



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:38 AM UTC

PDB ID : 5U4I / pdb_00005u4i
EMDB ID : EMD-8505
Title : Structural Basis of Co-translational Quality Control by ArfA and RF2 Bound to Ribosome
Authors : Zeng, F.; Chen, Y.; Remis, J.; Shekhar, M.; Phillips, J.C.; Tajkhorshid, E.; Jin, H.
Deposited on : 2016-12-04
Resolution : 3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

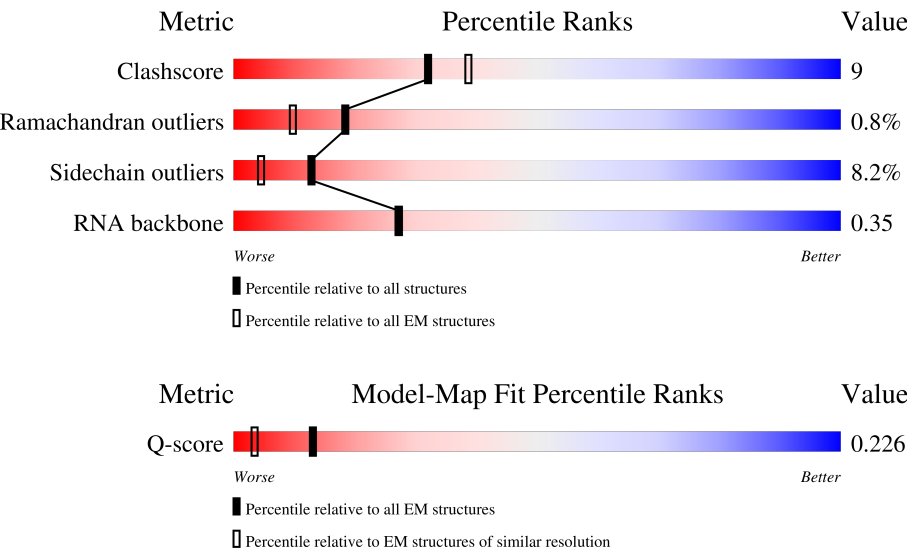
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2904	30% 40% 46% 13%
2	B	118	66% 43% 46% 11%
3	C	273	70% 78% 18% ..

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Mol	Chain	Length	Quality of chain
4	D	209	86% 83% 15% .
5	E	201	79% 80% 19% .
6	F	179	93% 82% 15% ..
7	G	177	96% 85% 14% ..
8	H	149	100% 87% 11% .
9	J	142	99% 82% 15% ..
10	K	142	96% 89% 11% .
11	L	123	82% 78% 16% 5% .
12	M	144	92% 83% 16% .
13	N	136	85% 82% 16% .
14	O	127	85% 72% 21% . 6%
15	P	117	94% 87% 12% .
16	Q	115	96% 89% 10% .
17	R	118	84% 79% 19% ..
18	S	103	83% 78% 19% ..
19	T	110	48% 78% 20% .
20	U	100	81% 81% 12% 7%
21	V	104	83% 80% 18% .
22	W	94	96% 80% 18% .
23	X	85	87% 75% 12% . 9%
24	Y	78	97% 74% 22% ..
25	Z	63	84% 86% 11% ..
26	0	59	83% 92% 7% .
27	1	57	75% 86% 11% ..
28	2	55	89% 75% 15% . 9%

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Mol	Chain	Length	Quality of chain
29	3	46	
30	4	65	
31	5	38	
32	a	1533	
33	b	241	
34	c	233	
35	d	206	
36	e	167	
37	f	135	
38	g	179	
39	h	129	
40	i	130	
41	j	103	
42	k	117	
43	l	123	
44	m	118	
45	n	100	
46	o	88	
47	p	82	
48	q	84	
49	r	75	
50	s	82	
51	t	86	
52	u	71	
53	v	383	

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Mol	Chain	Length	Quality of chain
54	w	57	
55	x	77	
55	y	77	
56	z	18	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PSU	A	2504	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 149495 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2904	Total	C	N	O	P	0	0
			62351	27820	11472	20155	2904		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	887	A	U	conflict	GB 42756

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- 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 L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

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

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

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

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 22 is a protein called 50S ribosomal protein L25.

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

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	77	Total	C	N	O	S	0	0
			588	363	118	106	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	0	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	50	Total	C	N	O		0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1533	Total	C	N	O	P	0	0
			32906	14683	6036	10654	1533		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	527	A	G	conflict	GB 817573384

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- 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	204	Total	C	N	O	S	0	0
			1633	1020	313	296	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
			1156	719	218	213	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	117	Total	C	N	O	S	0	0
			877	540	174	160	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	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- 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	S	0	0
			539	341	100	97	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	15	GLU	ALA	conflict	UNP P0A7T7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 53 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	357	Total	C	N	O	S	0	0
			2836	1744	498	584	10		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	-17	HIS	-	expression tag	UNP P07012
v	-16	HIS	-	expression tag	UNP P07012
v	-15	HIS	-	expression tag	UNP P07012
v	-14	HIS	-	expression tag	UNP P07012
v	-13	HIS	-	expression tag	UNP P07012
v	-12	HIS	-	expression tag	UNP P07012
v	-11	SER	-	expression tag	UNP P07012
v	-10	ALA	-	expression tag	UNP P07012
v	-9	ALA	-	expression tag	UNP P07012
v	-8	LEU	-	expression tag	UNP P07012
v	-7	GLU	-	expression tag	UNP P07012
v	-6	VAL	-	expression tag	UNP P07012
v	-5	LEU	-	expression tag	UNP P07012
v	-4	PHE	-	expression tag	UNP P07012
v	-3	GLN	-	expression tag	UNP P07012
v	-2	GLY	-	expression tag	UNP P07012
v	-1	PRO	-	expression tag	UNP P07012
v	0	GLY	-	expression tag	UNP P07012

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	47	Total	C	N	O	S	0	0
			388	239	82	66	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	-1	GLY	-	expression tag	UNP P36675
w	0	SER	-	expression tag	UNP P36675

- Molecule 55 is a RNA chain called P-site or E-site fMet-tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
55	x	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

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Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	A	100	Total	Mg	0
			100	100	
57	B	4	Total	Mg	0
			4	4	
57	a	20	Total	Mg	0
			20	20	

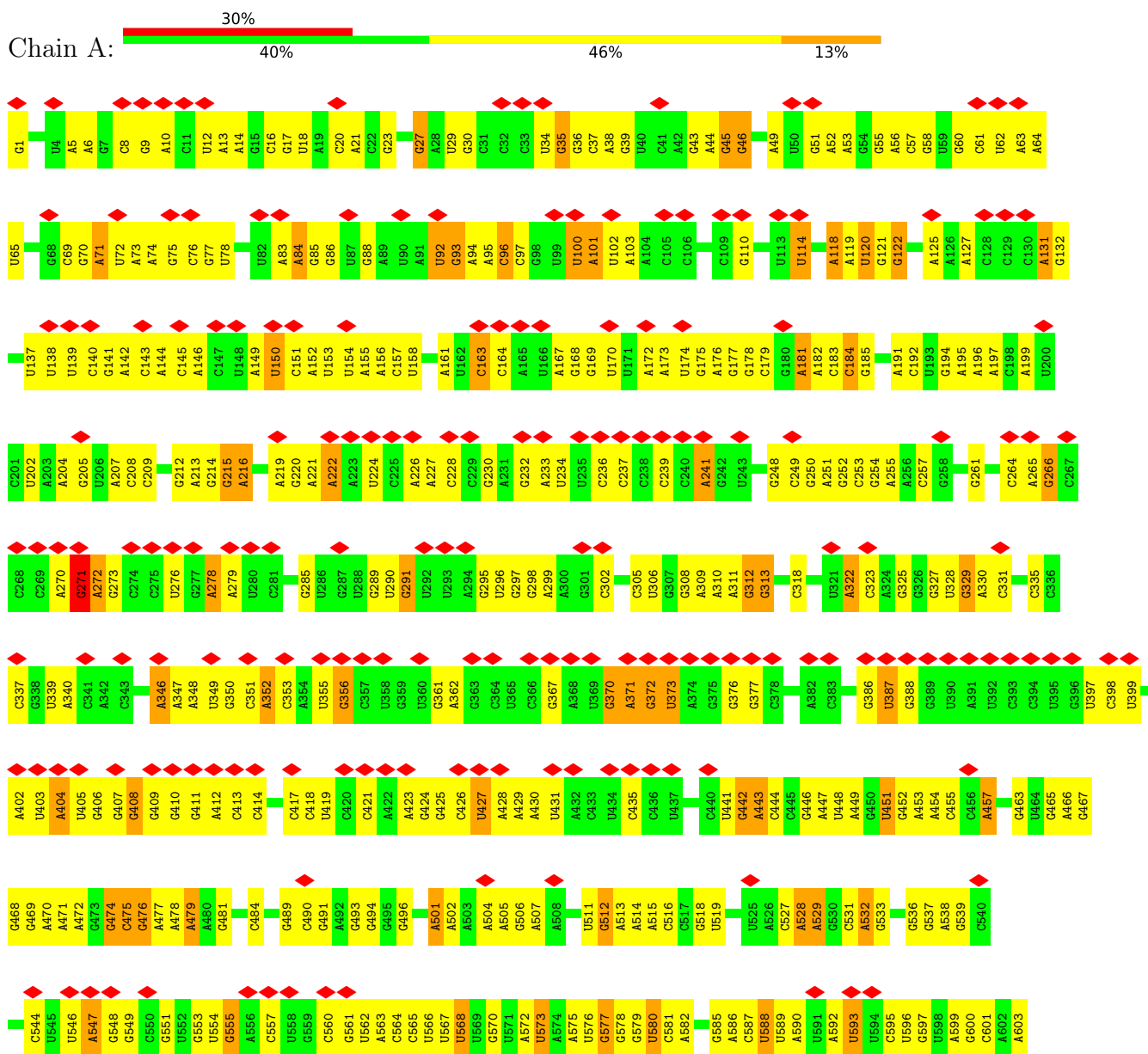
- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

