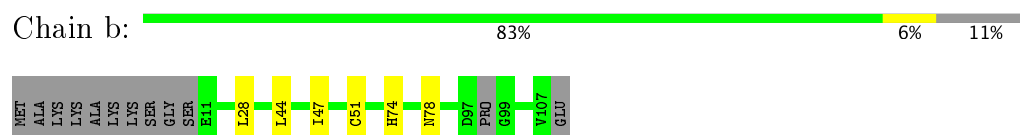
- Molecule 29: Ribosomal protein uL15



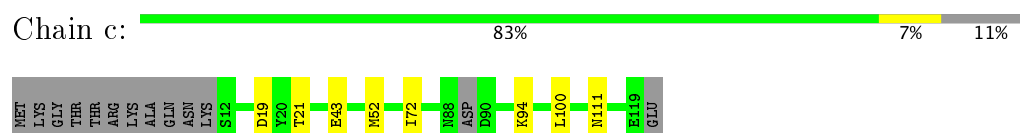
- Molecule 30: Ribosomal protein eL29



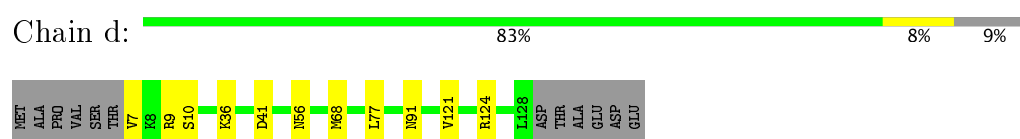
- Molecule 31: Ribosomal protein eL30



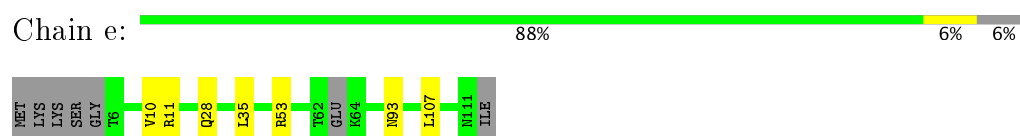
- Molecule 32: Ribosomal protein eL31



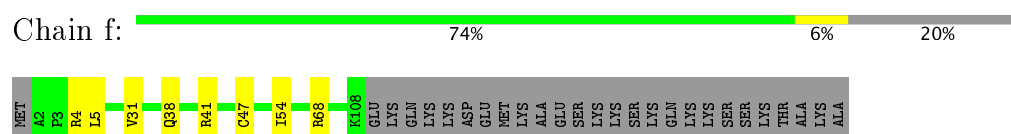
- Molecule 33: Ribosomal protein eL32




- Molecule 34: Ribosomal protein eL33



- Molecule 35: Ribosomal protein eL34



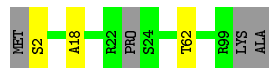
- Molecule 36: Ribosomal protein uL29

Chain g:  91% 7% .




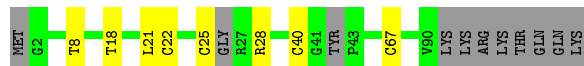
- Molecule 37: Ribosomal protein eL36

Chain h:  93% . .




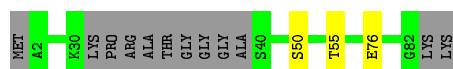
- Molecule 38: Ribosomal protein eL37

Chain i:  81% 8% 11%




- Molecule 39: Ribosomal protein eL38

Chain j:  82% . 14%



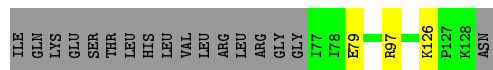
- Molecule 40: Ribosomal protein eL39

Chain k:  84% 10% . .




- Molecule 41: Ribosomal protein eL40

Chain l:  38% . 60%



- Molecule 42: Ribosomal protein eL42

Chain n:  88% 5% 8%



- Molecule 43: Ribosomal protein eL43

Chain o:  92% • 6%



- Molecule 44: Ribosomal protein eL28

Chain p:  92% • 5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	108162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	1	0.22	0/73347	0.68	0/114257
10	G	0.37	0/1905	0.57	0/2546
11	H	0.35	0/1500	0.53	0/2019
12	I	0.40	0/1570	0.62	0/2099
13	J	0.37	0/1366	0.54	0/1823
14	K	0.34	0/1621	0.60	0/2172
15	L	0.39	0/1077	0.63	0/1438
16	M	0.39	0/1715	0.65	0/2289
17	N	0.36	0/1671	0.59	0/2233
18	O	0.42	0/1308	0.66	0/1744
19	P	0.34	0/1498	0.62	0/1992
2	3	0.20	0/2813	0.66	0/4379
20	Q	0.34	0/1491	0.57	0/1970
21	R	0.37	0/1523	0.61	0/2043
22	S	0.40	0/1257	0.59	0/1685
23	T	0.39	0/840	0.59	0/1120
24	U	0.36	0/984	0.58	0/1326
25	V	0.37	0/547	0.59	0/728
26	W	0.36	0/1054	0.62	0/1420
27	X	0.38	0/1026	0.63	0/1367
28	Y	0.40	0/1182	0.59	0/1573
29	Z	0.48	0/1161	0.72	0/1549
3	4	0.23	0/3731	0.67	0/5808
30	a	0.30	0/408	0.59	0/531
31	b	0.39	0/732	0.56	0/980
32	c	0.38	0/925	0.65	0/1239
33	d	0.36	0/1029	0.71	0/1370
34	e	0.35	0/872	0.60	0/1170
35	f	0.37	0/881	0.68	0/1183
36	g	0.37	0/987	0.62	0/1306
37	h	0.37	0/779	0.66	0/1033
38	i	0.47	0/700	0.79	0/923
39	j	0.37	0/599	0.55	0/800
4	A	0.33	0/1918	0.61	0/2572

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
40	k	0.47	0/428	0.77	0/566
41	l	0.42	0/426	0.64	0/566
42	n	0.33	0/802	0.54	0/1057
43	o	0.36	0/693	0.60	0/923
44	p	0.34	0/984	0.60	0/1307
5	B	0.37	0/3006	0.58	0/4023
6	C	0.35	0/3104	0.59	0/4164
7	D	0.35	0/2158	0.56	0/2891
8	E	0.35	0/981	0.54	0/1311
9	F	0.36	0/2102	0.55	0/2811
All	All	0.29	0/130701	0.66	0/192306

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	65598	0	33041	211	0
2	3	2519	0	1277	0	0
3	4	3339	0	1684	3	0
4	A	1882	0	1944	8	0
5	B	2942	0	3034	54	0
6	C	3060	0	3193	22	0
7	D	2123	0	2166	8	0
8	E	971	0	1047	4	0
9	F	2059	0	2185	11	0
10	G	1877	0	2005	15	0
11	H	1478	0	1549	7	0
12	I	1540	0	1584	11	0
13	J	1343	0	1370	24	0
14	K	1593	0	1711	13	0
15	L	1063	0	1142	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	M	1683	0	1768	55	0
17	N	1645	0	1747	20	0
18	O	1286	0	1325	40	0
19	P	1477	0	1587	43	0
20	Q	1473	0	1600	22	0
21	R	1492	0	1571	40	0
22	S	1231	0	1272	56	0
23	T	827	0	865	50	0
24	U	968	0	1014	14	0
25	V	533	0	555	3	0
26	W	1038	0	1095	4	0
27	X	1011	0	1089	13	0
28	Y	1163	0	1268	70	0
29	Z	1136	0	1194	91	0
30	a	404	0	436	0	0
31	b	725	0	747	0	0
32	c	908	0	942	0	0
33	d	1011	0	1080	0	0
34	e	854	0	897	0	0
35	f	863	0	912	0	0
36	g	981	0	1102	0	0
37	h	772	0	856	0	0
38	i	688	0	703	0	0
39	j	591	0	636	0	0
40	k	419	0	464	0	0
41	l	419	0	464	0	0
42	n	790	0	886	0	0
43	o	684	0	738	0	0
44	p	974	0	1058	0	0
All	All	121433	0	88803	754	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 5.