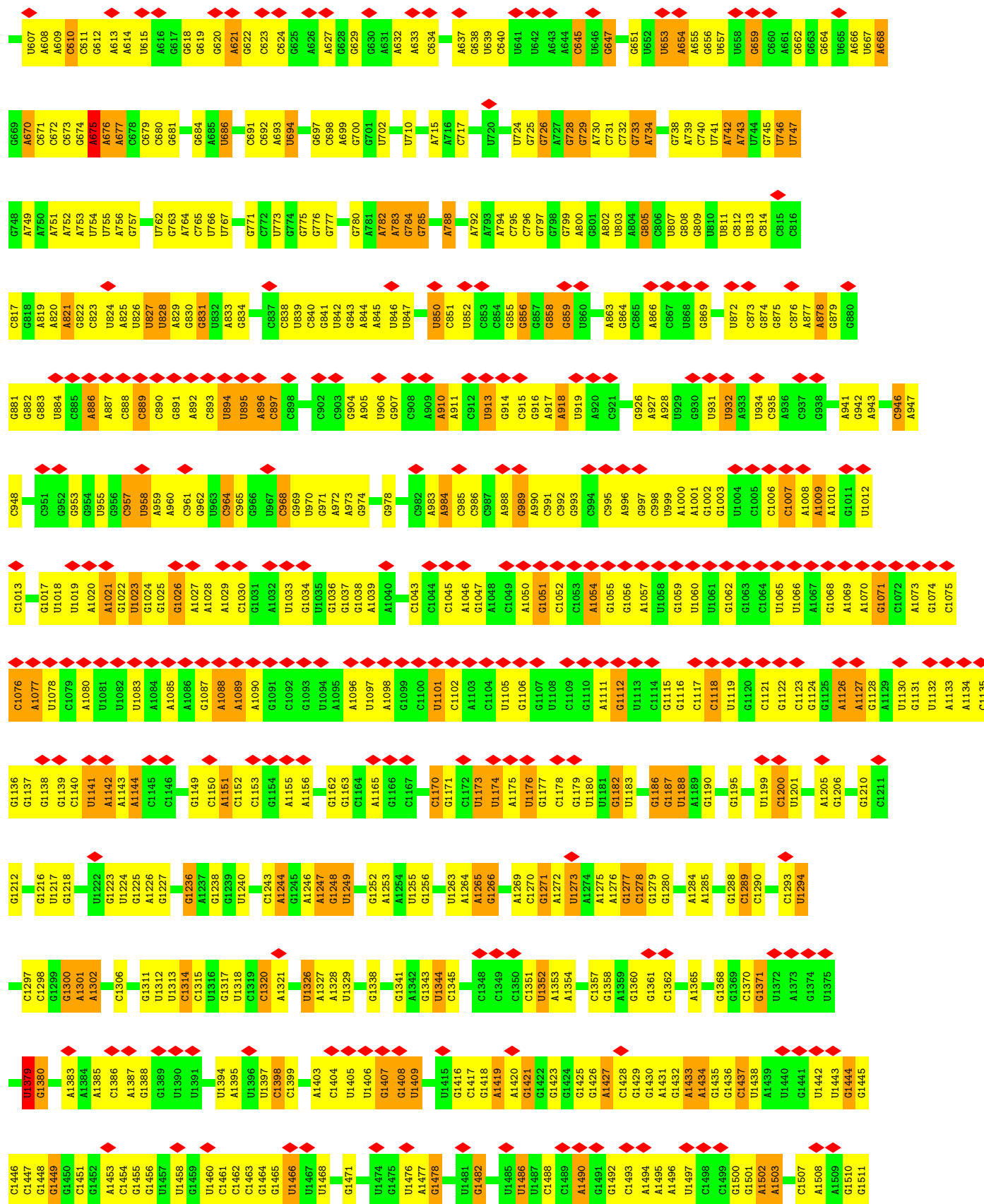
Mol	Chain	Residues	Atoms		AltConf
58	5	1	Total	Zn	0
			1	1	

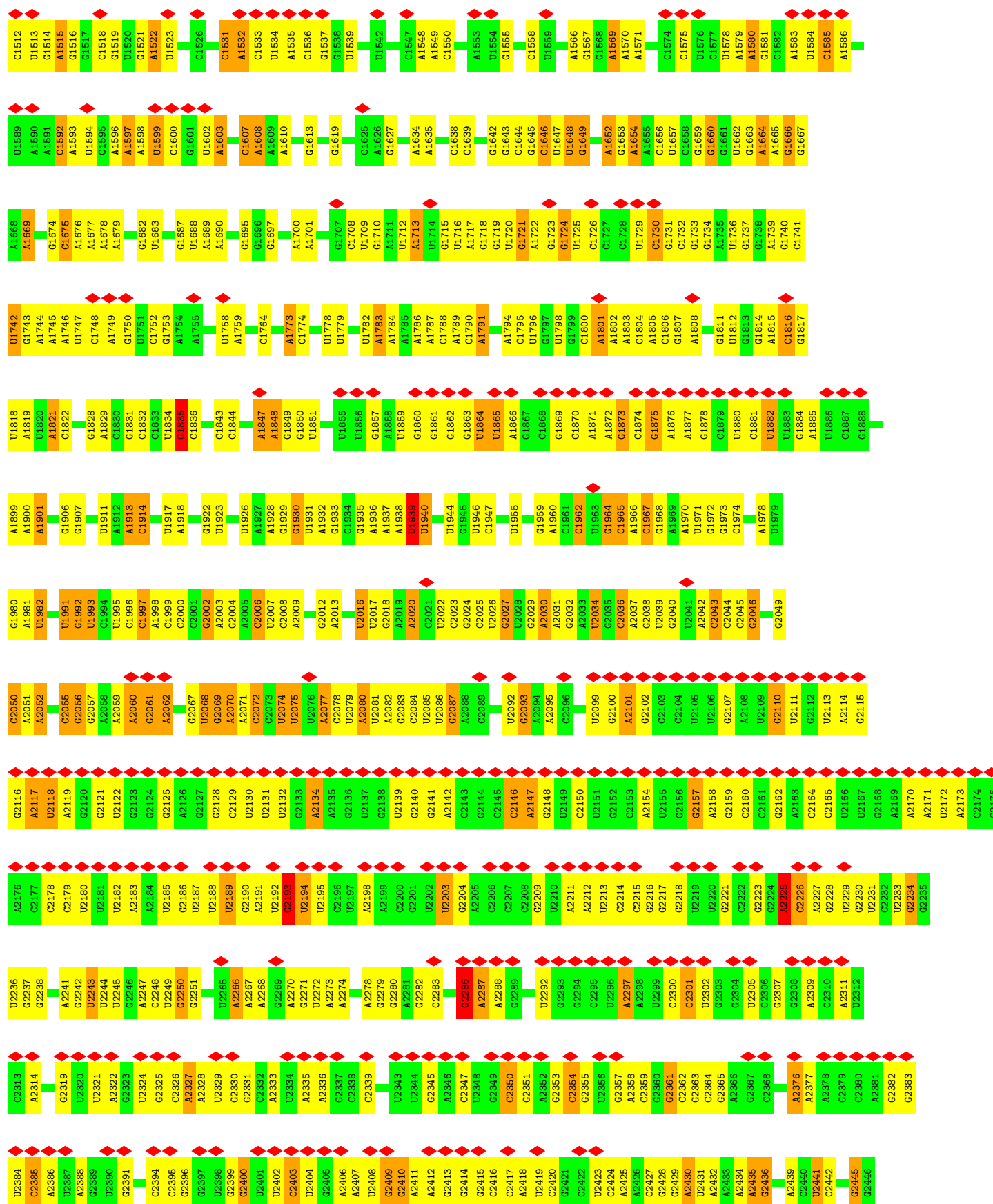
3 Residue-property plots

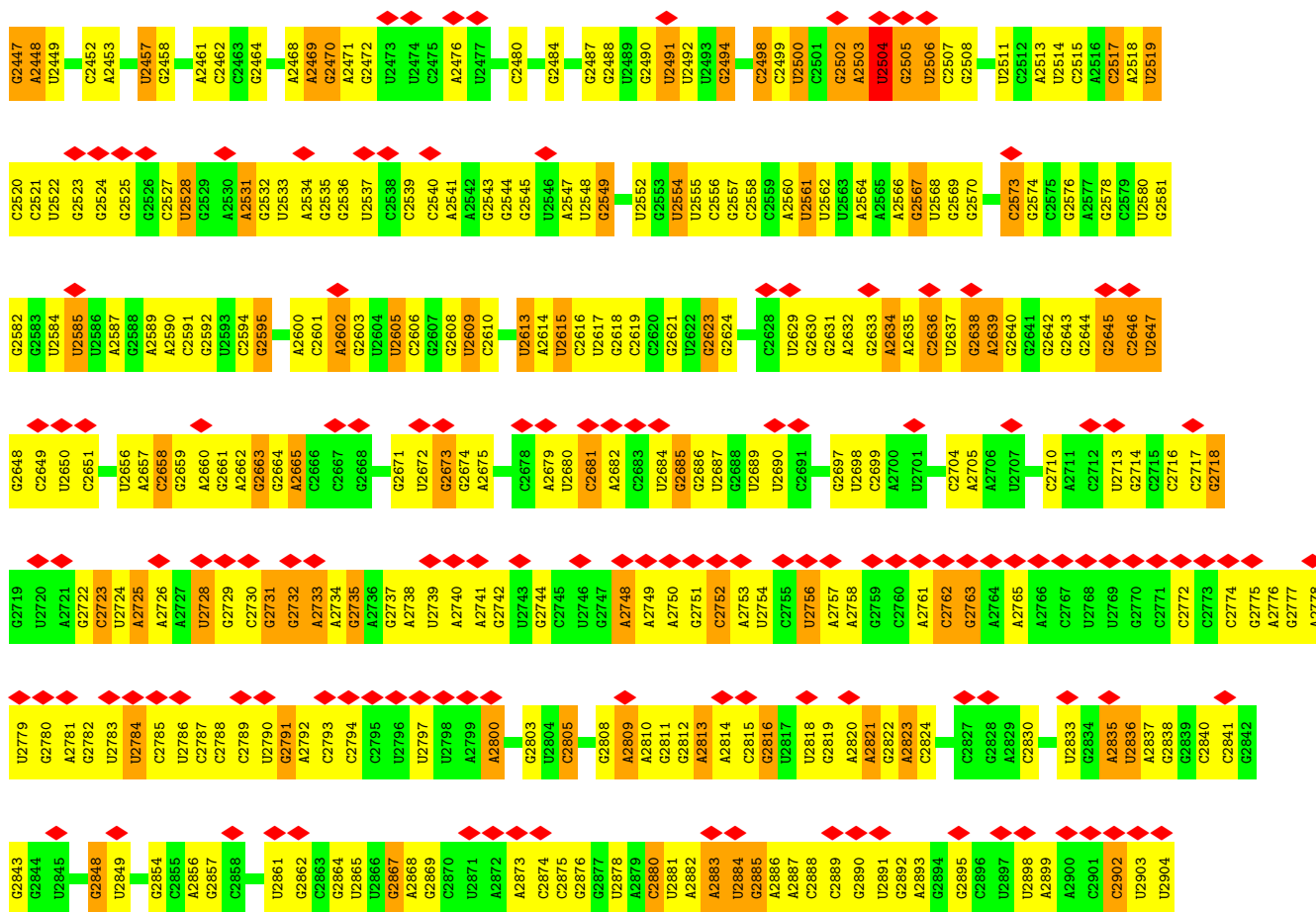
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 rRNA

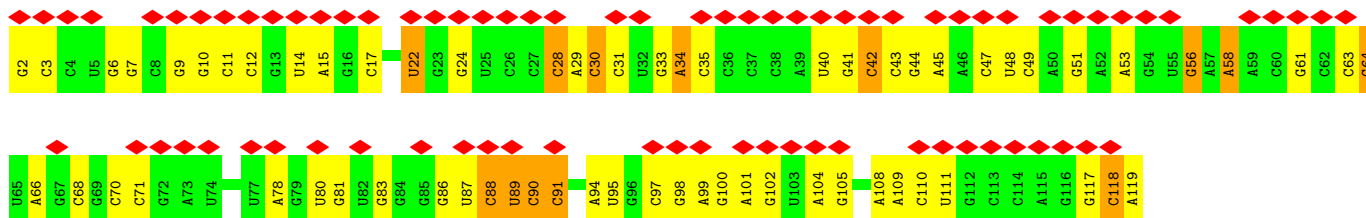
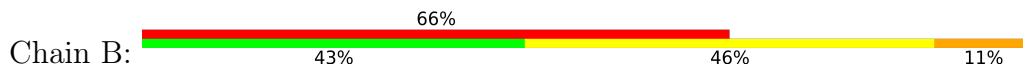




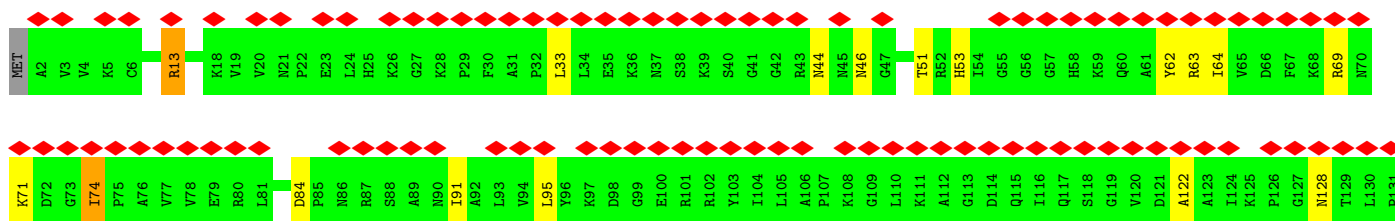
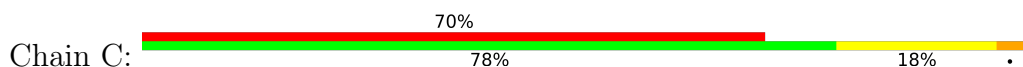


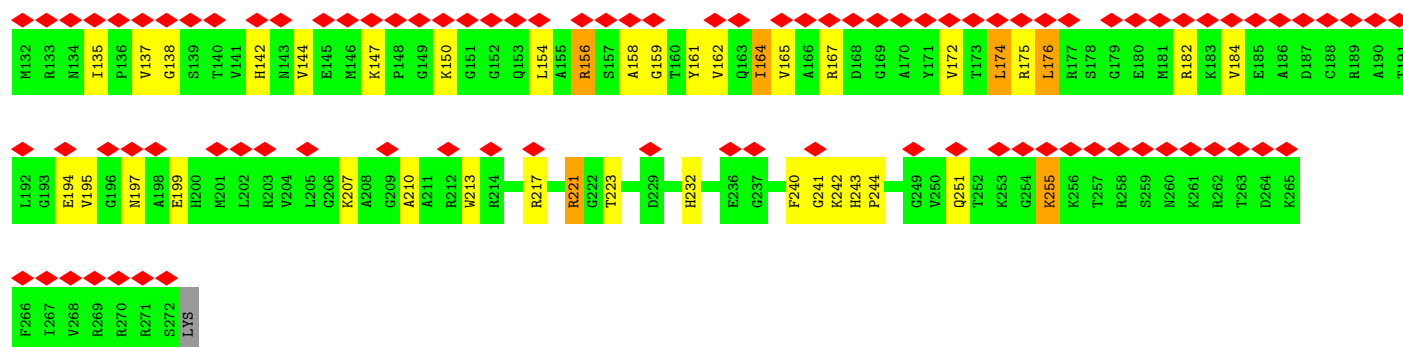


• Molecule 2: 5S rRNA

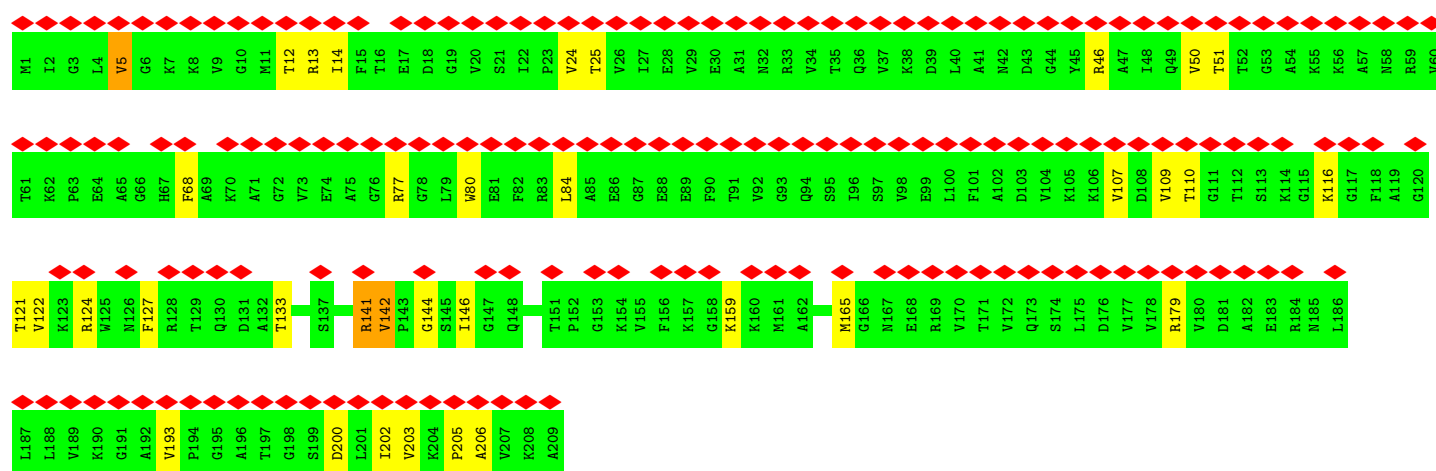
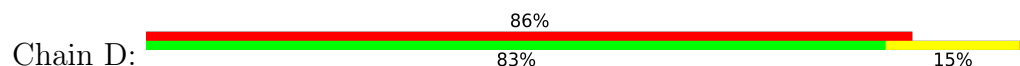


• Molecule 3: 50S ribosomal protein L2

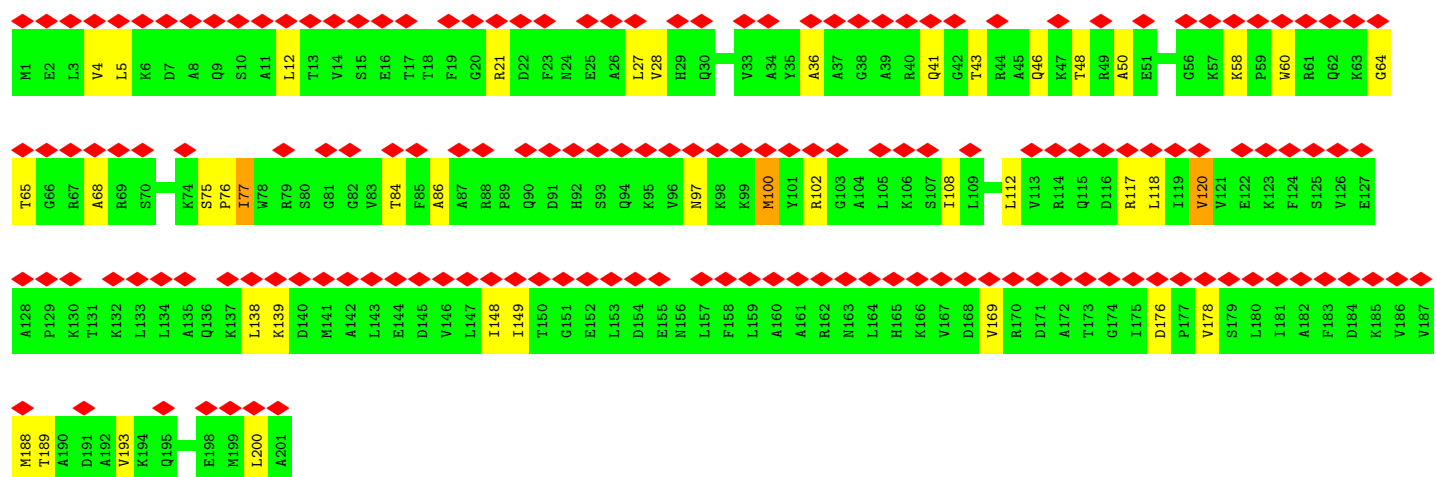
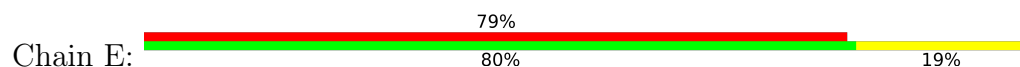




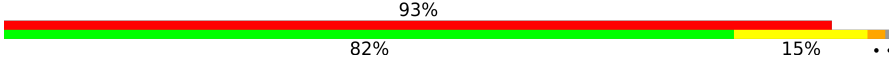
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4

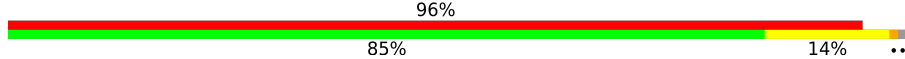


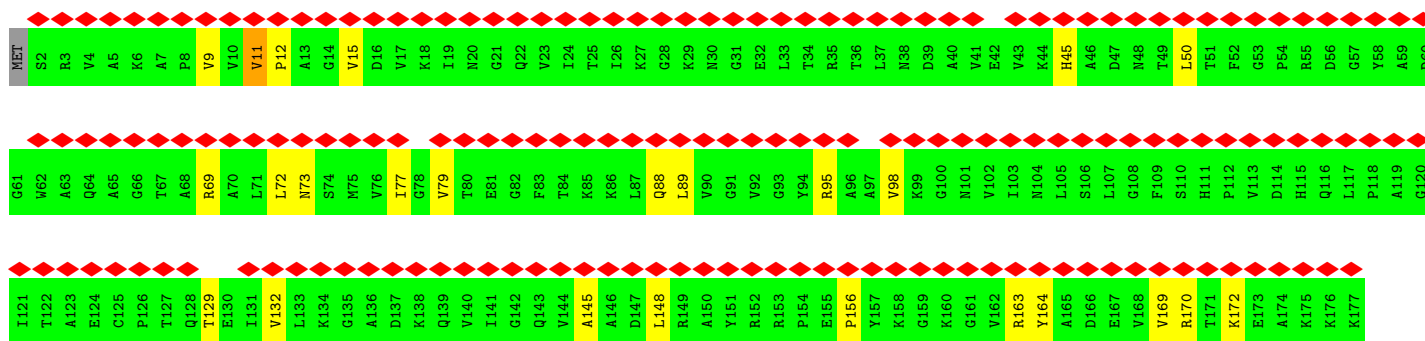
• Molecule 6: 50S ribosomal protein L5

Chain F: 