All (754) 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)
1:1:1436:A:C2	6:C:299:GLU:HG3	1.28	1.67
22:S:49:GLN:HA	22:S:52:MET:CE	1.01	1.47
22:S:49:GLN:CA	22:S:52:MET:CE	1.92	1.44
1:1:1436:A:N1	6:C:299:GLU:HG3	1.31	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:122:PHE:CD2	28:Y:141:ARG:HG2	1.57	1.38
22:S:49:GLN:CA	22:S:52:MET:HE3	1.51	1.37
1:1:496:C:C5	29:Z:82:VAL:HG11	1.58	1.36
28:Y:122:PHE:CD2	28:Y:141:ARG:CG	2.11	1.33
1:1:1436:A:C2	6:C:299:GLU:CG	2.15	1.28
13:J:17:LYS:HE2	13:J:131:GLN:CD	1.52	1.28
29:Z:90:ALA:O	29:Z:119:ILE:HD11	1.32	1.27
21:R:100:GLU:OE1	21:R:141:CYS:SG	1.94	1.26
17:N:172:GLU:OE1	17:N:219:VAL:HG21	1.29	1.26
16:M:187:PRO:HD2	16:M:192:CYS:SG	1.77	1.23
21:R:100:GLU:CD	21:R:141:CYS:SG	2.17	1.22
1:1:2045:U:C5	20:Q:73:ARG:NH1	2.06	1.22
22:S:15:PHE:O	22:S:46:PRO:HG3	1.36	1.21
18:O:20:GLN:O	18:O:151:HIS:HD2	1.24	1.20
18:O:135:THR:OG1	18:O:145:TYR:CD1	1.95	1.20
1:1:496:C:N4	29:Z:82:VAL:HG21	1.59	1.18
1:1:1949:C:N3	18:O:142:ILE:HD11	1.57	1.18
13:J:17:LYS:HE2	13:J:131:GLN:OE1	1.45	1.16
29:Z:90:ALA:O	29:Z:119:ILE:CD1	1.93	1.16
16:M:64:VAL:HG21	16:M:106:VAL:CG2	1.76	1.16
28:Y:122:PHE:HD2	28:Y:141:ARG:CG	1.49	1.15
1:1:496:C:C5	29:Z:82:VAL:CG1	2.31	1.13
23:T:109:ARG:HH21	23:T:111:VAL:CG2	1.64	1.11
18:O:20:GLN:O	18:O:151:HIS:CD2	2.03	1.10
1:1:3313:U:O4	21:R:169:LYS:HE3	1.51	1.10
1:1:2045:U:C6	20:Q:73:ARG:NH1	2.16	1.10
16:M:64:VAL:CG2	16:M:106:VAL:CG2	2.30	1.09
1:1:1039:C:OP1	19:P:10:ARG:NH2	1.85	1.08
12:I:14:ASN:O	12:I:128:ARG:NH2	1.87	1.08
1:1:1436:A:N1	6:C:299:GLU:CG	2.16	1.05
1:1:180:G:O2'	1:1:181:C:H6	1.39	1.05
16:M:68:ARG:HH22	16:M:124:GLN:NE2	1.54	1.04
23:T:109:ARG:HH21	23:T:111:VAL:HG22	1.18	1.04
17:N:172:GLU:OE1	17:N:219:VAL:CG2	2.07	1.02
28:Y:122:PHE:CD2	28:Y:141:ARG:HG3	1.91	1.02
1:1:99:A:OP1	16:M:196:ARG:HD3	1.60	1.01
23:T:57:LYS:HA	23:T:61:LYS:O	1.61	1.01
28:Y:122:PHE:CE2	28:Y:141:ARG:CG	2.43	1.00
29:Z:79:TRP:CH2	29:Z:121:VAL:HG11	1.96	1.00
29:Z:76:ASP:HB2	29:Z:114:GLY:HA3	1.42	1.00
16:M:187:PRO:CD	16:M:192:CYS:SG	2.49	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1039:C:P	19:P:10:ARG:NH2	2.34	1.00
1:1:300:G:OP2	16:M:68:ARG:NH1	1.93	1.00
9:F:146:TYR:CZ	9:F:245:ASN:HB3	1.97	1.00
5:B:60:LEU:HD21	5:B:62:LYS:CG	1.93	0.98
10:G:95:LEU:H	10:G:95:LEU:HD22	4.54	0.98
1:1:2795:C:OP1	13:J:17:LYS:NZ	1.96	0.98
28:Y:122:PHE:CE2	28:Y:141:ARG:HG3	1.98	0.98
1:1:2899:C:OP1	29:Z:56:VAL:O	1.82	0.98
16:M:68:ARG:NH2	16:M:124:GLN:NE2	2.13	0.97
1:1:299:C:OP1	16:M:68:ARG:HG2	1.66	0.96
1:1:85:A:OP2	29:Z:65:LYS:HE3	1.65	0.96
13:J:14:ARG:HE	13:J:135:PRO:HG3	1.30	0.95
22:S:49:GLN:HA	22:S:52:MET:HE1	0.95	0.95
16:M:64:VAL:HG21	16:M:106:VAL:HG23	1.49	0.94
23:T:25:PRO:CB	23:T:83:GLU:OE2	2.15	0.94
16:M:122:VAL:HG11	16:M:132:GLU:HG3	1.47	0.94
18:O:132:ARG:HB3	18:O:132:ARG:NH1	1.83	0.94
1:1:1039:C:P	19:P:10:ARG:HH21	1.92	0.92
22:S:49:GLN:HA	22:S:52:MET:HE3	1.00	0.92
28:Y:100:ALA:HB1	28:Y:106:ASP:CG	1.90	0.91
13:J:17:LYS:HE2	13:J:131:GLN:NE2	1.83	0.91
22:S:49:GLN:HA	22:S:52:MET:HE2	1.51	0.91
22:S:49:GLN:C	22:S:52:MET:HE3	1.91	0.91
1:1:1436:A:H2	6:C:299:GLU:CG	1.67	0.91
10:G:95:LEU:HB2	10:G:99:GLN:HG3	5.42	0.90
1:1:2040:U:O2	20:Q:77:LYS:NZ	2.03	0.90
21:R:155:LYS:O	21:R:156:LEU:HD12	1.71	0.90
28:Y:122:PHE:HD2	28:Y:141:ARG:HG2	0.88	0.90
16:M:68:ARG:HH22	16:M:124:GLN:HE21	1.20	0.89
22:S:15:PHE:O	22:S:46:PRO:CG	2.18	0.89
5:B:60:LEU:HD21	5:B:62:LYS:HG3	1.55	0.89
1:1:299:C:OP1	16:M:68:ARG:CG	2.20	0.88
1:1:496:C:N4	29:Z:82:VAL:CG2	2.35	0.88
28:Y:118:PHE:O	28:Y:122:PHE:HD1	1.56	0.88
29:Z:124:LYS:HG2	29:Z:144:VAL:HB	1.56	0.88
7:D:8:LYS:O	7:D:8:LYS:NZ	7.59	0.87
1:1:2868:U:H5"	22:S:7:LYS:HE2	1.55	0.87
1:1:836:C:OP1	19:P:141:ALA:HB1	1.75	0.87
29:Z:12:ARG:HH11	29:Z:12:ARG:HG3	1.38	0.87
1:1:607:U:O2'	21:R:155:LYS:NZ	2.08	0.87
18:O:4:TYR:CE2	18:O:16:LYS:HD3	2.10	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:54:THR:HA	23:T:63:ASN:ND2	1.89	0.87
28:Y:74:ILE:CB	28:Y:79:LEU:HD21	2.04	0.87
1:1:1643:A:O2'	16:M:108:ARG:NH2	2.08	0.86
23:T:25:PRO:HB2	23:T:83:GLU:OE2	1.73	0.86
23:T:108:MET:HE2	23:T:122:TYR:CZ	2.10	0.86
29:Z:78:LEU:O	29:Z:81:LEU:HB2	1.75	0.85
16:M:127:VAL:HG23	16:M:128:TYR:CD2	2.11	0.85
1:1:1436:A:C2	6:C:299:GLU:HA	2.12	0.85
16:M:64:VAL:HG21	16:M:106:VAL:HG21	1.59	0.85
5:B:51:ALA:O	5:B:331:LYS:HG2	1.77	0.85
28:Y:74:ILE:HB	28:Y:79:LEU:HD21	1.59	0.85
22:S:41:ASP:OD1	22:S:61:THR:OG1	1.94	0.84
13:J:17:LYS:CE	13:J:131:GLN:NE2	2.40	0.84
23:T:109:ARG:NH2	23:T:111:VAL:HG22	1.92	0.84
29:Z:79:TRP:HH2	29:Z:121:VAL:HG11	1.42	0.84
17:N:93:LEU:O	17:N:167:ARG:NH1	2.10	0.84
1:1:1855:C:OP1	20:Q:15:LYS:NZ	2.11	0.84
1:1:1212:U:OP1	12:I:15:LYS:HE3	1.77	0.83
14:K:10:ASN:OD1	19:P:167:ARG:NH1	2.12	0.82
1:1:180:G:O2'	1:1:181:C:C6	2.24	0.82
1:1:872:U:O2'	1:1:873:U:H5'	1.80	0.82
21:R:165:THR:HB	21:R:169:LYS:HD3	1.61	0.82
23:T:102:GLN:O	23:T:104:LEU:CD2	2.27	0.82
1:1:180:G:O6	1:1:245:U:O4	1.97	0.82
28:Y:101:MET:CE	28:Y:107:ARG:HE	1.92	0.82
1:1:180:G:O2'	1:1:181:C:O5'	1.97	0.81
16:M:64:VAL:CG2	16:M:106:VAL:HG21	2.10	0.81
16:M:125:ASP:OD1	16:M:126:ALA:N	2.13	0.81
29:Z:79:TRP:HE1	29:Z:117:PRO:HD2	1.45	0.81
23:T:102:GLN:HB2	23:T:104:LEU:HG	1.64	0.80
1:1:2898:G:H1'	29:Z:58:MET:HE2	1.64	0.80
17:N:102:VAL:CG1	17:N:174:VAL:HG22	2.11	0.80
16:M:189:ARG:HA	16:M:189:ARG:HE	1.46	0.80
23:T:102:GLN:O	23:T:104:LEU:HD21	1.82	0.80
5:B:50:LYS:HB2	5:B:335:ILE:HD11	1.62	0.80
1:1:3313:U:O4	21:R:169:LYS:CE	2.29	0.79
29:Z:84:PRO:HD2	29:Z:85:ALA:H	1.47	0.79
1:1:872:U:H2'	1:1:873:U:C6	2.17	0.79
13:J:17:LYS:CE	13:J:131:GLN:CD	2.44	0.79
13:J:18:LEU:HD12	13:J:19:THR:N	1.98	0.79
28:Y:74:ILE:CG2	28:Y:79:LEU:HD21	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2835:U:OP1	22:S:57:TYR:OH	2.00	0.78
22:S:49:GLN:CA	22:S:52:MET:HE1	1.85	0.78
28:Y:102:ARG:HH11	28:Y:107:ARG:CZ	1.96	0.78
23:T:25:PRO:HB3	23:T:83:GLU:OE2	1.82	0.78
28:Y:5:LEU:CD1	28:Y:76:VAL:HG23	2.14	0.78
1:1:2729:G:OP1	12:I:116:ARG:HD3	1.83	0.77
29:Z:119:ILE:HD12	29:Z:120:PRO:CD	2.14	0.77
1:1:2741:C:OP1	22:S:5:PHE:O	2.02	0.77
29:Z:116:LEU:H	29:Z:116:LEU:HD12	1.49	0.77
15:L:4:PHE:CZ	21:R:159:ILE:HG12	2.20	0.77
1:1:496:C:H5	29:Z:82:VAL:HG11	1.44	0.77
14:K:10:ASN:CG	19:P:167:ARG:NH1	2.38	0.76
19:P:6:GLU:O	19:P:7:ARG:HB3	1.85	0.76
29:Z:79:TRP:CZ2	29:Z:119:ILE:CG2	2.68	0.76
28:Y:122:PHE:CE2	28:Y:141:ARG:HG2	2.12	0.76
23:T:68:ARG:HG3	23:T:83:GLU:HB2	1.68	0.76
1:1:179:A:O2'	1:1:180:G:H5'	1.86	0.75
1:1:1949:C:C4	18:O:142:ILE:HD11	2.22	0.75
27:X:21:ALA:O	27:X:26:ARG:NH1	2.19	0.75
5:B:21:ARG:NH1	5:B:268:GLN:NE2	2.34	0.75
10:G:95:LEU:HD23	10:G:100:THR:OG1	6.28	0.75
9:F:148:TYR:CD2	9:F:247:GLU:O	2.40	0.75
1:1:179:A:C2'	1:1:180:G:H5'	2.17	0.75
1:1:180:G:C6	1:1:245:U:O4	2.40	0.75
1:1:496:C:H41	29:Z:82:VAL:HG21	1.48	0.75
16:M:189:ARG:HE	16:M:189:ARG:CA	1.99	0.74
28:Y:122:PHE:HE2	28:Y:141:ARG:HA	1.52	0.74
15:L:4:PHE:HZ	21:R:159:ILE:HG12	1.52	0.74
15:L:33:ASN:HA	21:R:149:LEU:HD21	1.67	0.74
1:1:496:C:C6	29:Z:82:VAL:CG1	2.70	0.74
29:Z:79:TRP:HH2	29:Z:121:VAL:CG1	2.00	0.74
18:O:22:LEU:HD23	18:O:22:LEU:N	2.03	0.73
23:T:104:LEU:HD23	23:T:104:LEU:N	2.03	0.73
5:B:60:LEU:HD23	5:B:61:ASP:N	2.04	0.73
16:M:64:VAL:HG22	16:M:106:VAL:HG22	1.69	0.73
18:O:135:THR:OG1	18:O:145:TYR:HD1	1.66	0.73
1:1:1436:A:C2	6:C:299:GLU:CA	2.71	0.73
16:M:184:ARG:O	16:M:189:ARG:NH1	2.21	0.73
22:S:49:GLN:C	22:S:52:MET:CE	2.53	0.73
23:T:109:ARG:HH21	23:T:111:VAL:HG21	1.50	0.73
27:X:22:PRO:HG2	27:X:25:VAL:HG23	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:146:TYR:CE2	9:F:245:ASN:HB3	2.24	0.73
21:R:100:GLU:OE2	21:R:141:CYS:SG	2.45	0.73
1:1:872:U:H2'	1:1:873:U:H6	1.52	0.72
1:1:889:G:OP2	29:Z:32:ARG:NH1	2.22	0.72
1:1:2862:A:OP1	22:S:50:LYS:HE2	1.88	0.72
23:T:108:MET:CE	23:T:122:TYR:CZ	2.72	0.72
16:M:64:VAL:HG22	16:M:106:VAL:CG2	2.19	0.72
16:M:64:VAL:CG2	16:M:106:VAL:HG22	2.20	0.72
17:N:102:VAL:HG13	17:N:174:VAL:HG22	1.70	0.72
1:1:796:A:N3	29:Z:58:MET:HE3	2.04	0.72
14:K:15:LYS:HD2	16:M:197:GLN:HE22	1.55	0.72
18:O:132:ARG:HH11	18:O:132:ARG:HB3	1.52	0.72
5:B:21:ARG:HH12	5:B:268:GLN:HE22	1.36	0.72
1:1:2811:G:H5"	22:S:17:LYS:HG2	1.69	0.72
10:G:207:PRO:O	10:G:208:VAL:HG22	1.90	0.71
21:R:166:PRO:HD2	21:R:169:LYS:CD	2.20	0.71
29:Z:36:GLY:HA3	29:Z:40:HIS:CE1	2.26	0.71
1:1:802:A:OP1	29:Z:131:ILE:HB	1.90	0.71
1:1:836:C:P	19:P:141:ALA:HB1	2.31	0.71
28:Y:122:PHE:HE2	28:Y:141:ARG:CA	2.04	0.71
21:R:167:LYS:O	21:R:168:ASP:HB3	1.90	0.71
23:T:54:THR:HA	23:T:63:ASN:HD21	1.55	0.70
28:Y:102:ARG:NH1	28:Y:107:ARG:HG3	2.06	0.70
1:1:3157:G:OP1	5:B:19:ARG:NH2	2.24	0.70
27:X:21:ALA:HB3	27:X:26:ARG:NH1	2.05	0.70
1:1:496:C:C4	29:Z:82:VAL:CG2	2.75	0.70
19:P:13:LYS:CE	19:P:17:ARG:HH12	2.04	0.70
1:1:496:C:C4	29:Z:82:VAL:HG21	2.26	0.70
21:R:136:ILE:CG2	21:R:140:GLN:HB3	2.21	0.70
28:Y:74:ILE:HG21	28:Y:79:LEU:CD2	2.22	0.70
29:Z:119:ILE:HD12	29:Z:120:PRO:HD2	1.73	0.70
1:1:2469:A:N3	18:O:137:ARG:NH2	2.39	0.69
5:B:60:LEU:HD23	5:B:61:ASP:H	1.57	0.69
23:T:26:VAL:HG12	23:T:27:LYS:N	2.07	0.69
29:Z:90:ALA:O	29:Z:119:ILE:HD13	1.87	0.69
28:Y:2:VAL:HG13	28:Y:6:LYS:NZ	2.07	0.69
28:Y:74:ILE:HG21	28:Y:79:LEU:HD21	1.72	0.69
5:B:50:LYS:HB2	5:B:335:ILE:CD1	2.22	0.69
10:G:95:LEU:N	10:G:95:LEU:HD22	4.43	0.69
18:O:128:ALA:HB3	18:O:149:PRO:O	1.92	0.69
5:B:21:ARG:HH12	5:B:268:GLN:NE2	1.89	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:166:PRO:HD2	21:R:169:LYS:HD3	1.75	0.69
28:Y:5:LEU:HD12	28:Y:76:VAL:HG23	1.75	0.69
1:1:1949:C:C2	18:O:142:ILE:HD11	2.27	0.69
1:1:835:A:O3'	19:P:141:ALA:HA	1.93	0.69
1:1:1781:U:O4	23:T:60:GLY:N	2.23	0.68
1:1:3284:U:H2'	17:N:163:LYS:HD3	1.73	0.68
28:Y:101:MET:HE1	28:Y:107:ARG:HE	1.58	0.68
19:P:92:VAL:CG1	29:Z:87:LEU:HD21	2.24	0.68
13:J:17:LYS:CE	13:J:131:GLN:OE1	2.35	0.68
21:R:166:PRO:O	21:R:169:LYS:HB3	1.94	0.68
23:T:103:MET:C	23:T:104:LEU:HD23	2.13	0.68
17:N:154:LEU:HD12	17:N:165:LEU:HD21	1.75	0.68
27:X:47:LEU:HD11	27:X:118:LEU:HD21	1.74	0.68
19:P:13:LYS:HE3	19:P:17:ARG:HH12	1.57	0.68
1:1:1978:G:O6	20:Q:19:ARG:NH1	2.26	0.68
24:U:12:LYS:HG3	24:U:127:LEU:HD21	1.76	0.68
22:S:49:GLN:CB	22:S:52:MET:HE3	2.22	0.68
29:Z:12:ARG:CG	29:Z:12:ARG:HH11	2.04	0.68
28:Y:101:MET:HG3	28:Y:102:ARG:H	1.57	0.67
29:Z:76:ASP:CB	29:Z:114:GLY:HA3	2.21	0.67
22:S:21:ARG:HG3	22:S:21:ARG:HH11	1.58	0.67
23:T:108:MET:CE	23:T:122:TYR:OH	2.42	0.67
1:1:802:A:H5'	29:Z:131:ILE:HD12	1.76	0.67
10:G:95:LEU:N	10:G:95:LEU:HD13	4.92	0.67
15:L:21:ASP:OD1	15:L:21:ASP:N	2.27	0.67
22:S:50:LYS:HG2	22:S:92:ARG:HH21	1.60	0.66
1:1:2868:U:C5'	22:S:7:LYS:HE2	2.24	0.66
1:1:178:A:N6	1:1:179:A:C6	2.63	0.66
1:1:1578:A:O2'	1:1:1961:A:H1'	1.94	0.66
1:1:180:G:HO2'	1:1:181:C:H6	1.10	0.66
22:S:44:CYS:H	22:S:58:HIS:CD2	2.13	0.66
1:1:1039:C:P	19:P:10:ARG:HH22	2.19	0.66
18:O:21:ASP:OD2	18:O:149:PRO:HB2	1.96	0.65
28:Y:2:VAL:HG13	28:Y:6:LYS:CE	2.27	0.65
27:X:22:PRO:HG2	27:X:25:VAL:CG2	2.27	0.65
1:1:3161:C:O2'	5:B:55:HIS:HD2	1.79	0.65
16:M:196:ARG:O	16:M:196:ARG:HG3	1.95	0.65
1:1:299:C:OP1	16:M:68:ARG:HG3	1.97	0.65
1:1:496:C:C5	29:Z:82:VAL:HG13	2.30	0.65
9:F:146:TYR:CZ	9:F:245:ASN:CB	2.78	0.65
21:R:141:CYS:O	21:R:147:GLN:NE2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:7:SER:OG	28:Y:26:VAL:O	2.07	0.65
29:Z:79:TRP:NE1	29:Z:117:PRO:HD2	2.11	0.65
1:1:1135:A:H5''	12:I:16:PRO:HG3	1.78	0.65
1:1:719:C:OP1	17:N:159:GLU:HB2	1.97	0.65
28:Y:75:ASN:HB3	28:Y:78:HIS:CD2	2.32	0.65
13:J:14:ARG:HD2	13:J:135:PRO:HD3	1.79	0.65
14:K:10:ASN:CG	19:P:167:ARG:HH11	1.98	0.65
23:T:102:GLN:O	23:T:104:LEU:HD23	1.95	0.65
28:Y:121:LYS:O	28:Y:125:PRO:HB3	1.97	0.65
1:1:180:G:O2'	1:1:181:C:P	2.54	0.64
23:T:68:ARG:HG3	23:T:83:GLU:CB	2.27	0.64
1:1:1038:C:O3'	19:P:10:ARG:NH2	2.30	0.64
28:Y:100:ALA:HB1	28:Y:106:ASP:OD2	1.97	0.64
28:Y:119:TYR:O	28:Y:123:THR:HG22	1.97	0.64
28:Y:118:PHE:O	28:Y:122:PHE:CD1	2.46	0.63