• Molecule 7: 50S ribosomal protein L6

Chain G: 

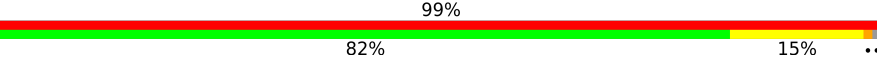


• Molecule 8: 50S ribosomal protein L9

Chain H: 



• Molecule 9: 50S ribosomal protein L11

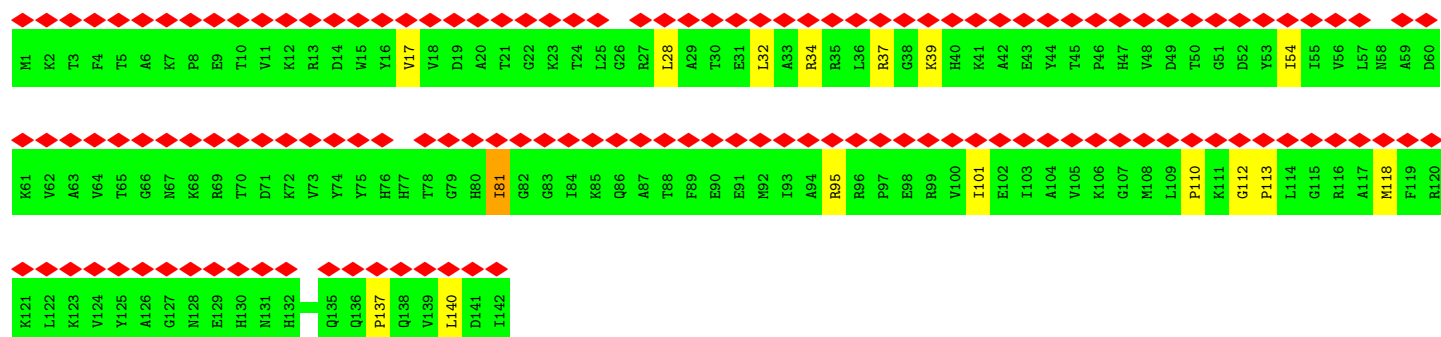
Chain J: 





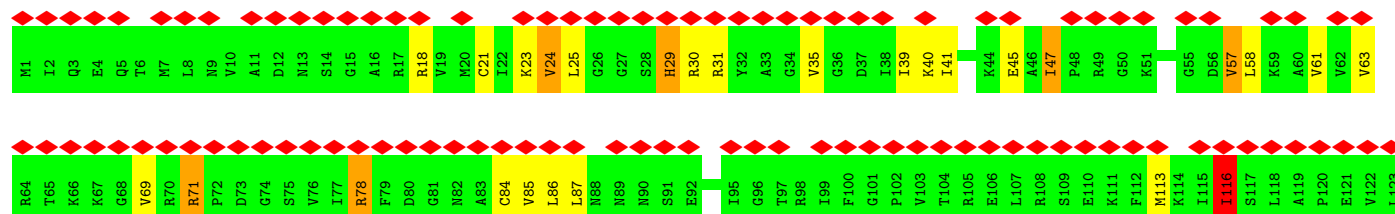
• Molecule 10: 50S ribosomal protein L13

Chain K: 96%
89% 11%



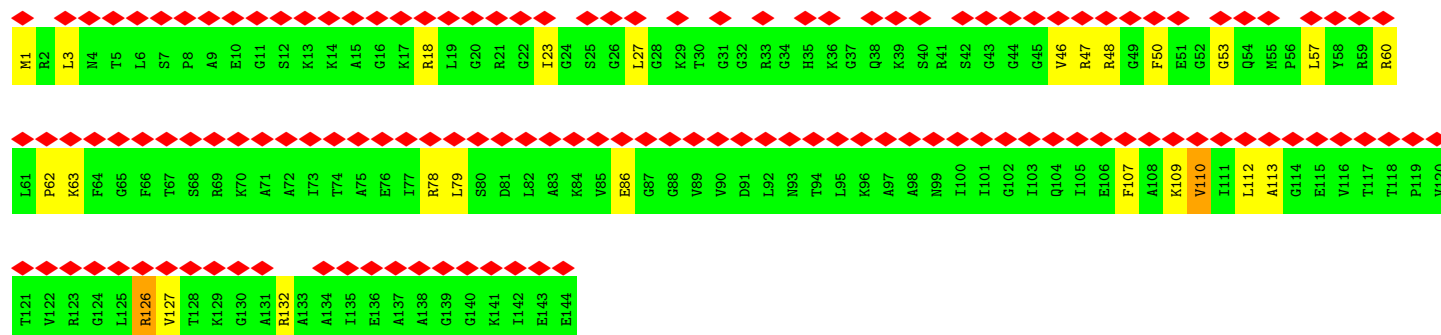
• Molecule 11: 50S ribosomal protein L14

Chain L: 82%
78% 16% 5%



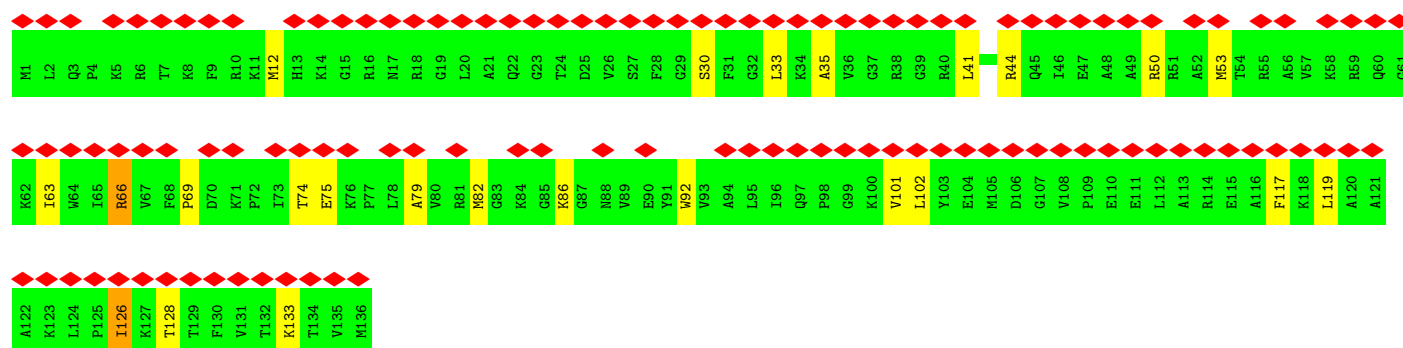
• Molecule 12: 50S ribosomal protein L15

Chain M: 92%
83% 16%



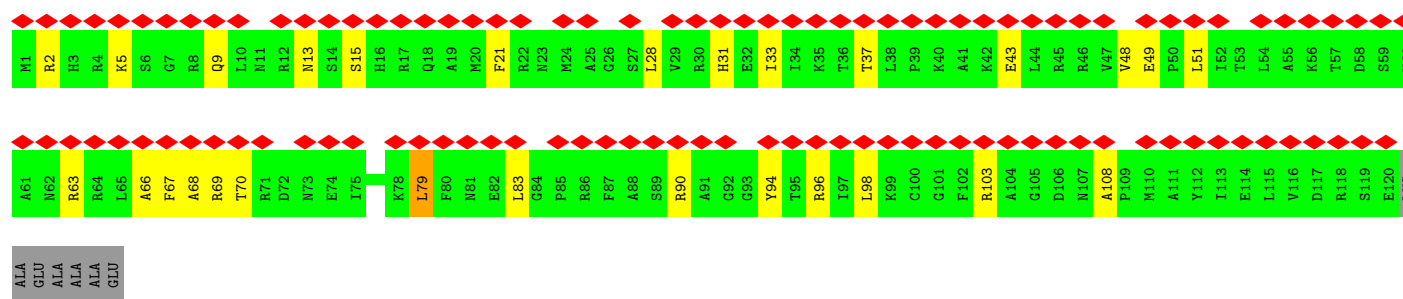
• Molecule 13: 50S ribosomal protein L16

Chain N: 

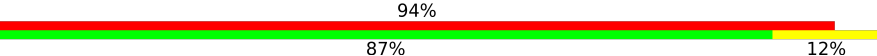


• Molecule 14: 50S ribosomal protein L17

Chain O: 

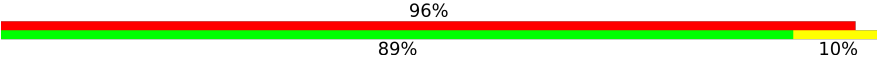


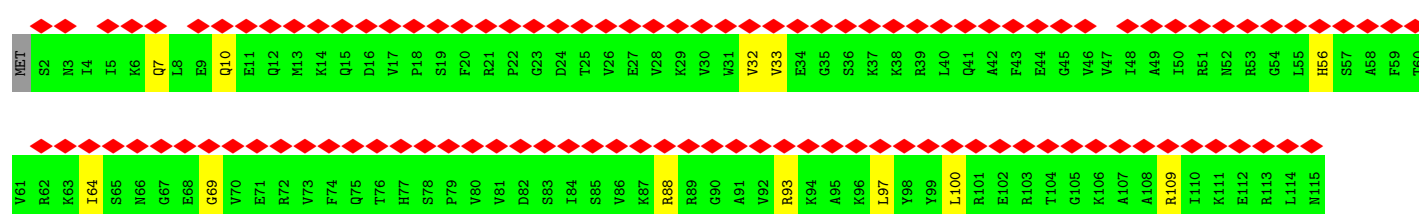
• Molecule 15: 50S ribosomal protein L18

Chain P: 



• Molecule 16: 50S ribosomal protein L19

Chain Q: 



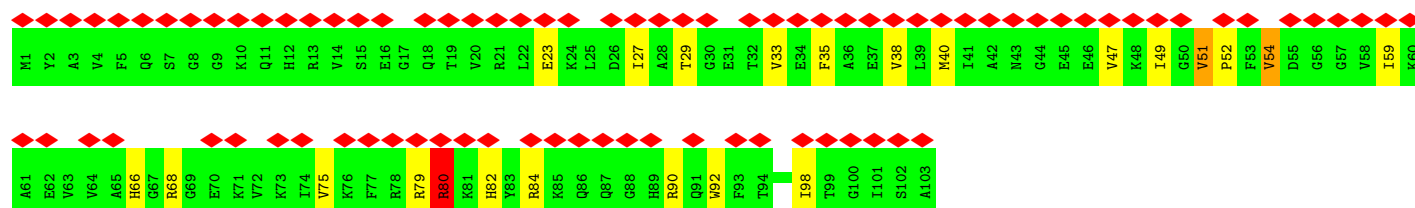
• Molecule 17: 50S ribosomal protein L20

Chain R: 



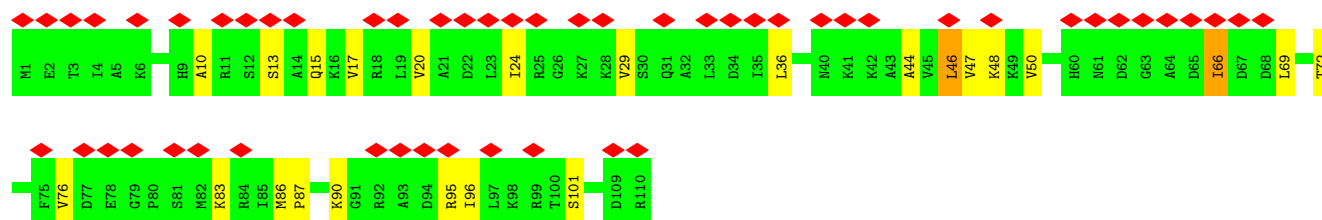
- Molecule 18: 50S ribosomal protein L21

Chain S: 



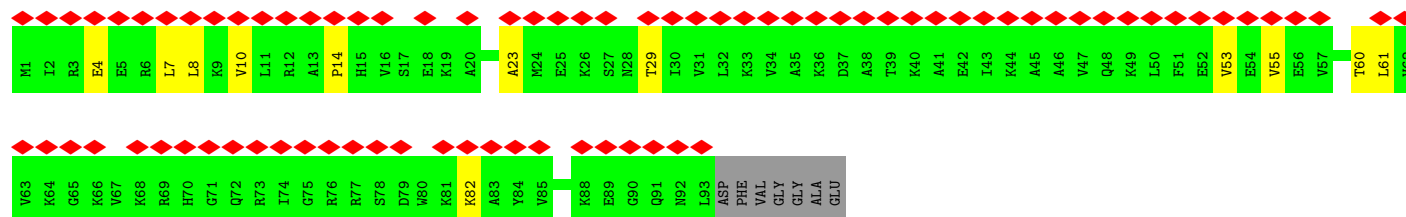
- Molecule 19: 50S ribosomal protein L22

Chain T: 



- Molecule 20: 50S ribosomal protein L23

Chain U: 



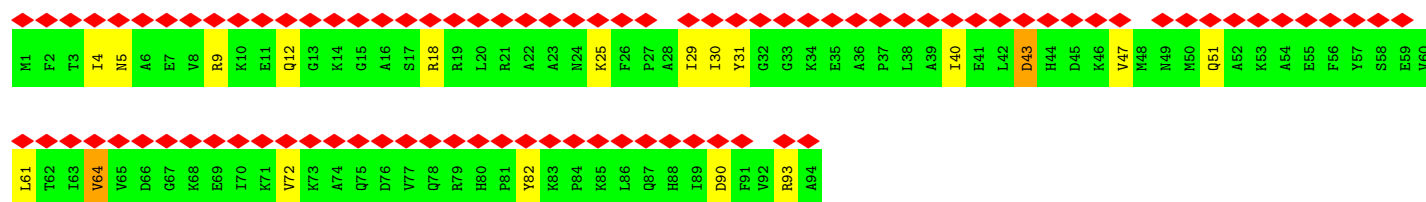
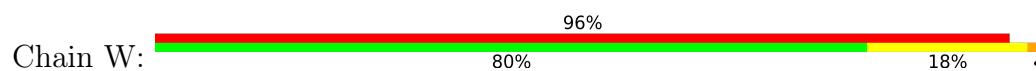
- Molecule 21: 50S ribosomal protein L24

Chain V: 

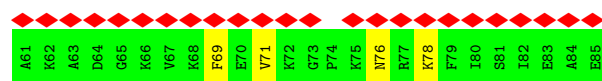
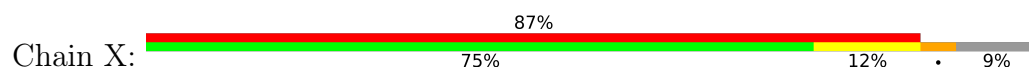




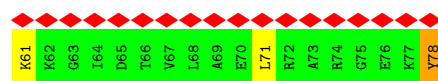
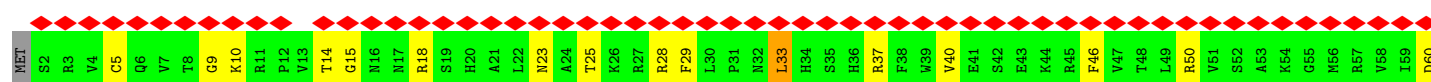
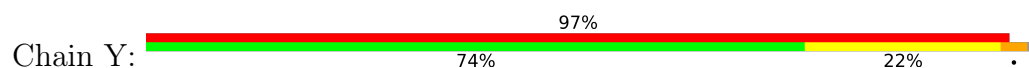
• Molecule 22: 50S ribosomal protein L25



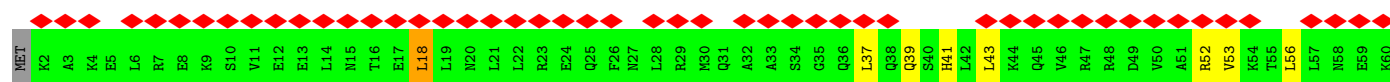
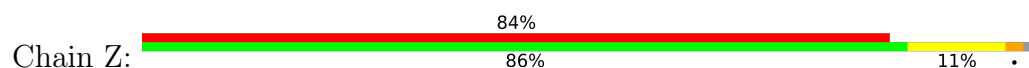
• Molecule 23: 50S ribosomal protein L27



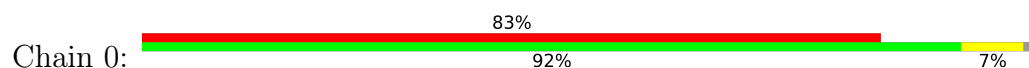
• Molecule 24: 50S ribosomal protein L28

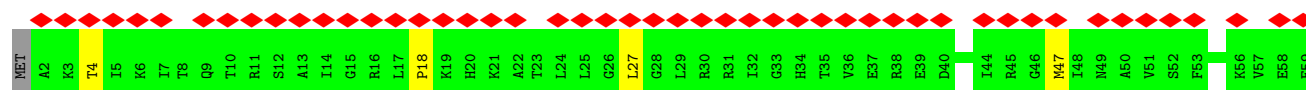


• Molecule 25: 50S ribosomal protein L29

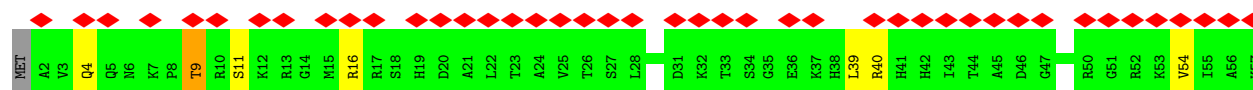
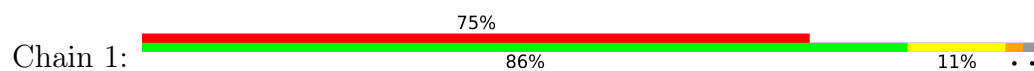


• Molecule 26: 50S ribosomal protein L30

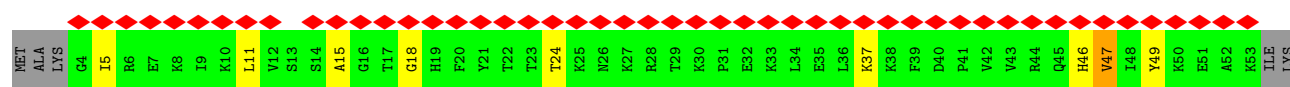
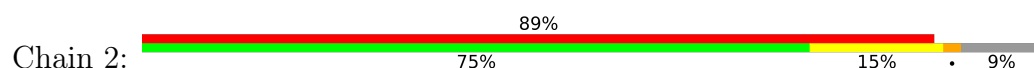




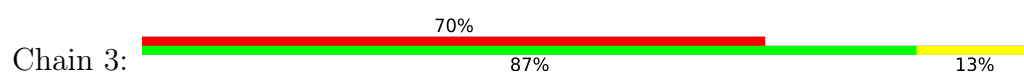
- Molecule 27: 50S ribosomal protein L32



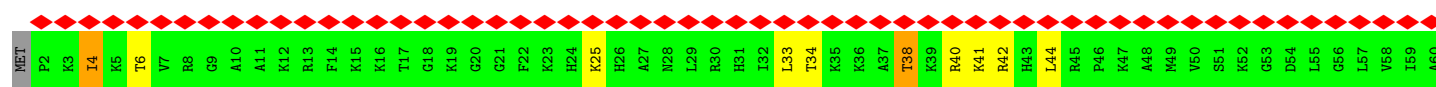
- Molecule 28: 50S ribosomal protein L33



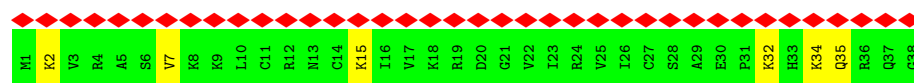
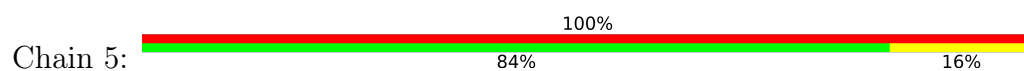
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