28:Y:40:CYS:SG	28:Y:79:LEU:CD1	2.87	0.63
29:Z:84:PRO:CD	29:Z:85:ALA:H	2.12	0.63
20:Q:68:ALA:O	20:Q:71:ALA:HB3	1.98	0.63
28:Y:2:VAL:HG13	28:Y:6:LYS:HE3	1.81	0.63
1:1:874:G:O2'	19:P:90:ARG:NH1	2.31	0.62
28:Y:75:ASN:OD1	28:Y:76:VAL:N	2.32	0.62
18:O:4:TYR:CZ	18:O:16:LYS:HD3	2.34	0.62
5:B:53:MET:CE	5:B:75:ALA:HB1	2.30	0.62
29:Z:79:TRP:CZ2	29:Z:119:ILE:HG21	2.35	0.62
6:C:236:LEU:HD22	6:C:241:LEU:HD11	1.82	0.62
14:K:10:ASN:ND2	19:P:167:ARG:HH11	1.97	0.62
23:T:109:ARG:NH2	23:T:111:VAL:CG2	2.49	0.61
1:1:2745:G:O6	22:S:3:THR:HG21	2.00	0.61
5:B:60:LEU:CD2	5:B:62:LYS:CG	2.74	0.61
1:1:802:A:OP2	29:Z:111:LEU:HB3	2.01	0.61
19:P:13:LYS:HE3	19:P:17:ARG:NH1	2.14	0.61
1:1:2835:U:P	22:S:57:TYR:OH	2.58	0.61
18:O:138:ALA:O	18:O:139:HIS:HB2	2.01	0.61
22:S:4:SER:O	22:S:10:ARG:NH1	2.34	0.61
12:I:115:MET:O	12:I:116:ARG:HB2	2.00	0.60
1:1:3313:U:C4	21:R:169:LYS:HE3	2.33	0.60
23:T:108:MET:HE3	23:T:122:TYR:CE1	2.36	0.60
1:1:2749:C:O2	22:S:60:ARG:NH2	2.35	0.60
21:R:165:THR:OG1	21:R:170:LYS:HG3	2.02	0.60
29:Z:82:VAL:HG12	29:Z:82:VAL:O	2.01	0.60
1:1:2468:G:H4'	18:O:145:TYR:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:10:ASN:ND2	19:P:167:ARG:NH1	2.50	0.60
1:1:1436:A:H2	6:C:299:GLU:CD	2.04	0.59
28:Y:5:LEU:HD11	28:Y:76:VAL:HG23	1.84	0.59
1:1:496:C:C4	29:Z:82:VAL:CG1	2.83	0.59
13:J:161:ILE:HG23	13:J:172:VAL:HG11	1.84	0.59
16:M:103:GLU:OE2	16:M:119:SER:OG	2.13	0.59
5:B:16:PHE:O	5:B:17:LEU:HG	2.02	0.59
29:Z:116:LEU:N	29:Z:116:LEU:HD12	2.18	0.59
19:P:143:LYS:HB3	19:P:143:LYS:NZ	2.18	0.59
21:R:136:ILE:HG23	21:R:140:GLN:HB3	1.84	0.59
13:J:18:LEU:HD12	13:J:19:THR:H	1.64	0.59
1:1:294:U:O2	16:M:184:ARG:NH1	2.36	0.59
1:1:3058:G:N3	5:B:249:ALA:HB1	2.17	0.59
22:S:44:CYS:H	22:S:58:HIS:HD2	1.51	0.59
23:T:57:LYS:CA	23:T:61:LYS:O	2.44	0.59
29:Z:111:LEU:HD23	29:Z:129:SER:HB3	1.85	0.59
23:T:96:LYS:HG2	23:T:105:ARG:NH1	2.18	0.59
28:Y:40:CYS:SG	28:Y:79:LEU:HD12	2.43	0.59
28:Y:5:LEU:O	28:Y:6:LYS:HG2	2.02	0.58
1:1:178:A:C5	1:1:179:A:C5	2.91	0.58
23:T:26:VAL:HG12	23:T:27:LYS:H	1.68	0.58
28:Y:73:TYR:OH	28:Y:101:MET:HG2	2.03	0.58
1:1:3253:A:OP1	5:B:23:LYS:NZ	2.37	0.58
1:1:970:G:C8	18:O:138:ALA:CB	2.87	0.58
5:B:93:ILE:HD11	5:B:102:LEU:HG	1.86	0.58
5:B:60:LEU:HD12	5:B:72:ILE:HD11	1.85	0.58
15:L:38:LEU:HD12	21:R:79:VAL:HG23	1.86	0.58
6:C:289:ASN:HB2	6:C:295:ILE:HD11	1.86	0.58
16:M:196:ARG:O	16:M:197:GLN:HG2	2.03	0.58
1:1:3456:U:O2'	1:1:3459:C:OP2	2.22	0.58
18:O:132:ARG:HB3	18:O:132:ARG:CZ	2.33	0.58
28:Y:104:VAL:O	28:Y:104:VAL:HG12	2.03	0.58
10:G:95:LEU:HB2	10:G:99:GLN:CG	5.65	0.58
22:S:48:VAL:O	22:S:52:MET:CE	2.52	0.58
22:S:9:ALA:O	22:S:10:ARG:HB2	2.04	0.58
23:T:83:GLU:OE1	23:T:83:GLU:HA	2.03	0.58
28:Y:122:PHE:CE2	28:Y:141:ARG:HA	2.36	0.58
5:B:60:LEU:HD21	5:B:62:LYS:CB	2.33	0.57
23:T:108:MET:HE2	23:T:122:TYR:OH	2.03	0.57
23:T:29:LYS:HE3	23:T:79:PHE:HB3	1.85	0.57
20:Q:59:ARG:O	20:Q:63:ARG:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:13:ILE:HD11	13:J:159:ASP:OD2	2.04	0.57
29:Z:47:LYS:O	29:Z:48:TYR:HB2	2.05	0.57
1:1:1949:C:N3	18:O:142:ILE:CD1	2.50	0.57
29:Z:11:ARG:NE	29:Z:11:ARG:HA	2.19	0.57
29:Z:79:TRP:HZ2	29:Z:119:ILE:CG2	2.18	0.56
1:1:1436:A:N1	6:C:299:GLU:HA	2.19	0.56
6:C:12:LYS:HG2	6:C:18:ALA:HB2	1.86	0.56
28:Y:40:CYS:SG	28:Y:79:LEU:HD11	2.45	0.56
23:T:62:CYS:O	23:T:63:ASN:HB2	2.05	0.56
27:X:22:PRO:CG	27:X:25:VAL:HG23	2.35	0.56
28:Y:38:ALA:O	28:Y:76:VAL:HB	2.05	0.56
13:J:14:ARG:HE	13:J:135:PRO:CG	2.12	0.56
1:1:2045:U:H6	20:Q:73:ARG:HH11	1.39	0.56
1:1:178:A:C6	1:1:179:A:C5	2.93	0.56
28:Y:126:VAL:HG22	28:Y:132:LYS:O	2.05	0.56
1:1:496:C:C6	29:Z:82:VAL:HG13	2.39	0.56
1:1:38:U:H4'	29:Z:32:ARG:HD2	1.86	0.56
1:1:1578:A:O2'	1:1:1961:A:N3	2.33	0.56
18:O:36:ILE:HD11	18:O:54:LEU:HD21	1.87	0.56
16:M:68:ARG:HH12	16:M:124:GLN:HE22	1.52	0.56
16:M:68:ARG:CZ	16:M:124:GLN:NE2	2.69	0.56
16:M:68:ARG:NH1	16:M:124:GLN:HE22	2.04	0.56
1:1:2745:G:O6	22:S:3:THR:CG2	2.54	0.56
22:S:49:GLN:O	22:S:52:MET:HE3	2.05	0.56
1:1:1642:U:OP1	16:M:67:ARG:HD3	2.06	0.55
11:H:88:GLN:HA	11:H:146:THR:HG22	1.88	0.55
21:R:166:PRO:HD2	21:R:169:LYS:HD2	1.86	0.55
22:S:43:VAL:O	22:S:95:HIS:O	2.24	0.55
29:Z:16:SER:O	29:Z:17:ALA:HB3	2.06	0.55
29:Z:79:TRP:CH2	29:Z:121:VAL:CG1	2.76	0.55
1:1:1436:A:C2	6:C:299:GLU:CB	2.87	0.55
1:1:2261:A:OP2	4:A:200:ARG:NH1	2.39	0.55
1:1:923:A:OP1	20:Q:83:THR:HG21	2.06	0.55
28:Y:79:LEU:HD23	28:Y:79:LEU:N	2.20	0.55
1:1:178:A:N7	1:1:179:A:N7	2.54	0.55
1:1:875:G:OP1	19:P:66:LYS:HD3	2.06	0.55
1:1:3161:C:H5'	5:B:53:MET:O	2.07	0.55
22:S:11:THR:O	22:S:14:LYS:N	2.40	0.55
23:T:108:MET:CE	23:T:122:TYR:CE1	2.90	0.55
1:1:796:A:C2	29:Z:58:MET:HE1	2.42	0.55
1:1:1436:A:C2	6:C:299:GLU:CD	2.78	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:122:VAL:HG11	16:M:132:GLU:CG	2.29	0.55
29:Z:115:ASP:OD2	29:Z:116:LEU:N	2.40	0.55
7:D:214:LEU:HD21	7:D:221:LYS:HB3	1.90	0.54
21:R:165:THR:HB	21:R:169:LYS:CD	2.36	0.54
22:S:17:LYS:HD3	22:S:47:SER:HB2	1.88	0.54
27:X:22:PRO:CG	27:X:25:VAL:CG2	2.85	0.54
1:1:796:A:C2	29:Z:58:MET:CE	2.90	0.54
29:Z:75:VAL:CG2	29:Z:112:GLY:HA2	2.37	0.54
5:B:58:ARG:HH21	5:B:353:VAL:HA	1.72	0.54
18:O:132:ARG:HG2	18:O:146:MET:SD	2.47	0.54
22:S:49:GLN:CA	22:S:52:MET:HE2	2.21	0.54
28:Y:101:MET:HE1	28:Y:107:ARG:NE	2.21	0.54
1:1:606:G:N3	1:1:606:G:H2'	2.22	0.54
1:1:796:A:H2	29:Z:58:MET:HE1	1.72	0.54
28:Y:101:MET:HG3	28:Y:102:ARG:N	2.23	0.54
1:1:796:A:N3	29:Z:58:MET:CE	2.71	0.54
1:1:836:C:H5''	19:P:143:LYS:HG2	1.89	0.54
28:Y:119:TYR:O	28:Y:123:THR:CG2	2.56	0.54
13:J:16:GLU:OE2	13:J:137:ASN:ND2	2.41	0.54
24:U:12:LYS:HG3	24:U:127:LEU:HD11	1.89	0.54
29:Z:46:ASP:O	29:Z:47:LYS:HG2	2.08	0.54
1:1:2497:A:H61	17:N:162:GLN:NE2	2.05	0.54
20:Q:69:LYS:HZ3	20:Q:69:LYS:HB2	1.72	0.53
1:1:1651:A:O2'	1:1:1652:U:O4'	2.26	0.53
17:N:160:ARG:HG3	17:N:161:GLY:N	2.22	0.53
1:1:2834:U:O3'	22:S:57:TYR:OH	2.27	0.53
1:1:719:C:H5''	17:N:160:ARG:HB3	1.89	0.53
9:F:146:TYR:CE1	9:F:245:ASN:CB	2.92	0.53
18:O:142:ILE:C	18:O:143:ASN:HD22	2.12	0.53
22:S:43:VAL:HG13	22:S:43:VAL:O	2.08	0.53
28:Y:2:VAL:CG1	28:Y:6:LYS:HE3	2.37	0.53
5:B:248:ILE:HD11	5:B:264:PRO:HG2	1.89	0.53
5:B:44:THR:HG21	5:B:183:ASN:HD22	1.74	0.53
17:N:82:LEU:HD21	17:N:149:THR:HG21	1.91	0.53
1:1:1730:U:O2'	28:Y:78:HIS:CD2	2.62	0.53
1:1:3099:C:O2	5:B:265:ARG:NH1	2.41	0.52
5:B:304:ILE:HD11	5:B:322:LEU:HD21	1.90	0.52
9:F:102:ILE:HD11	19:P:2:GLY:C	2.30	0.52
12:I:9:TYR:CG	12:I:97:LEU:HD21	2.43	0.52
6:C:134:PRO:HG3	6:C:150:LEU:HD12	1.91	0.52
28:Y:90:MET:HB3	28:Y:121:LYS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:86:PHE:CE1	23:T:90:TYR:HD2	2.27	0.52
5:B:53:MET:HB3	5:B:77:THR:HA	1.90	0.52
1:1:178:A:C5	1:1:179:A:N7	2.78	0.52
1:1:2663:U:O2	1:1:2663:U:C2'	2.57	0.52
1:1:2888:G:C5	29:Z:60:HIS:CE1	2.97	0.52
21:R:141:CYS:SG	21:R:146:MET:HG3	2.50	0.52
29:Z:79:TRP:HE1	29:Z:117:PRO:CD	2.21	0.52
15:L:8:TYR:CD1	15:L:59:LEU:HD21	2.44	0.52
19:P:13:LYS:CE	19:P:17:ARG:NH1	2.73	0.52
1:1:2001:G:O2'	24:U:20:PRO:HD2	2.10	0.52
12:I:60:ILE:HD12	12:I:129:VAL:HG21	1.91	0.52
14:K:15:LYS:HD2	16:M:197:GLN:NE2	2.23	0.52
15:L:21:ASP:OD2	15:L:47:VAL:HG13	2.10	0.52
1:1:970:G:C8	18:O:138:ALA:HB1	2.45	0.52
1:1:1924:A:H2'	1:1:1924:A:N3	2.25	0.52
5:B:60:LEU:CD2	5:B:61:ASP:N	2.73	0.52
13:J:60:ILE:HD13	13:J:66:ILE:HD12	1.91	0.52
18:O:137:ARG:HB2	18:O:141:ARG:HB2	1.92	0.52
20:Q:114:ILE:HD11	20:Q:141:ILE:HD13	1.92	0.51
23:T:25:PRO:O	23:T:26:VAL:HB	2.10	0.51
24:U:95:ILE:HD13	25:V:27:ARG:HB2	1.92	0.51
1:1:995:U:O2'	4:A:12:ARG:NH2	2.43	0.51
5:B:23:LYS:O	5:B:23:LYS:HG3	2.10	0.51
16:M:187:PRO:HD3	16:M:192:CYS:SG	2.45	0.51
23:T:106:ASP:OD1	23:T:106:ASP:N	2.42	0.51
16:M:189:ARG:NE	16:M:189:ARG:CA	2.73	0.51
19:P:9:GLY:HA3	19:P:11:LYS:HG3	1.91	0.51
5:B:305:THR:HG22	5:B:315:THR:O	2.11	0.51
9:F:124:ALA:HB3	9:F:219:PHE:HB2	1.93	0.51
27:X:21:ALA:CB	27:X:26:ARG:NH1	2.73	0.51
23:T:26:VAL:CG1	23:T:27:LYS:N	2.73	0.51
1:1:2947:C:O2	1:1:2947:C:O4'	2.28	0.51
1:1:871:G:C2'	1:1:872:U:H5'	2.41	0.51
18:O:145:TYR:O	18:O:146:MET:HG2	2.11	0.51
1:1:836:C:P	19:P:141:ALA:CB	2.99	0.51
1:1:802:A:C8	29:Z:113:LYS:HD2	2.45	0.51
15:L:33:ASN:HA	21:R:149:LEU:CD2	2.37	0.51
1:1:85:A:P	29:Z:65:LYS:HE3	2.51	0.51
13:J:17:LYS:HE3	13:J:131:GLN:NE2	2.23	0.50
29:Z:119:ILE:O	29:Z:121:VAL:HG13	2.11	0.50
14:K:63:ARG:CB	29:Z:69:THR:HG21	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1769:G:OP1	23:T:87:SER:OG	2.29	0.50
1:1:970:G:C8	18:O:138:ALA:HB2	2.46	0.50
5:B:53:MET:HB3	5:B:77:THR:HG22	1.92	0.50
20:Q:83:THR:HG23	20:Q:86:ALA:H	1.75	0.50
22:S:48:VAL:O	22:S:52:MET:HE2	2.11	0.50
1:1:2729:G:OP1	12:I:116:ARG:CD	2.57	0.50
1:1:288:C:H4'	16:M:184:ARG:HH21	1.77	0.50
21:R:165:THR:CB	21:R:169:LYS:HD3	2.37	0.50
27:X:55:VAL:HG22	27:X:103:VAL:HG22	1.92	0.50
21:R:81:ASN:ND2	21:R:150:PHE:CZ	2.80	0.50
29:Z:132:ALA:O	29:Z:136:ILE:HG13	2.11	0.50
1:1:1468:G:OP1	29:Z:16:SER:HB3	2.10	0.50
9:F:95:LEU:HD11	9:F:124:ALA:HB1	1.93	0.50
16:M:177:THR:HG23	16:M:182:ALA:HB2	1.94	0.50
28:Y:126:VAL:HG13	28:Y:132:LYS:O	2.11	0.50
29:Z:41:MET:O	29:Z:45:TYR:HD2	1.94	0.50
29:Z:84:PRO:CD	29:Z:85:ALA:N	2.73	0.50
5:B:60:LEU:CD2	5:B:62:LYS:HB2	2.41	0.50
1:1:1279:C:N4	1:1:1389:A:OP2	2.45	0.49
19:P:145:ARG:O	19:P:146:GLU:C	2.48	0.49
28:Y:102:ARG:NH1	28:Y:107:ARG:NH1	2.60	0.49
11:H:127:MET:HE3	11:H:145:LEU:HD11	1.94	0.49
22:S:48:VAL:O	22:S:52:MET:HE1	2.12	0.49
1:1:1436:A:N1	6:C:299:GLU:CB	2.74	0.49
22:S:42:ILE:O	22:S:59:GLY:N	2.41	0.49
1:1:55:G:O2'	16:M:108:ARG:NH1	2.45	0.49
19:P:92:VAL:HG13	29:Z:87:LEU:HD21	1.92	0.49
1:1:405:A:H4'	1:1:406:A:OP1	2.12	0.49
23:T:30:PHE:O	23:T:31:THR:CG2	2.60	0.49
29:Z:7:LYS:O	29:Z:11:ARG:HB2	2.13	0.49
16:M:122:VAL:CG1	16:M:132:GLU:HG3	2.32	0.49
16:M:185:LEU:HD13	16:M:185:LEU:H	1.77	0.49
21:R:155:LYS:C	21:R:156:LEU:HD12	2.33	0.49
26:W:87:VAL:HA	26:W:110:VAL:HG12	1.94	0.49
18:O:4:TYR:CD2	18:O:16:LYS:HD3	2.47	0.49
9:F:58:THR:HG23	9:F:196:GLU:HG2	1.95	0.49
20:Q:73:ARG:O	20:Q:74:HIS:HB2	2.13	0.49
29:Z:79:TRP:CZ2	29:Z:119:ILE:HG23	2.46	0.49
1:1:2505:C:O2'	5:B:265:ARG:NH2	2.46	0.49
11:H:45:ILE:HG23	11:H:54:LEU:HD21	1.95	0.49
28:Y:5:LEU:HD11	28:Y:76:VAL:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2911:G:O6	29:Z:42:ARG:NH2	2.46	0.48
5:B:214:ILE:HD12	5:B:281:VAL:CG2	2.43	0.48
17:N:139:LEU:HD13	17:N:144:ARG:HG3	1.95	0.48
23:T:107:PHE:C	23:T:108:MET:HG3	2.34	0.48
5:B:60:LEU:HD22	5:B:62:LYS:N	2.28	0.48
14:K:6:ASN:O	29:Z:49:HIS:HE1	1.97	0.48
5:B:214:ILE:HD12	5:B:281:VAL:HG21	1.95	0.48
17:N:81:LEU:HD11	17:N:195:LEU:HD13	1.96	0.48
23:T:54:THR:HA	23:T:63:ASN:HD22	1.77	0.48
1:1:180:G:C2'	1:1:181:C:C6	2.96	0.48
1:1:1592:U:H5	1:1:1938:A:N1	2.11	0.48
5:B:60:LEU:CD2	5:B:62:LYS:CB	2.91	0.48
11:H:34:ILE:HD11	11:H:148:THR:HB	1.96	0.48
15:L:8:TYR:CE1	15:L:59:LEU:HD21	2.49	0.48
18:O:4:TYR:CE2	18:O:16:LYS:CD	2.91	0.48
24:U:15:VAL:HG13	24:U:87:TRP:CD1	2.49	0.48
28:Y:74:ILE:CG2	28:Y:79:LEU:CD2	2.85	0.48
28:Y:5:LEU:CD1	28:Y:76:VAL:CG2	2.90	0.48
1:1:2663:U:H2'	1:1:2663:U:O2	2.12	0.48
5:B:60:LEU:HD21	5:B:62:LYS:HG2	1.90	0.48
16:M:169:GLY:HA2	16:M:172:TYR:CE2	2.49	0.48
27:X:18:HIS:O	27:X:21:ALA:HB2	2.14	0.48
1:1:2264:G:H4'	18:O:22:LEU:HD21	91.98	0.48
15:L:5:THR:HG22	15:L:6:ARG:N	2.29	0.47
24:U:56:LEU:HD21	24:U:121:GLY:HA3	1.96	0.47
1:1:2957:U:O4'	1:1:2957:U:O2	2.30	0.47
28:Y:101:MET:CG	28:Y:102:ARG:H	2.24	0.47
1:1:1710:A:OP2	1:1:1924:A:N6	2.47	0.47
22:S:21:ARG:HG3	22:S:21:ARG:NH1	2.26	0.47
23:T:26:VAL:CG1	23:T:27:LYS:H	2.27	0.47
28:Y:4:LEU:HD12	28:Y:81:PRO:HG2	1.96	0.47
1:1:2925:G:P	6:C:75:ARG:HH22	2.37	0.47
13:J:17:LYS:CE	13:J:131:GLN:HE22	2.21	0.47
18:O:132:ARG:HH11	18:O:132:ARG:CB	2.24	0.47
19:P:9:GLY:HA2	19:P:10:ARG:C	2.34	0.47
21:R:136:ILE:HG22	21:R:137:LYS:O	2.14	0.47
24:U:21:VAL:HG13	24:U:22:GLY:N	2.29	0.47
28:Y:24:VAL:HG12	28:Y:25:VAL:O	2.15	0.47
1:1:2045:U:C5	20:Q:73:ARG:CZ	2.92	0.47