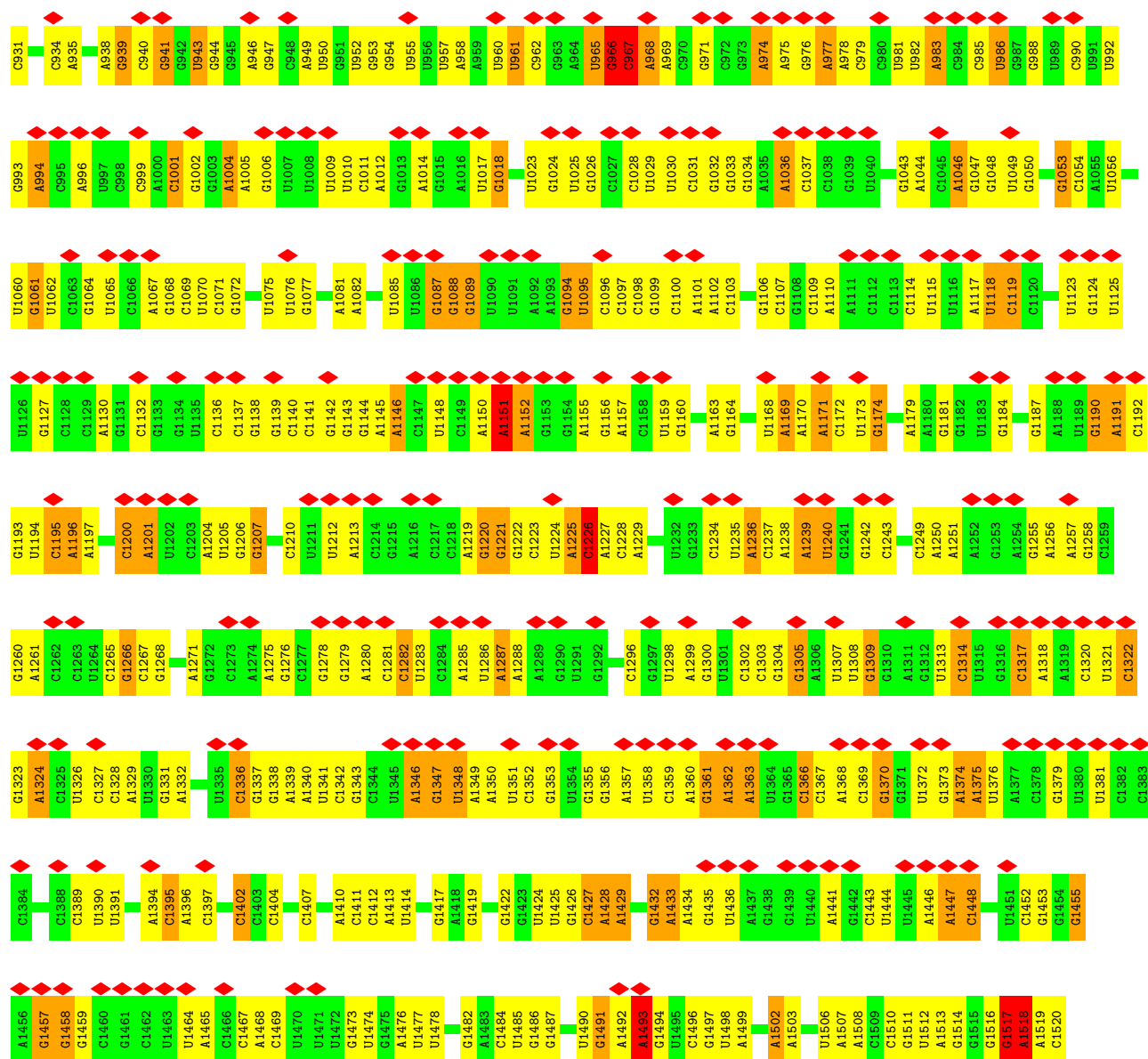
- Molecule 31: 50S ribosomal protein L36



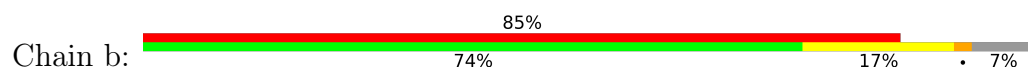
- Molecule 32: 16S rRNA

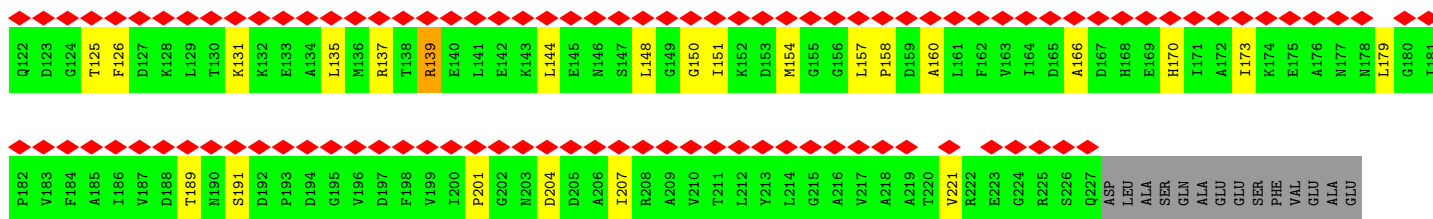




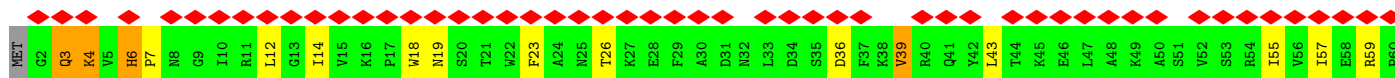


• Molecule 33: 30S ribosomal protein S2

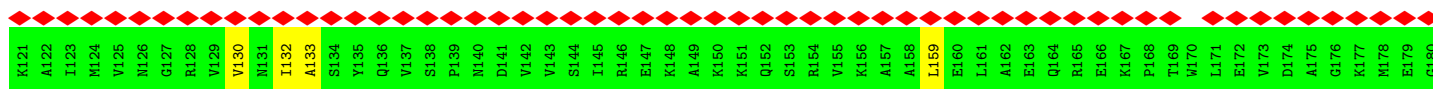
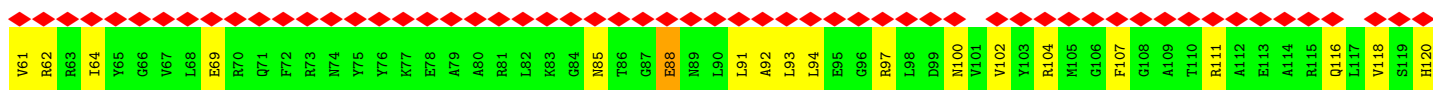
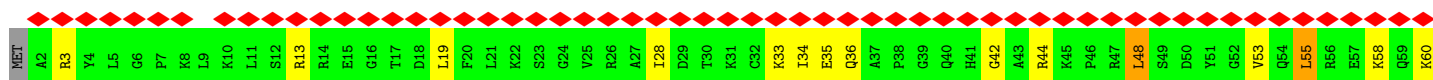
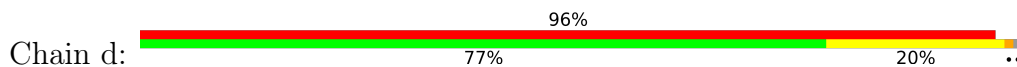




• Molecule 34: 30S ribosomal protein S3

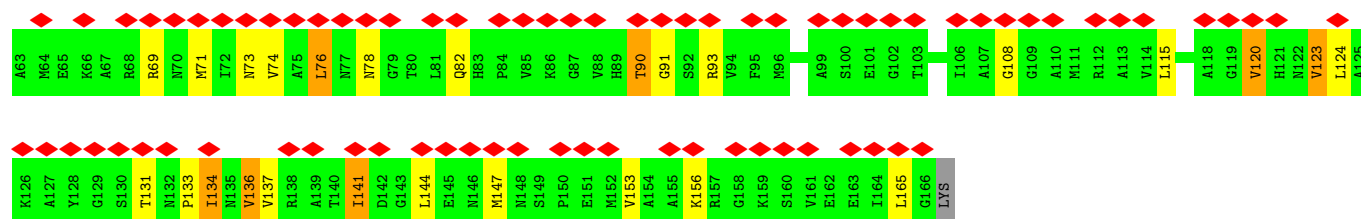


• Molecule 35: 30S ribosomal protein S4

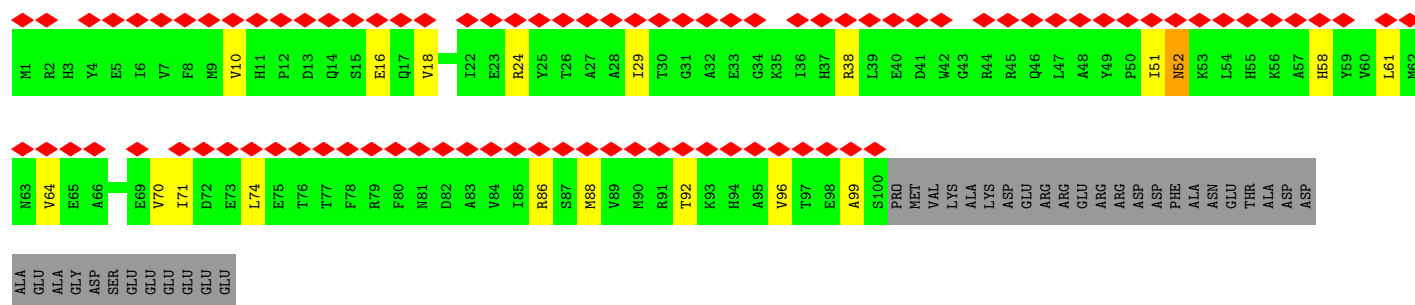


• Molecule 36: 30S ribosomal protein S5

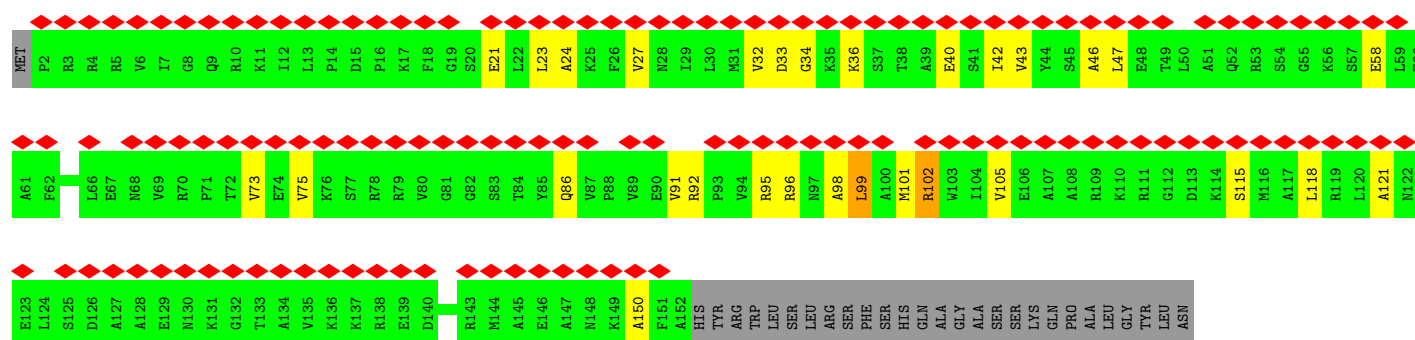
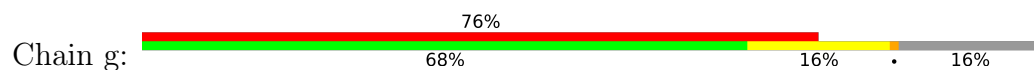