11:H:93:PHE:CE1	11:H:178:ILE:HD12	2.49	0.47
24:U:24:LEU:HD11	24:U:35:ASN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:73:THR:OG1	8:E:83:LEU:HD23	2.13	0.47
17:N:154:LEU:CD1	17:N:165:LEU:HD21	2.44	0.47
27:X:21:ALA:HB3	27:X:26:ARG:CZ	2.44	0.47
28:Y:100:ALA:HB1	28:Y:106:ASP:OD1	2.12	0.47
1:1:889:G:P	29:Z:32:ARG:NH1	2.88	0.47
10:G:174:VAL:HG13	10:G:177:ILE:HD12	1.96	0.47
21:R:152:SER:O	21:R:153:LYS:HB2	2.14	0.47
22:S:11:THR:OG1	22:S:15:PHE:CG	2.67	0.47
1:1:1462:U:O2'	19:P:10:ARG:HD3	2.14	0.47
1:1:180:G:C6	1:1:245:U:C4	3.03	0.47
15:L:12:ARG:HD2	15:L:59:LEU:HD22	1.97	0.47
25:V:39:ILE:HD12	25:V:40:HIS:CD2	2.50	0.47
28:Y:103:THR:O	28:Y:104:VAL:HB	2.14	0.47
28:Y:98:GLU:OE1	28:Y:99:ASP:N	2.48	0.47
1:1:3010:C:O2'	1:1:3012:G:OP2	2.33	0.46
7:D:104:LEU:HD23	7:D:250:ILE:HG23	1.97	0.46
20:Q:16:CYS:HB3	20:Q:51:ARG:HD3	1.96	0.46
1:1:3281:G:C2	1:1:3367:A:C2	3.02	0.46
1:1:874:G:H5'	1:1:875:G:OP1	2.15	0.46
1:1:2745:G:O3'	12:I:15:LYS:NZ	2.48	0.46
17:N:120:TYR:CE2	17:N:211:VAL:HG11	2.50	0.46
22:S:9:ALA:CB	22:S:10:ARG:HH11	2.28	0.46
4:A:30:ARG:O	4:A:163:ARG:NH2	2.49	0.46
20:Q:69:LYS:HG3	20:Q:75:MET:CE	2.46	0.46
1:1:1858:C:H5''	23:T:109:ARG:HH22	1.81	0.46
29:Z:78:LEU:O	29:Z:81:LEU:CB	2.58	0.46
1:1:1069:G:N3	1:1:1069:G:H2'	2.31	0.46
1:1:970:G:N7	18:O:138:ALA:HB1	2.29	0.46
28:Y:101:MET:CG	28:Y:102:ARG:N	2.78	0.46
28:Y:82:THR:HG22	28:Y:84:TYR:H	1.81	0.46
21:R:84:VAL:HG11	21:R:113:LEU:CD2	2.46	0.46
4:A:201:GLY:HA3	4:A:209:HIS:CD2	2.51	0.46
14:K:74:PHE:O	14:K:75:THR:OG1	2.31	0.46
18:O:11:GLU:O	18:O:13:LYS:N	2.36	0.46
1:1:836:C:H5''	19:P:143:LYS:CG	2.45	0.46
29:Z:121:VAL:O	29:Z:141:GLY:HA2	2.16	0.46
15:L:5:THR:O	15:L:6:ARG:HB2	2.16	0.46
7:D:147:VAL:HG12	7:D:158:VAL:HG11	1.96	0.46
16:M:189:ARG:NE	16:M:189:ARG:O	2.48	0.46
1:1:115:A:H3'	1:1:116:A:C5'	2.46	0.45
5:B:60:LEU:HD21	5:B:62:LYS:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:36:LYS:HA	10:G:39:ILE:HD12	1.98	0.45
16:M:80:VAL:HG21	16:M:87:GLN:HA	1.98	0.45
20:Q:129:ASN:O	20:Q:131:PHE:N	2.49	0.45
10:G:84:VAL:HA	10:G:85:PRO:HD3	1.80	0.45
18:O:135:THR:OG1	18:O:145:TYR:CE1	2.46	0.45
24:U:15:VAL:HG13	24:U:87:TRP:CG	2.51	0.45
13:J:14:ARG:CD	13:J:135:PRO:HD3	2.47	0.45
28:Y:8:GLY:O	28:Y:85:THR:OG1	2.31	0.45
1:1:1919:U:H2'	1:1:1919:U:O2	2.17	0.45
1:1:3161:C:C4'	5:B:53:MET:O	2.65	0.45
21:R:81:ASN:HD21	21:R:150:PHE:HE1	1.65	0.45
7:D:214:LEU:HD21	7:D:221:LYS:CB	2.47	0.45
21:R:45:VAL:HG13	21:R:65:ILE:CD1	2.47	0.45
28:Y:122:PHE:HD2	28:Y:141:ARG:CD	2.21	0.45
16:M:185:LEU:C	16:M:185:LEU:CD2	2.86	0.45
1:1:3101:G:P	5:B:18:PRO:HB2	2.57	0.45
5:B:60:LEU:CD2	5:B:62:LYS:HG2	2.47	0.45
6:C:211:VAL:HG12	6:C:233:VAL:HG22	1.99	0.45
22:S:11:THR:HG23	22:S:12:ARG:N	2.32	0.45
29:Z:84:PRO:HD2	29:Z:85:ALA:N	2.23	0.45
1:1:3161:C:O2'	5:B:55:HIS:CD2	2.65	0.45
1:1:496:C:C4	29:Z:82:VAL:HG22	2.51	0.45
1:1:1480:G:OP2	6:C:191:ARG:NH2	2.49	0.45
1:1:2742:U:OP1	22:S:6:GLY:HA3	2.16	0.45
1:1:180:G:O2'	1:1:181:C:O4'	2.35	0.44
19:P:89:ILE:HG12	29:Z:80:SER:HB2	1.99	0.44
20:Q:3:LEU:O	20:Q:5:LEU:N	2.50	0.44
26:W:107:VAL:HG22	26:W:147:TYR:CD1	2.53	0.44
3:4:75:G:O4'	14:K:30:ARG:HA	53.70	0.44
22:S:9:ALA:HB1	22:S:10:ARG:HH11	1.82	0.44
23:T:107:PHE:H	23:T:107:PHE:HD2	1.65	0.44
29:Z:59:ARG:H	29:Z:59:ARG:HG2	1.56	0.44
6:C:54:VAL:HG21	6:C:101:MET:CE	2.47	0.44
10:G:201:VAL:HG21	10:G:209:LEU:HD21	1.98	0.44
1:1:1136:A:N3	1:1:2744:U:O2'	2.50	0.44
1:1:842:A:H61	1:1:872:U:H3	1.66	0.44
5:B:55:HIS:H	5:B:55:HIS:CD2	2.35	0.44
29:Z:79:TRP:CH2	29:Z:119:ILE:HG21	2.53	0.44
1:1:2786:C:N4	13:J:23:CYS:SG	2.91	0.44
29:Z:79:TRP:CH2	29:Z:119:ILE:CG2	3.01	0.44
5:B:44:THR:HG21	5:B:183:ASN:ND2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:9:TYR:CD2	12:I:97:LEU:HD21	2.53	0.44
23:T:96:LYS:HG2	23:T:105:ARG:HH12	1.82	0.44
23:T:107:PHE:CD2	23:T:107:PHE:N	2.84	0.44
16:M:114:LEU:HB2	16:M:135:LEU:HD23	1.99	0.44
16:M:114:LEU:CB	16:M:135:LEU:HD23	2.48	0.44
20:Q:96:ARG:O	20:Q:100:VAL:HG23	2.18	0.44
5:B:256:PRO:HG2	5:B:260:GLN:HE21	1.83	0.44
23:T:108:MET:HG2	23:T:121:ARG:O	2.18	0.44
1:I:89:A:N7	19:P:172:LYS:NZ	2.59	0.44
10:G:93:HIS:CD2	10:G:239:VAL:HG11	2.52	0.44
16:M:185:LEU:C	16:M:185:LEU:HD22	2.38	0.44
11:H:93:PHE:CZ	11:H:143:ILE:HG13	2.53	0.43
19:P:143:LYS:HZ3	19:P:143:LYS:HB3	1.83	0.43
3:4:104:A:C8	3:4:105:A:C8	3.06	0.43
7:D:8:LYS:HA	7:D:8:LYS:HD2	4.59	0.43
28:Y:102:ARG:NH1	28:Y:107:ARG:CZ	2.73	0.43
7:D:122:VAL:HG21	7:D:129:TYR:CG	2.53	0.43
11:H:89:TYR:CZ	11:H:183:THR:HG22	2.53	0.43
23:T:27:LYS:HE3	23:T:81:THR:CG2	2.48	0.43
1:I:1651:A:O2'	1:I:1652:U:O5'	2.33	0.43
1:I:3100:U:H2'	1:I:3101:G:O4'	2.18	0.43
22:S:80:VAL:O	22:S:80:VAL:HG23	2.18	0.43
22:S:52:MET:HB3	22:S:95:HIS:NE2	2.32	0.43
26:W:109:LEU:HD23	26:W:109:LEU:HA	1.92	0.43
12:I:89:ILE:HD13	12:I:136:MET:HG2	1.99	0.43
15:L:89:ASN:HD21	15:L:98:LEU:HD11	1.83	0.43
9:F:94:ILE:HD12	9:F:146:TYR:CD1	2.54	0.43
18:O:11:GLU:C	18:O:13:LYS:N	2.72	0.43
22:S:5:PHE:N	22:S:5:PHE:CD2	2.86	0.43
1:I:2634:U:OP1	4:A:123:ARG:NH1	2.52	0.43
1:I:871:G:H2'	1:I:872:U:H5'	1.99	0.43
1:I:1825:G:N3	1:I:1825:G:C2'	2.81	0.43
20:Q:69:LYS:NZ	20:Q:69:LYS:HB2	2.32	0.43
1:I:178:A:C4	1:I:179:A:C8	3.07	0.43
9:F:146:TYR:CE1	9:F:245:ASN:HB2	2.53	0.43
18:O:11:GLU:O	18:O:12:ASN:HB2	2.19	0.43
1:I:1695:U:OP2	20:Q:41:ARG:NH2	2.52	0.43
20:Q:69:LYS:HG3	20:Q:75:MET:HE2	2.01	0.43
29:Z:37:GLY:HA2	29:Z:45:TYR:CE2	2.54	0.43
1:I:3319:U:O3'	8:E:178:THR:HG22	2.19	0.43
21:R:150:PHE:O	21:R:151:ASP:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:12:LYS:HG3	24:U:127:LEU:CD2	2.45	0.43
10:G:63:VAL:HG21	26:W:44:ARG:HD2	2.01	0.43
4:A:104:LEU:CD1	4:A:148:ILE:HD11	2.49	0.42
5:B:56:VAL:HG23	5:B:358:ILE:HA	2.00	0.42
5:B:53:MET:HB3	5:B:77:THR:CG2	2.48	0.42
24:U:19:LEU:HD21	24:U:100:ASN:OD1	2.17	0.42
5:B:53:MET:HE1	5:B:75:ALA:HB1	2.01	0.42
16:M:103:GLU:OE2	16:M:119:SER:CB	2.66	0.42
29:Z:75:VAL:HB	29:Z:112:GLY:HA2	2.01	0.42
19:P:145:ARG:NH1	19:P:147:ALA:HB3	2.34	0.42
15:L:8:TYR:O	15:L:31:ILE:HD11	2.18	0.42
19:P:9:GLY:HA2	19:P:10:ARG:CB	2.49	0.42
19:P:98:THR:HG23	19:P:118:GLU:HB3	2.01	0.42
22:S:17:LYS:HG2	22:S:46:PRO:HG2	2.02	0.42
29:Z:62:HIS:CG	29:Z:62:HIS:O	2.70	0.42
16:M:65:ARG:HD2	16:M:128:TYR:CD1	2.55	0.42
10:G:194:LYS:HE3	10:G:205:ASN:ND2	2.35	0.42
22:S:57:TYR:HA	22:S:60:ARG:HG3	2.01	0.42
23:T:30:PHE:C	23:T:31:THR:HG23	2.39	0.42
1:1:1005:A:H2'	1:1:1005:A:N3	2.35	0.42
1:1:85:A:OP2	29:Z:65:LYS:CE	2.51	0.42
18:O:22:LEU:CD2	18:O:22:LEU:N	2.73	0.42
1:1:480:U:HO2'	1:1:481:C:P	2.43	0.42
18:O:11:GLU:C	18:O:13:LYS:H	2.22	0.42
19:P:89:ILE:HG12	29:Z:80:SER:CB	2.50	0.42
1:1:1268:U:H3'	21:R:170:LYS:NZ	2.34	0.42
29:Z:118:LYS:HE3	29:Z:118:LYS:HB3	1.86	0.42
1:1:2496:C:OP2	17:N:151:ARG:NH2	2.53	0.42
1:1:475:A:H3'	1:1:476:U:H5''	2.02	0.42
13:J:8:ASN:N	13:J:9:PRO:HD2	2.34	0.42
19:P:7:ARG:C	19:P:8:ASN:ND2	2.73	0.42
1:1:2741:C:P	22:S:5:PHE:O	2.77	0.42
24:U:15:VAL:HB	24:U:55:SER:HB2	2.00	0.42
1:1:1265:A:N3	1:1:1415:C:O2'	2.53	0.42
4:A:148:ILE:HD12	4:A:158:VAL:HG21	2.02	0.42
10:G:208:VAL:HG23	10:G:208:VAL:O	2.20	0.42
16:M:187:PRO:HD2	16:M:192:CYS:HG	1.73	0.42
19:P:145:ARG:O	19:P:147:ALA:N	2.53	0.42
22:S:43:VAL:HG11	22:S:97:ARG:HH11	1.84	0.42
1:1:3102:A:OP1	5:B:20:LYS:HB2	2.20	0.41
13:J:60:ILE:HD13	13:J:66:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:192:ILE:O	21:R:160:ARG:NH2	2.53	0.41
22:S:11:THR:CG2	22:S:12:ARG:N	2.83	0.41
1:1:872:U:C2'	1:1:873:U:C6	2.97	0.41
1:1:872:U:C2'	1:1:873:U:H6	2.27	0.41
3:4:79:A:H3'	3:4:80:A:H4'	2.02	0.41
5:B:13:SER:OG	5:B:16:PHE:HD2	2.03	0.41
18:O:17:ALA:HB3	18:O:100:LEU:HD23	2.01	0.41
15:L:55:ARG:NH1	21:R:164:PRO:HB3	2.35	0.41
1:1:872:U:H2'	1:1:873:U:C5	2.52	0.41
8:E:47:ILE:HG22	8:E:57:ARG:HG2	2.02	0.41
13:J:18:LEU:HD12	13:J:129:TYR:O	2.21	0.41
19:P:171:ARG:O	19:P:172:LYS:CB	2.68	0.41
23:T:29:LYS:HG3	23:T:81:THR:OG1	2.20	0.41
1:1:825:C:O2'	1:1:826:A:O5'	2.38	0.41
15:L:18:TYR:CG	15:L:19:GLY:N	2.87	0.41
18:O:21:ASP:OD2	18:O:149:PRO:CB	2.66	0.41
21:R:150:PHE:O	21:R:151:ASP:CB	2.69	0.41
29:Z:12:ARG:NH1	29:Z:12:ARG:CG	2.72	0.41
1:1:3058:G:C2	5:B:249:ALA:HB1	2.56	0.41
8:E:49:LEU:HD11	8:E:92:ILE:HG13	2.02	0.41
5:B:55:HIS:HE1	25:V:22:PRO:O	2.02	0.41
27:X:81:ILE:HD11	27:X:98:ILE:HD11	2.03	0.41
28:Y:11:VAL:HG22	28:Y:23:GLY:O	2.21	0.41
21:R:19:ARG:HB3	21:R:31:LEU:HD23	2.02	0.41
1:1:1730:U:O2'	28:Y:78:HIS:HD2	2.02	0.41
1:1:180:G:O2'	1:1:181:C:C5'	2.69	0.41
1:1:1825:G:H2'	1:1:1825:G:N3	2.35	0.41
1:1:581:U:O4'	1:1:581:U:O2	2.37	0.41
1:1:761:G:OP1	6:C:33:ARG:NH2	2.53	0.41
16:M:127:VAL:HG23	16:M:128:TYR:CE2	2.51	0.41
19:P:13:LYS:HD3	19:P:17:ARG:NH2	2.36	0.41
1:1:178:A:H2'	1:1:179:A:O4'	2.20	0.41
5:B:260:GLN:O	5:B:263:VAL:HG12	2.21	0.41
1:1:311:G:C2	1:1:321:A:C2	3.09	0.41
21:R:81:ASN:ND2	21:R:150:PHE:CE1	2.88	0.41
1:1:1435:U:OP1	19:P:38:ARG:NH1	2.53	0.41
14:K:63:ARG:HB3	29:Z:69:THR:HG21	2.02	0.41
1:1:344:A:O2'	6:C:50:GLN:NE2	2.54	0.41
13:J:111:ILE:HD13	13:J:123:ILE:HD12	2.03	0.40
1:1:873:U:O2'	1:1:874:G:P	2.79	0.40
4:A:104:LEU:HD13	4:A:148:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:103:ARG:HG3	17:N:174:VAL:CG2	2.52	0.40
17:N:158:VAL:CG1	17:N:159:GLU:N	2.84	0.40
22:S:11:THR:OG1	22:S:15:PHE:HB2	2.22	0.40
24:U:59:LEU:HD12	24:U:78:ALA:O	2.21	0.40
7:D:8:LYS:CG	7:D:8:LYS:O	4.32	0.40
14:K:50:SER:OG	14:K:51:GLY:N	2.55	0.40
1:1:1924:A:C2'	1:1:1924:A:N3	2.85	0.40
1:1:2868:U:C5'	22:S:7:LYS:CE	2.97	0.40
16:M:189:ARG:HE	16:M:189:ARG:C	2.25	0.40
24:U:12:LYS:CG	24:U:127:LEU:HD21	2.47	0.40
27:X:21:ALA:HB1	27:X:26:ARG:HG3	2.03	0.40
28:Y:102:ARG:HD3	28:Y:107:ARG:NH2	2.37	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	
4	A	244/260 (94%)	228 (93%)	15 (6%)	1 (0%)	38	76
5	B	351/389 (90%)	312 (89%)	33 (9%)	6 (2%)	11	48
6	C	380/416 (91%)	345 (91%)	30 (8%)	5 (1%)	14	54
7	D	253/310 (82%)	225 (89%)	24 (10%)	4 (2%)	11	49
8	E	114/193 (59%)	101 (89%)	12 (10%)	1 (1%)	20	63
9	F	246/258 (95%)	226 (92%)	19 (8%)	1 (0%)	38	76
10	G	225/276 (82%)	209 (93%)	12 (5%)	4 (2%)	10	46
11	H	185/190 (97%)	169 (91%)	16 (9%)	0	100	100
12	I	185/221 (84%)	168 (91%)	15 (8%)	2 (1%)	17	58
13	J	164/175 (94%)	145 (88%)	16 (10%)	3 (2%)	10	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	K	193/355 (54%)	167 (86%)	20 (10%)	6 (3%)	5	30
15	L	129/134 (96%)	118 (92%)	8 (6%)	3 (2%)	7	39
16	M	196/205 (96%)	180 (92%)	15 (8%)	1 (0%)	32	74
17	N	196/269 (73%)	187 (95%)	6 (3%)	3 (2%)	12	51
18	O	154/195 (79%)	140 (91%)	13 (8%)	1 (1%)	28	71
19	P	184/187 (98%)	172 (94%)	10 (5%)	2 (1%)	17	58
20	Q	174/187 (93%)	165 (95%)	7 (4%)	2 (1%)	17	58
21	R	180/183 (98%)	159 (88%)	16 (9%)	5 (3%)	6	33
22	S	152/157 (97%)	141 (93%)	6 (4%)	5 (3%)	4	28
23	T	95/133 (71%)	85 (90%)	7 (7%)	3 (3%)	5	28
24	U	127/139 (91%)	117 (92%)	10 (8%)	0	100	100
25	V	61/155 (39%)	60 (98%)	1 (2%)	0	100	100
26	W	125/167 (75%)	107 (86%)	16 (13%)	2 (2%)	11	49
27	X	122/141 (86%)	111 (91%)	10 (8%)	1 (1%)	22	64
28	Y	140/146 (96%)	123 (88%)	11 (8%)	6 (4%)	3	22
29	Z	141/147 (96%)	126 (89%)	11 (8%)	4 (3%)	6	33
30	a	45/54 (83%)	42 (93%)	1 (2%)	2 (4%)	3	21
31	b	92/108 (85%)	83 (90%)	9 (10%)	0	100	100
32	c	103/120 (86%)	93 (90%)	7 (7%)	3 (3%)	5	32
33	d	120/134 (90%)	111 (92%)	6 (5%)	3 (2%)	6	36
34	e	101/112 (90%)	94 (93%)	6 (6%)	1 (1%)	18	61
35	f	105/134 (78%)	98 (93%)	6 (6%)	1 (1%)	18	61
36	g	119/123 (97%)	113 (95%)	4 (3%)	2 (2%)	11	48
37	h	93/101 (92%)	89 (96%)	2 (2%)	2 (2%)	8	40
38	i	81/98 (83%)	77 (95%)	3 (4%)	1 (1%)	15	56
39	j	68/84 (81%)	63 (93%)	4 (6%)	1 (2%)	12	51
40	k	47/51 (92%)	45 (96%)	1 (2%)	1 (2%)	8	41
41	l	50/129 (39%)	48 (96%)	1 (2%)	1 (2%)	9	43
42	n	95/105 (90%)	86 (90%)	7 (7%)	2 (2%)	8	41
43	o	88/96 (92%)	82 (93%)	5 (6%)	1 (1%)	17	58
44	p	118/129 (92%)	107 (91%)	10 (8%)	1 (1%)	22	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6041/7166 (84%)	5517 (91%)	431 (7%)	93 (2%)	17	51

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	5	LYS
6	C	191	ARG
7	D	156	ASN
14	K	60	PRO
20	Q	130	GLN
21	R	151	ASP
22	S	12	ARG
23	T	26	VAL
28	Y	104	VAL
32	c	72	ILE
33	d	124	ARG
36	g	94	ARG
40	k	37	TYR
44	p	44	ILE
5	B	30	LYS
5	B	38	SER
12	I	144	ASN
13	J	115	ILE
14	K	74	PHE
14	K	154	LYS
14	K	155	ILE
15	L	22	ALA
16	M	197	GLN
17	N	176	THR
19	P	146	GLU
21	R	168	ASP
22	S	120	HIS
22	S	124	GLU
23	T	75	LYS
28	Y	8	GLY
29	Z	77	LYS
29	Z	78	LEU
30	a	4	SER
32	c	111	ASN
38	i	28	ARG
43	o	13	LYS
6	C	85	HIS

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Mol	Chain	Res	Type
7	D	20	TYR
7	D	21	ARG
7	D	44	TYR
13	J	119	PRO
15	L	8	TYR
17	N	198	LYS
20	Q	128	GLY
21	R	31	LEU
27	X	21	ALA
29	Z	47	LYS
29	Z	66	ASN
30	a	29	LYS
32	c	94	LYS
36	g	84	ARG
42	n	95	ALA
4	A	3	ARG
6	C	57	ASN
6	C	133	LEU
10	G	157	LYS
10	G	168	VAL
10	G	208	VAL
13	J	56	ARG
15	L	36	ARG
18	O	3	LYS
19	P	154	ALA
21	R	140	GLN
26	W	62	LYS
28	Y	35	ARG
28	Y	129	LYS
28	Y	134	SER
33	d	9	ARG
35	f	68	ARG
37	h	62	THR
41	l	79	GLU
5	B	24	ARG
5	B	186	SER
5	B	316	VAL
6	C	323	LEU
14	K	145	SER
21	R	177	LYS
22	S	68	THR
23	T	41	ASN