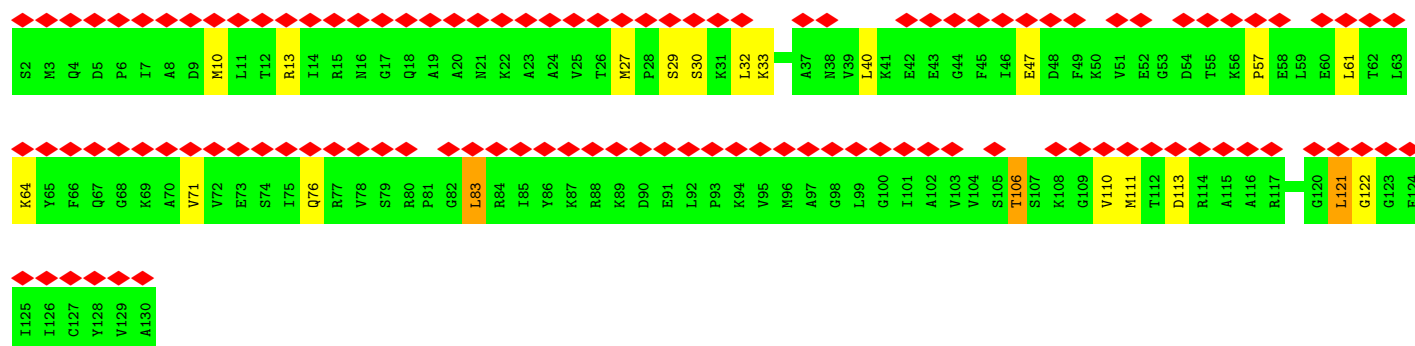
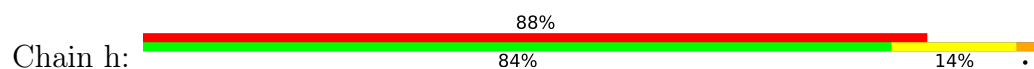
• Molecule 37: 30S ribosomal protein S6



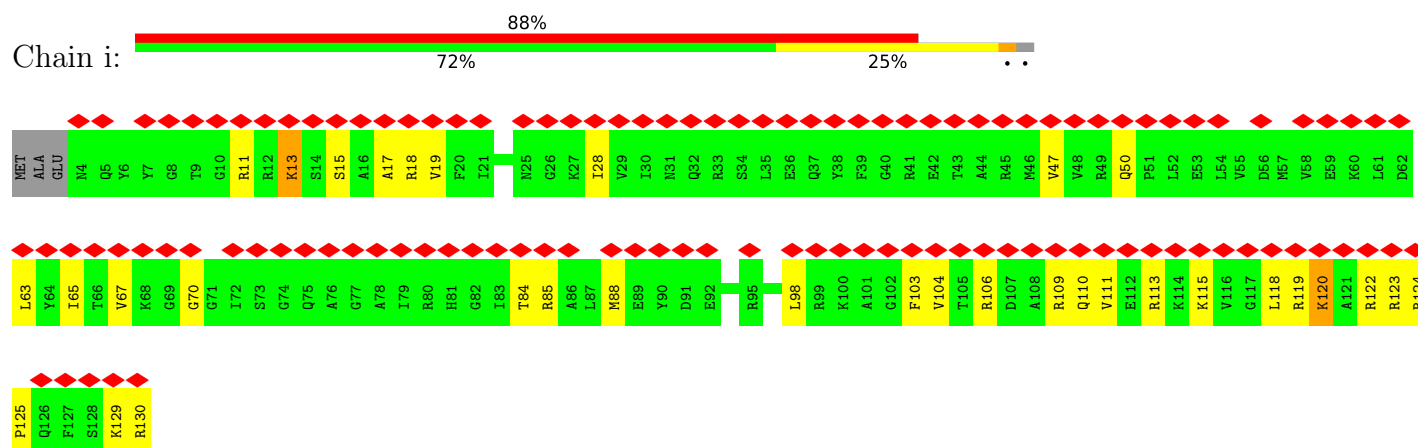
• Molecule 38: 30S ribosomal protein S7



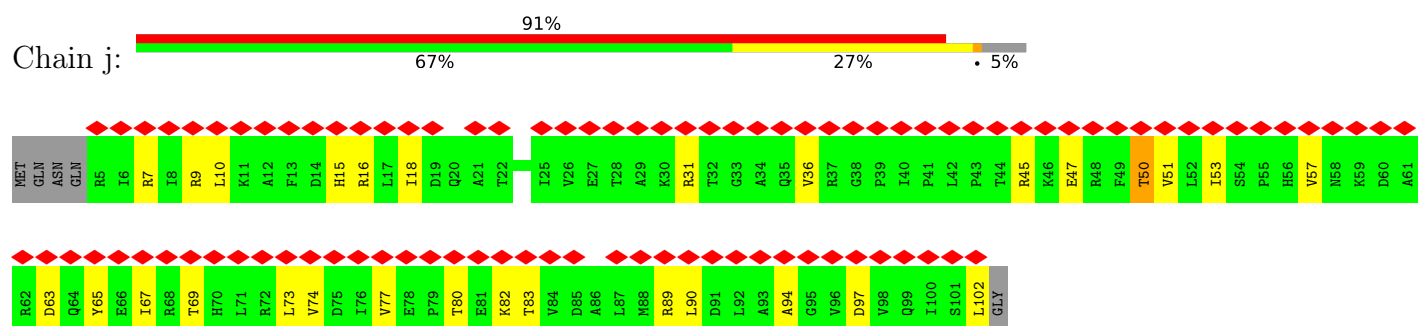
• Molecule 39: 30S ribosomal protein S8



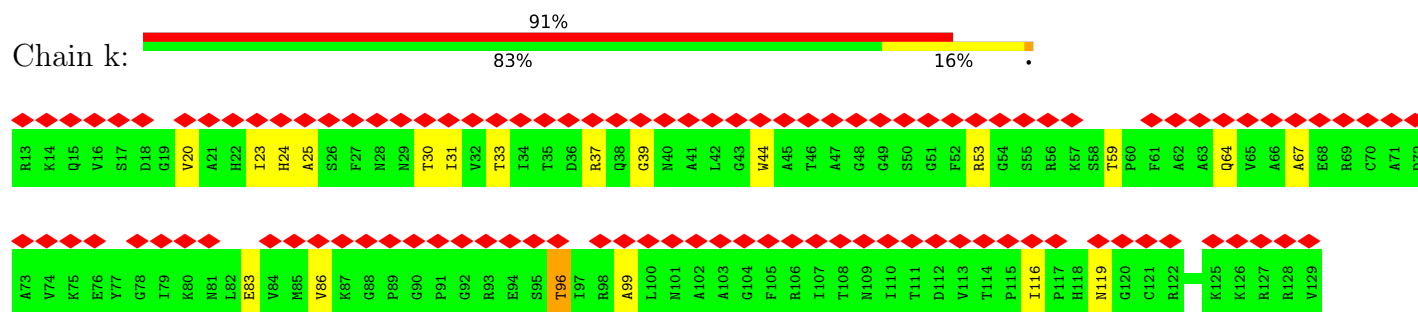
- Molecule 40: 30S ribosomal protein S9



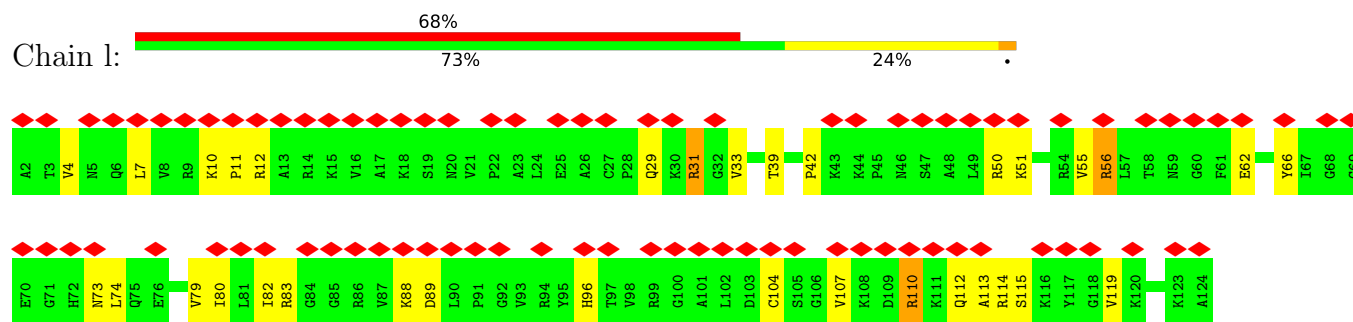
- Molecule 41: 30S ribosomal protein S10



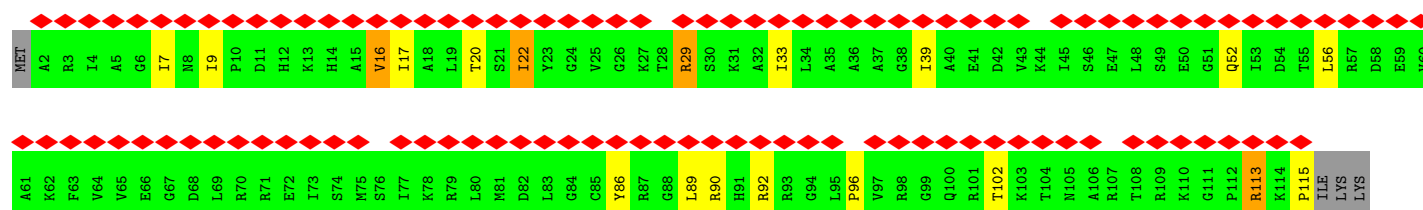
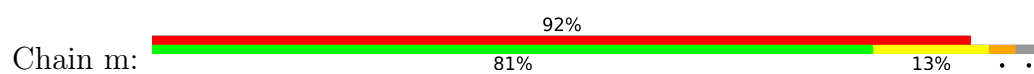
- Molecule 42: 30S ribosomal protein S11



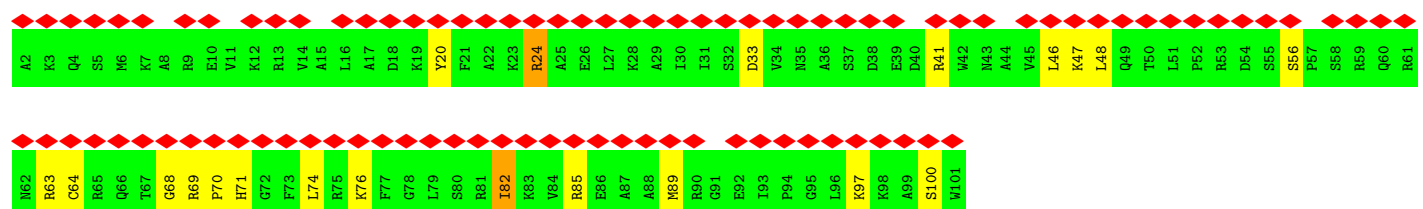
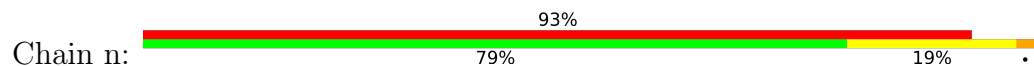
- Molecule 43: 30S ribosomal protein S12