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Mol	Chain	Res	Type
26	W	141	ASP
28	Y	89	ASP
33	d	10	SER
39	j	76	GLU
34	e	10	VAL
37	h	18	ALA
22	S	81	GLY
10	G	132	GLY
14	K	51	GLY
17	N	175	PRO
42	n	36	VAL
9	F	237	GLU
12	I	196	GLY
8	E	184	GLY

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	
4	A	190/200 (95%)	181 (95%)	9 (5%)	30	69
5	B	315/330 (96%)	298 (95%)	17 (5%)	26	63
6	C	313/326 (96%)	302 (96%)	11 (4%)	41	76
7	D	218/253 (86%)	213 (98%)	5 (2%)	56	84
8	E	110/163 (68%)	106 (96%)	4 (4%)	40	75
9	F	216/223 (97%)	206 (95%)	10 (5%)	31	69
10	G	204/233 (88%)	198 (97%)	6 (3%)	48	80
11	H	167/169 (99%)	159 (95%)	8 (5%)	30	68
12	I	159/180 (88%)	153 (96%)	6 (4%)	38	74
13	J	141/151 (93%)	136 (96%)	5 (4%)	41	76
14	K	170/303 (56%)	163 (96%)	7 (4%)	35	71
15	L	116/118 (98%)	109 (94%)	7 (6%)	22	60
16	M	171/176 (97%)	159 (93%)	12 (7%)	18	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	N	178/240 (74%)	172 (97%)	6 (3%)	42	77
18	O	139/168 (83%)	129 (93%)	10 (7%)	17	51
19	P	154/155 (99%)	146 (95%)	8 (5%)	27	64
20	Q	154/162 (95%)	153 (99%)	1 (1%)	89	96
21	R	162/163 (99%)	152 (94%)	10 (6%)	21	58
22	S	134/137 (98%)	128 (96%)	6 (4%)	32	69
23	T	93/111 (84%)	86 (92%)	7 (8%)	16	50
24	U	100/105 (95%)	96 (96%)	4 (4%)	36	72
25	V	56/131 (43%)	54 (96%)	2 (4%)	40	75
26	W	116/139 (84%)	110 (95%)	6 (5%)	27	64
27	X	113/128 (88%)	106 (94%)	7 (6%)	21	58
28	Y	128/130 (98%)	119 (93%)	9 (7%)	18	53
29	Z	116/118 (98%)	110 (95%)	6 (5%)	27	64
30	a	44/48 (92%)	43 (98%)	1 (2%)	56	84
31	b	80/89 (90%)	74 (92%)	6 (8%)	16	50
32	c	99/110 (90%)	94 (95%)	5 (5%)	28	65
33	d	112/122 (92%)	104 (93%)	8 (7%)	17	52
34	e	91/97 (94%)	85 (93%)	6 (7%)	19	56
35	f	91/115 (79%)	84 (92%)	7 (8%)	15	49
36	g	103/105 (98%)	96 (93%)	7 (7%)	18	54
37	h	79/82 (96%)	78 (99%)	1 (1%)	73	91
38	i	69/79 (87%)	62 (90%)	7 (10%)	9	33
39	j	66/73 (90%)	64 (97%)	2 (3%)	46	79
40	k	44/45 (98%)	38 (86%)	6 (14%)	4	20
41	l	47/116 (40%)	45 (96%)	2 (4%)	33	70
42	n	88/93 (95%)	85 (97%)	3 (3%)	42	77
43	o	68/71 (96%)	67 (98%)	1 (2%)	70	90
44	p	108/114 (95%)	106 (98%)	2 (2%)	62	87
All	All	5322/6071 (88%)	5069 (95%)	253 (5%)	34	68

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	6	ARG
4	A	15	VAL
4	A	30	ARG
4	A	41	ILE
4	A	80	GLU
4	A	163	ARG
4	A	174	ARG
4	A	193	ARG
4	A	242	ARG
5	B	10	ARG
5	B	36	ASP
5	B	58	ARG
5	B	60	LEU
5	B	102	LEU
5	B	163	THR
5	B	172	SER
5	B	189	GLU
5	B	209	THR
5	B	230	SER
5	B	243	ARG
5	B	321	LEU
5	B	323	LEU
5	B	324	LYS
5	B	336	THR
5	B	346	THR
5	B	382	LEU
6	C	73	VAL
6	C	95	MET
6	C	107	THR
6	C	108	TRP
6	C	122	HIS
6	C	140	ARG
6	C	180	LEU
6	C	182	ARG
6	C	191	ARG
6	C	277	LYS
6	C	372	ARG
7	D	68	THR
7	D	122	VAL
7	D	151	ARG
7	D	196	GLU
7	D	240	GLU
8	E	46	LEU

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Mol	Chain	Res	Type
8	E	54	ARG
8	E	94	THR
8	E	179	ARG
9	F	21	ARG
9	F	110	LYS
9	F	144	ILE
9	F	153	THR
9	F	172	HIS
9	F	173	SER
9	F	222	ASN
9	F	232	ARG
9	F	246	ARG
9	F	255	GLN
10	G	70	LEU
10	G	161	LEU
10	G	189	CYS
10	G	192	LYS
10	G	214	VAL
10	G	218	ASP
11	H	23	ARG
11	H	40	HIS
11	H	57	GLU
11	H	65	ASP
11	H	138	ASN
11	H	141	ASP
11	H	170	ASP
11	H	176	ASP
12	I	23	CYS
12	I	63	GLU
12	I	99	ILE
12	I	130	ASP
12	I	133	GLN
12	I	199	TRP
13	J	14	ARG
13	J	23	CYS
13	J	113	LEU
13	J	115	ILE
13	J	118	ASP
14	K	52	LEU
14	K	54	ARG
14	K	155	ILE
14	K	167	ARG

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Mol	Chain	Res	Type
14	K	168	CYS
14	K	177	GLU
14	K	180	PHE
15	L	4	PHE
15	L	6	ARG
15	L	21	ASP
15	L	38	LEU
15	L	54	VAL
15	L	72	SER
15	L	82	ASP
16	M	10	LEU
16	M	39	CYS
16	M	66	VAL
16	M	75	VAL
16	M	104	GLU
16	M	118	ASN
16	M	146	ASP
16	M	160	ARG
16	M	161	GLU
16	M	175	LEU
16	M	185	LEU
16	M	189	ARG
17	N	84	ARG
17	N	117	ARG
17	N	121	GLN
17	N	172	GLU
17	N	224	GLU
17	N	226	ARG
18	O	22	LEU
18	O	24	VAL
18	O	47	LEU
18	O	56	ASP
18	O	63	CYS
18	O	100	LEU
18	O	113	LEU
18	O	116	ASP
18	O	145	TYR
18	O	147	SER
19	P	8	ASN
19	P	29	LEU
19	P	32	LEU
19	P	39	ARG

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Mol	Chain	Res	Type
19	P	41	ASN
19	P	143	LYS
19	P	148	ASP
19	P	171	ARG
20	Q	33	MET
21	R	17	VAL
21	R	65	ILE
21	R	72	ARG
21	R	94	THR
21	R	97	MET
21	R	103	ASP
21	R	120	ARG
21	R	141	CYS
21	R	168	ASP
21	R	183	HIS
22	S	13	GLN
22	S	67	VAL
22	S	68	THR
22	S	100	ARG
22	S	103	GLU
22	S	140	PHE
23	T	40	ASP
23	T	62	CYS
23	T	63	ASN
23	T	67	ASP
23	T	104	LEU
23	T	106	ASP
23	T	116	THR
24	U	47	CYS
24	U	73	LYS
24	U	77	MET
24	U	131	ILE
25	V	24	ARG
25	V	56	LEU
26	W	68	TYR
26	W	78	LEU
26	W	111	ASP
26	W	137	LEU
26	W	139	ARG
26	W	149	ARG
27	X	6	GLN
27	X	23	SER

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Mol	Chain	Res	Type
27	X	47	LEU
27	X	55	VAL
27	X	59	ARG
27	X	64	ASP
27	X	73	TYR
28	Y	65	MET
28	Y	72	LYS
28	Y	74	ILE
28	Y	80	MET
28	Y	89	ASP
28	Y	91	ASP
28	Y	98	GLU
28	Y	121	LYS
28	Y	123	THR
29	Z	11	ARG
29	Z	12	ARG
29	Z	73	VAL
29	Z	95	ASP
29	Z	116	LEU
29	Z	129	SER
30	a	6	ASN
31	b	28	LEU
31	b	44	LEU
31	b	47	ILE
31	b	51	CYS
31	b	74	HIS
31	b	78	ASN
32	c	19	ASP
32	c	21	THR
32	c	43	GLU
32	c	52	MET
32	c	100	LEU
33	d	7	VAL
33	d	36	LYS
33	d	41	ASP
33	d	56	ASN
33	d	68	MET
33	d	77	LEU
33	d	91	ASN
33	d	121	VAL
34	e	11	ARG
34	e	28	GLN

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Mol	Chain	Res	Type
34	e	35	LEU
34	e	53	ARG
34	e	93	ASN
34	e	107	LEU
35	f	4	ARG
35	f	5	LEU
35	f	31	VAL
35	f	38	GLN
35	f	41	ARG
35	f	47	CYS
35	f	54	ILE
36	g	21	LEU
36	g	58	LEU
36	g	81	ASN
36	g	83	LEU
36	g	95	LEU
36	g	101	ARG
36	g	121	LEU
37	h	2	SER
38	i	8	THR
38	i	18	THR
38	i	21	LEU
38	i	22	CYS
38	i	25	CYS
38	i	40	CYS
38	i	67	CYS
39	j	50	SER
39	j	55	THR
40	k	3	SER
40	k	9	LEU
40	k	13	LEU
40	k	23	ILE
40	k	37	TYR
40	k	38	ASN
41	l	97	ARG
41	l	126	LYS
42	n	33	ASP
42	n	46	LYS
42	n	53	GLN
43	o	73	THR
44	p	16	CYS
44	p	117	LYS

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

Mol	Chain	Res	Type
4	A	209	HIS
5	B	55	HIS
5	B	152	ASN
5	B	260	GLN
5	B	268	GLN
6	C	50	GLN
6	C	94	ASN
9	F	130	ASN
9	F	214	ASN
9	F	251	ASN
10	G	93	HIS
12	I	185	GLN
13	J	40	GLN
13	J	131	GLN
13	J	137	ASN
14	K	18	GLN
14	K	32	GLN
16	M	124	GLN
17	N	162	GLN
18	O	20	GLN
18	O	143	ASN
18	O	151	HIS
19	P	8	ASN
19	P	41	ASN
20	Q	98	GLN
20	Q	129	ASN
21	R	21	GLN
21	R	81	ASN
21	R	147	GLN
22	S	13	GLN
22	S	58	HIS
22	S	90	HIS
23	T	63	ASN
28	Y	78	HIS
29	Z	14	HIS
29	Z	25	HIS
29	Z	49	HIS
29	Z	60	HIS
30	a	6	ASN
30	a	17	HIS
32	c	64	ASN

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Mol	Chain	Res	Type
33	d	91	ASN
33	d	116	GLN
34	e	28	GLN
35	f	34	ASN
36	g	99	GLN
40	k	38	ASN
40	k	43	HIS
42	n	47	GLN
42	n	53	GLN
44	p	55	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3053/3477 (87%)	732 (23%)	91 (2%)
2	3	115/124 (92%)	21 (18%)	1 (0%)
3	4	155/158 (98%)	35 (22%)	2 (1%)
All	All	3323/3759 (88%)	788 (23%)	94 (2%)

All (788) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	7	C
1	1	31	C
1	1	40	A
1	1	43	A
1	1	49	U
1	1	57	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	69	U
1	1	74	A
1	1	75	U
1	1	77	A
1	1	85	A
1	1	92	G
1	1	109	A
1	1	110	G
1	1	115	A

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Mol	Chain	Res	Type
1	1	116	A
1	1	117	G
1	1	119	G
1	1	121	A
1	1	122	A
1	1	129	U
1	1	132	U
1	1	147	G
1	1	159	C
1	1	160	G
1	1	164	G
1	1	168	U
1	1	169	U
1	1	174	G
1	1	176	G
1	1	180	G
1	1	181	C
1	1	190	A
1	1	193	U
1	1	194	U
1	1	195	U
1	1	203	A
1	1	213	U
1	1	214	A
1	1	215	G
1	1	216	A
1	1	221	G
1	1	222	A
1	1	245	U
1	1	246	U
1	1	247	U
1	1	248	U
1	1	249	U
1	1	250	G
1	1	251	U
1	1	252	U
1	1	253	C
1	1	254	C
1	1	259	A
1	1	260	C
1	1	261	G
1	1	262	G

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Mol	Chain	Res	Type
1	1	270	U
1	1	271	U
1	1	272	A
1	1	273	U
1	1	277	G
1	1	278	U
1	1	283	U
1	1	291	G
1	1	293	U
1	1	294	U
1	1	303	A
1	1	323	A
1	1	337	U
1	1	338	G
1	1	358	C
1	1	360	A
1	1	379	G
1	1	380	A
1	1	383	A
1	1	384	G
1	1	387	C
1	1	393	A
1	1	403	A
1	1	405	A
1	1	406	A
1	1	408	U
1	1	428	G
1	1	429	A
1	1	431	G
1	1	436	U
1	1	451	U
1	1	459	G
1	1	461	G
1	1	466	C
1	1	467	G
1	1	476	U
1	1	477	C
1	1	481	C
1	1	484	U
1	1	485	U
1	1	488	C
1	1	496	C

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Mol	Chain	Res	Type
1	1	497	U
1	1	499	U
1	1	500	C
1	1	501	A
1	1	502	C
1	1	503	C
1	1	504	A
1	1	509	U
1	1	514	U
1	1	515	U
1	1	517	G
1	1	522	C
1	1	523	U
1	1	526	A
1	1	527	U
1	1	535	C
1	1	537	G
1	1	538	U
1	1	539	U
1	1	540	C
1	1	541	A
1	1	546	U
1	1	547	U
1	1	548	U
1	1	552	G
1	1	554	G
1	1	572	G
1	1	573	G
1	1	576	U
1	1	580	U
1	1	581	U
1	1	582	U
1	1	587	C
1	1	594	G
1	1	595	G
1	1	596	U
1	1	600	U
1	1	601	U
1	1	603	C
1	1	606	G
1	1	608	G
1	1	613	G

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Mol	Chain	Res	Type
1	1	615	U
1	1	616	A
1	1	618	A
1	1	619	U
1	1	622	U
1	1	625	U
1	1	628	U
1	1	629	U
1	1	630	U
1	1	637	C
1	1	638	C
1	1	639	U
1	1	640	U
1	1	641	G
1	1	649	G
1	1	650	G
1	1	652	G
1	1	653	U
1	1	655	U
1	1	656	U
1	1	657	C
1	1	663	U
1	1	665	C
1	1	666	G
1	1	667	A
1	1	668	G
1	1	686	C
1	1	691	U
1	1	696	G
1	1	697	A
1	1	698	U
1	1	699	G
1	1	700	C
1	1	721	G
1	1	723	C
1	1	736	A
1	1	746	G
1	1	747	A
1	1	763	G
1	1	764	A
1	1	767	A
1	1	774	U

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Mol	Chain	Res	Type
1	1	776	U
1	1	777	U
1	1	778	A
1	1	792	A
1	1	796	A
1	1	799	G
1	1	802	A
1	1	817	U
1	1	820	U
1	1	821	U
1	1	824	C
1	1	826	A
1	1	827	U
1	1	828	U
1	1	830	U
1	1	831	U
1	1	833	G
1	1	835	A
1	1	851	G
1	1	855	U
1	1	856	C
1	1	857	U
1	1	858	G
1	1	864	G
1	1	866	U
1	1	867	U
1	1	870	A
1	1	871	G
1	1	873	U
1	1	874	G
1	1	875	G
1	1	876	A
1	1	889	G
1	1	896	A
1	1	898	A
1	1	907	A
1	1	908	C
1	1	909	U
1	1	920	A
1	1	927	A
1	1	931	A
1	1	947	G

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Mol	Chain	Res	Type
1	1	951	U
1	1	958	C
1	1	959	G
1	1	964	U
1	1	968	G
1	1	969	U
1	1	970	G
1	1	986	A
1	1	987	C
1	1	997	G
1	1	998	G
1	1	1001	C
1	1	1004	A
1	1	1006	G
1	1	1007	A
1	1	1008	C
1	1	1011	A
1	1	1013	C
1	1	1014	G
1	1	1015	A
1	1	1024	G
1	1	1027	G
1	1	1034	U
1	1	1036	U
1	1	1049	C
1	1	1050	U
1	1	1051	C
1	1	1052	A
1	1	1053	G
1	1	1065	U
1	1	1069	G
1	1	1070	U
1	1	1075	U
1	1	1080	C
1	1	1082	G
1	1	1083	G
1	1	1089	C
1	1	1090	G
1	1	1091	A
1	1	1099	G
1	1	1102	G
1	1	1121	C

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Mol	Chain	Res	Type
1	1	1123	C
1	1	1124	G
1	1	1125	A
1	1	1126	C
1	1	1134	C
1	1	1136	A
1	1	1138	C
1	1	1153	A
1	1	1154	U
1	1	1157	A
1	1	1160	G
1	1	1164	A
1	1	1165	C
1	1	1168	C
1	1	1170	U
1	1	1171	U
1	1	1183	A
1	1	1184	U
1	1	1185	U
1	1	1186	A
1	1	1191	G
1	1	1202	G
1	1	1204	G
1	1	1209	U
1	1	1218	G
1	1	1231	U
1	1	1240	C
1	1	1246	A
1	1	1249	C
1	1	1250	U
1	1	1268	U
1	1	1269	G
1	1	1278	U
1	1	1279	C
1	1	1283	U
1	1	1284	A
1	1	1288	U
1	1	1289	A
1	1	1293	G
1	1	1296	G
1	1	1299	G
1	1	1304	A

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Mol	Chain	Res	Type
1	1	1305	U
1	1	1382	G
1	1	1388	A
1	1	1392	U
1	1	1394	G
1	1	1396	U
1	1	1400	G
1	1	1403	G
1	1	1404	A
1	1	1409	G
1	1	1417	A
1	1	1427	A
1	1	1431	C
1	1	1432	U
1	1	1435	U
1	1	1436	A
1	1	1437	A
1	1	1438	U
1	1	1439	U
1	1	1440	A
1	1	1441	U
1	1	1442	C
1	1	1443	A
1	1	1449	C
1	1	1451	U
1	1	1452	U
1	1	1453	U
1	1	1454	U
1	1	1455	G
1	1	1456	U
1	1	1489	G
1	1	1496	U
1	1	1498	G
1	1	1514	G
1	1	1516	A
1	1	1517	C
1	1	1531	G
1	1	1533	U
1	1	1534	C
1	1	1543	A
1	1	1547	G
1	1	1549	A

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Mol	Chain	Res	Type
1	1	1552	U
1	1	1570	G
1	1	1572	A
1	1	1578	A
1	1	1579	A
1	1	1580	G
1	1	1599	G
1	1	1605	C
1	1	1620	U
1	1	1624	C
1	1	1628	C
1	1	1630	U
1	1	1633	G
1	1	1636	A
1	1	1637	C
1	1	1639	G
1	1	1644	A
1	1	1650	U
1	1	1651	A
1	1	1652	U
1	1	1653	A
1	1	1654	C
1	1	1672	C
1	1	1674	U
1	1	1675	U
1	1	1676	U
1	1	1678	G
1	1	1681	A
1	1	1683	A
1	1	1687	A
1	1	1691	G
1	1	1714	C
1	1	1717	G
1	1	1718	G
1	1	1722	C
1	1	1723	U
1	1	1724	G
1	1	1726	A
1	1	1731	A
1	1	1733	C
1	1	1736	A
1	1	1737	A

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Mol	Chain	Res	Type
1	1	1751	C
1	1	1777	G
1	1	1794	G
1	1	1818	C
1	1	1826	C
1	1	1829	G
1	1	1831	G
1	1	1841	G
1	1	1842	C
1	1	1843	U
1	1	1851	A
1	1	1852	G
1	1	1859	U
1	1	1861	G
1	1	1872	U
1	1	1877	G
1	1	1878	G
1	1	1882	G
1	1	1884	U
1	1	1899	A
1	1	1911	A
1	1	1916	U
1	1	1917	G
1	1	1918	U
1	1	1919	U
1	1	1920	A
1	1	1921	U
1	1	1922	U
1	1	1932	G
1	1	1942	A
1	1	1944	A
1	1	1945	A
1	1	1949	C
1	1	1950	A
1	1	1953	A
1	1	1961	A
1	1	1962	A
1	1	1969	U
1	1	1974	U
1	1	1981	G
1	1	1983	U
1	1	1987	A

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Mol	Chain	Res	Type
1	1	1989	A
1	1	1996	A
1	1	2009	G
1	1	2011	A
1	1	2013	A
1	1	2029	C
1	1	2033	A
1	1	2042	G
1	1	2055	G
1	1	2213	A
1	1	2215	C
1	1	2216	U
1	1	2217	C
1	1	2224	G
1	1	2225	G
1	1	2226	A
1	1	2227	G
1	1	2228	C
1	1	2232	C
1	1	2235	G
1	1	2236	G
1	1	2245	A
1	1	2258	A
1	1	2263	A
1	1	2264	G
1	1	2272	A
1	1	2274	G
1	1	2278	A
1	1	2283	U
1	1	2299	U
1	1	2307	G
1	1	2314	G
1	1	2318	U
1	1	2338	U
1	1	2357	A
1	1	2359	G
1	1	2362	G
1	1	2365	A
1	1	2373	U
1	1	2385	G
1	1	2386	G
1	1	2387	U

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Mol	Chain	Res	Type
1	1	2398	C
1	1	2401	G
1	1	2419	C
1	1	2420	G
1	1	2423	U
1	1	2426	A
1	1	2427	U
1	1	2428	G
1	1	2431	U
1	1	2448	G
1	1	2449	U
1	1	2476	A
1	1	2485	A
1	1	2486	A
1	1	2487	C
1	1	2488	G
1	1	2504	G
1	1	2506	G
1	1	2510	A
1	1	2514	A
1	1	2515	A
1	1	2516	G
1	1	2517	A
1	1	2518	C
1	1	2519	C
1	1	2524	U
1	1	2525	G
1	1	2535	C
1	1	2537	A
1	1	2548	G
1	1	2550	G
1	1	2624	A
1	1	2627	U
1	1	2628	A
1	1	2636	A
1	1	2638	G
1	1	2645	C
1	1	2646	U
1	1	2647	C
1	1	2651	C
1	1	2652	U
1	1	2653	C

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Mol	Chain	Res	Type
1	1	2655	G
1	1	2656	C
1	1	2657	A
1	1	2658	U
1	1	2659	G
1	1	2660	U
1	1	2661	G
1	1	2662	U
1	1	2663	U
1	1	2664	U
1	1	2665	U
1	1	2666	G
1	1	2667	G
1	1	2672	A
1	1	2673	A
1	1	2679	C
1	1	2695	A
1	1	2696	C
1	1	2702	A
1	1	2704	A
1	1	2705	C
1	1	2706	A
1	1	2717	G
1	1	2718	G
1	1	2725	G
1	1	2730	G
1	1	2731	G
1	1	2739	A
1	1	2749	C
1	1	2759	G
1	1	2763	U
1	1	2766	U
1	1	2767	A
1	1	2768	A
1	1	2785	A
1	1	2788	G
1	1	2791	A
1	1	2800	U
1	1	2801	G
1	1	2802	A
1	1	2805	A
1	1	2807	A

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Mol	Chain	Res	Type
1	1	2816	A
1	1	2820	U
1	1	2825	G
1	1	2827	U
1	1	2830	U
1	1	2836	U
1	1	2839	G
1	1	2840	U
1	1	2860	G
1	1	2863	U
1	1	2864	G
1	1	2866	C
1	1	2873	A
1	1	2883	U
1	1	2884	C
1	1	2888	G
1	1	2889	A
1	1	2907	G
1	1	2908	U
1	1	2911	G
1	1	2912	A
1	1	2913	A
1	1	2914	A
1	1	2915	A
1	1	2921	C
1	1	2925	G
1	1	2927	G
1	1	2928	A
1	1	2932	C
1	1	2949	A
1	1	2953	U
1	1	2954	U
1	1	2955	C
1	1	2956	A
1	1	2960	C
1	1	2974	G
1	1	2978	C
1	1	2982	G
1	1	2983	A
1	1	2984	U
1	1	2987	C
1	1	2998	A

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Mol	Chain	Res	Type
1	1	3010	C
1	1	3015	G
1	1	3021	A
1	1	3034	U
1	1	3041	G
1	1	3046	U
1	1	3047	A
1	1	3049	G
1	1	3052	A
1	1	3053	C
1	1	3058	G
1	1	3077	G
1	1	3079	G
1	1	3082	A
1	1	3091	U
1	1	3094	C
1	1	3101	G
1	1	3102	A
1	1	3108	U
1	1	3109	G
1	1	3115	G
1	1	3123	A
1	1	3124	A
1	1	3126	C
1	1	3140	G
1	1	3169	A
1	1	3170	U
1	1	3171	G
1	1	3181	G
1	1	3182	A
1	1	3185	A
1	1	3186	G
1	1	3190	G
1	1	3198	A
1	1	3204	C
1	1	3205	C
1	1	3208	C
1	1	3211	U
1	1	3213	G
1	1	3228	G
1	1	3229	C
1	1	3234	A

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Mol	Chain	Res	Type
1	1	3237	U
1	1	3242	A
1	1	3243	U
1	1	3253	A
1	1	3254	U
1	1	3255	A
1	1	3256	U
1	1	3257	G
1	1	3266	U
1	1	3267	U
1	1	3268	C
1	1	3269	A
1	1	3270	C
1	1	3279	U
1	1	3280	U
1	1	3282	U
1	1	3283	U
1	1	3284	U
1	1	3285	C
1	1	3286	A
1	1	3287	U
1	1	3288	G
1	1	3289	C
1	1	3290	A
1	1	3291	A
1	1	3292	U
1	1	3293	G
1	1	3295	U
1	1	3298	A
1	1	3299	G
1	1	3302	C
1	1	3303	U
1	1	3304	C
1	1	3305	U
1	1	3306	G
1	1	3310	U
1	1	3311	G
1	1	3312	C
1	1	3314	U
1	1	3320	C
1	1	3321	A
1	1	3322	A

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Mol	Chain	Res	Type
1	1	3323	A
1	1	3327	C
1	1	3345	G
1	1	3349	A
1	1	3350	G
1	1	3351	A
1	1	3355	U
1	1	3356	C
1	1	3357	A
1	1	3359	U
1	1	3361	U
1	1	3366	C
1	1	3374	G
1	1	3375	U
1	1	3376	G
1	1	3378	U
1	1	3379	A
1	1	3380	C
1	1	3389	C
1	1	3398	U
1	1	3401	U
1	1	3402	U
1	1	3403	G
1	1	3404	C
1	1	3423	U
1	1	3424	G
1	1	3428	G
1	1	3435	U
1	1	3436	G
1	1	3437	U
1	1	3443	A
1	1	3444	U
1	1	3449	U
1	1	3450	A
1	1	3456	U
1	1	3459	C
1	1	3463	C
1	1	3464	G
1	1	3467	G
1	1	3471	G
1	1	3477	G
2	3	2	C

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Mol	Chain	Res	Type
2	3	7	G
2	3	11	A
2	3	19	U
2	3	26	C
2	3	33	U
2	3	48	G
2	3	50	A
2	3	53	U
2	3	54	A
2	3	55	A
2	3	64	A
2	3	72	U
2	3	80	U
2	3	92	U
2	3	100	A
2	3	105	C
2	3	110	G
2	3	113	G
2	3	120	G
2	3	122	U
3	4	23	U
3	4	34	A
3	4	35	C
3	4	49	G
3	4	51	G
3	4	55	U
3	4	59	A
3	4	62	C
3	4	63	G
3	4	80	A
3	4	81	U
3	4	82	U
3	4	83	C
3	4	84	A
3	4	86	U
3	4	87	G
3	4	88	A
3	4	90	U
3	4	95	A
3	4	104	A
3	4	105	A
3	4	106	C

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Mol	Chain	Res	Type
3	4	108	C
3	4	109	A
3	4	111	A
3	4	113	G
3	4	122	G
3	4	124	G
3	4	127	A
3	4	130	C
3	4	139	A
3	4	152	U
3	4	153	G
3	4	156	U
3	4	157	U

All (94) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	116	A
1	1	180	G
1	1	193	U
1	1	259	A
1	1	405	A
1	1	407	G
1	1	413	G
1	1	460	U
1	1	537	G
1	1	547	U
1	1	578	G
1	1	580	U
1	1	581	U
1	1	614	U
1	1	649	G
1	1	654	G
1	1	748	G
1	1	823	G
1	1	826	A
1	1	873	U
1	1	874	G
1	1	875	G
1	1	890	G
1	1	906	A
1	1	986	A

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Mol	Chain	Res	Type
1	1	1006	G
1	1	1027	G
1	1	1049	C
1	1	1051	C
1	1	1082	G
1	1	1089	C
1	1	1153	A
1	1	1239	G
1	1	1241	U
1	1	1277	A
1	1	1283	U
1	1	1403	G
1	1	1436	A
1	1	1439	U
1	1	1440	A
1	1	1651	A
1	1	1675	U
1	1	1699	A
1	1	1723	U
1	1	1724	G
1	1	1737	A
1	1	1751	C
1	1	1825	G
1	1	1841	G
1	1	1897	U
1	1	1915	U
1	1	1937	U
1	1	1944	A
1	1	1961	A
1	1	1982	A
1	1	2212	U
1	1	2215	C
1	1	2224	G
1	1	2226	A
1	1	2258	A
1	1	2427	U
1	1	2485	A
1	1	2487	C
1	1	2635	U
1	1	2651	C
1	1	2663	U
1	1	2664	U

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Mol	Chain	Res	Type
1	1	2704	A
1	1	2738	C
1	1	2791	A
1	1	2800	U
1	1	2806	A
1	1	2839	G
1	1	2997	U
1	1	3090	U
1	1	3167	A
1	1	3204	C
1	1	3205	C
1	1	3233	U
1	1	3254	U
1	1	3255	A
1	1	3269	A
1	1	3281	G
1	1	3288	G
1	1	3290	A
1	1	3302	C
1	1	3348	G
1	1	3356	C
1	1	3358	A
1	1	3362	C
1	1	3456	U
2	3	112	U
3	4	83	C
3	4	87	G

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.