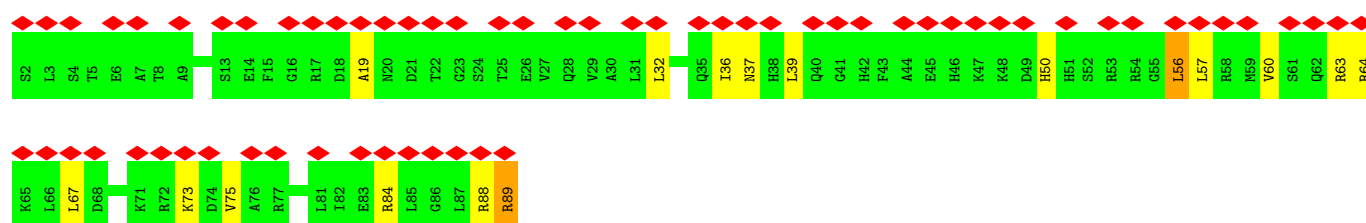
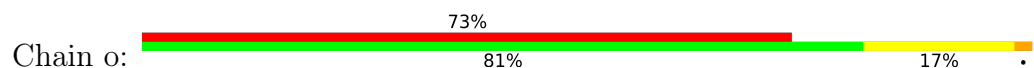
- Molecule 44: 30S ribosomal protein S13



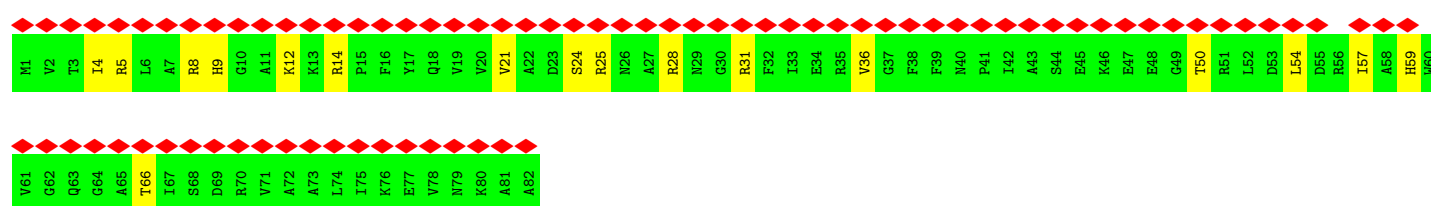
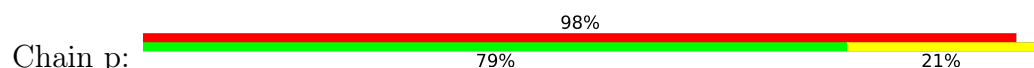
• Molecule 45: 30S ribosomal protein S14



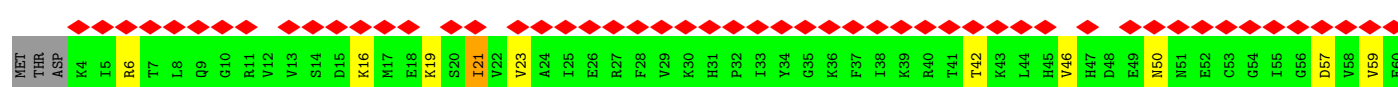
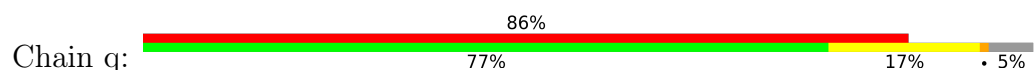
• Molecule 46: 30S ribosomal protein S15



• Molecule 47: 30S ribosomal protein S16

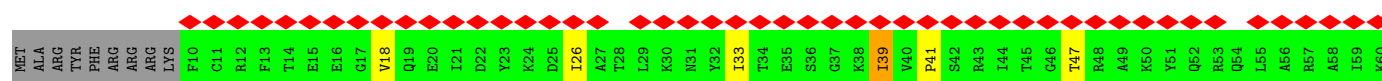
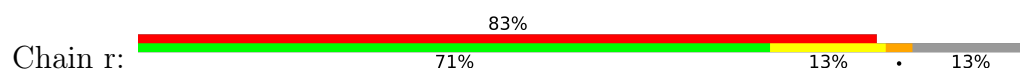


• Molecule 48: 30S ribosomal protein S17

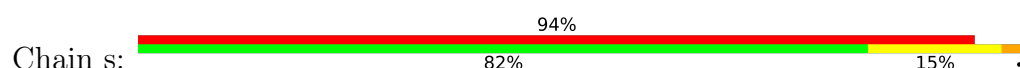




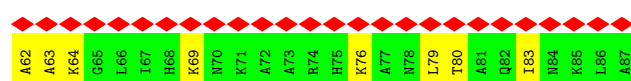
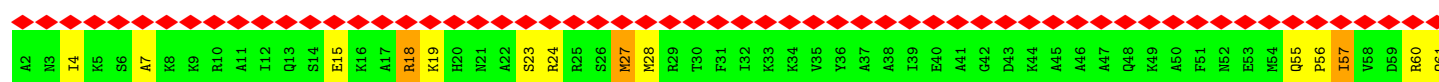
• Molecule 49: 30S ribosomal protein S18



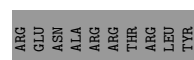
• Molecule 50: 30S ribosomal protein S19



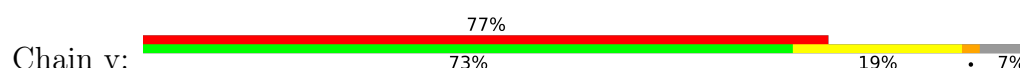
• Molecule 51: 30S ribosomal protein S20

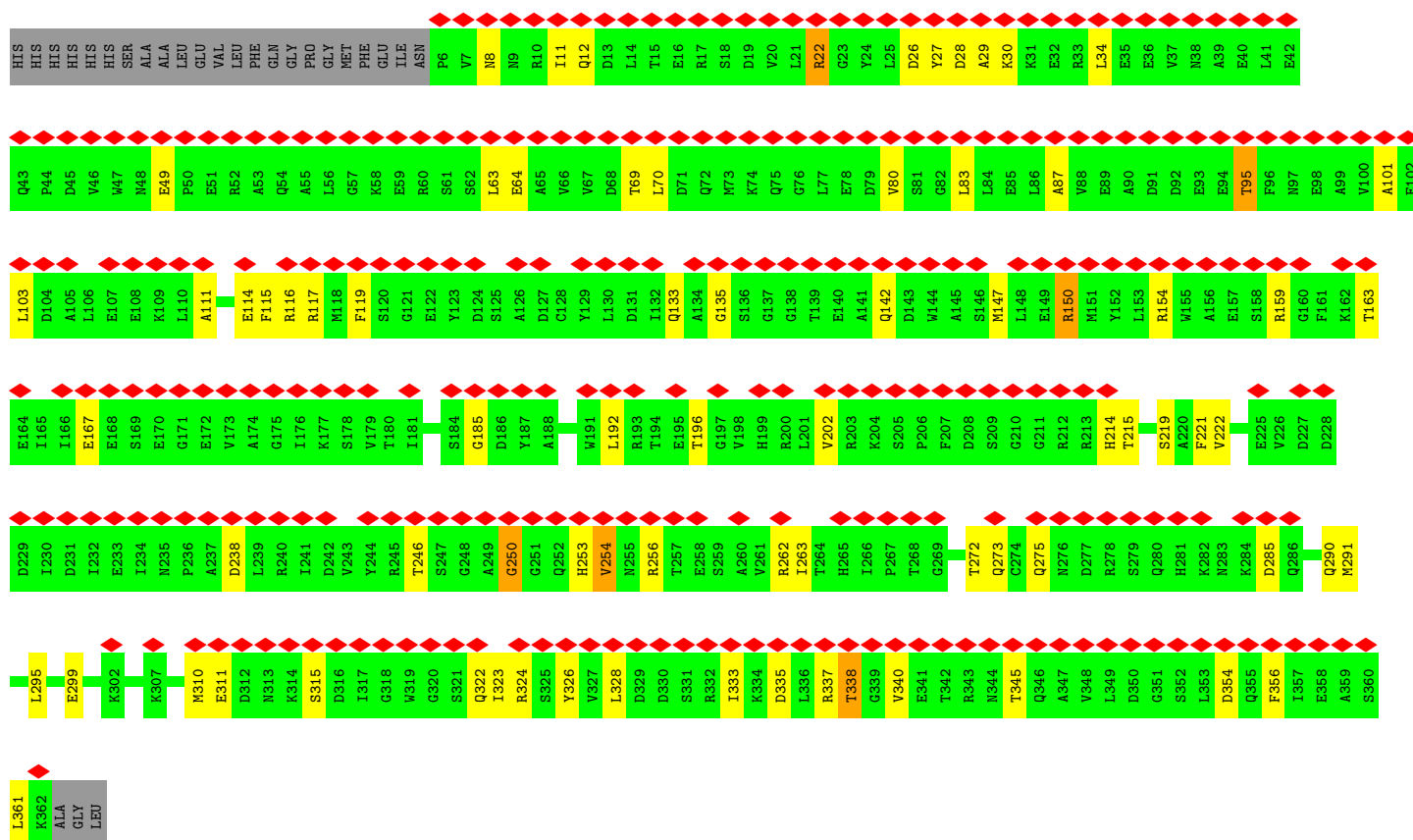


• Molecule 52: 30S ribosomal protein S21

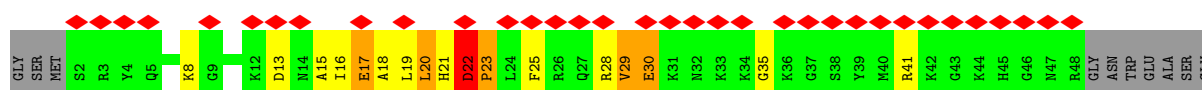


• Molecule 53: Peptide chain release factor 2

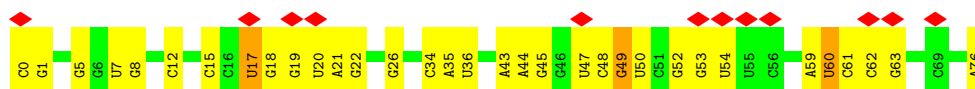




- Molecule 54: Alternative ribosome-rescue factor A



- Molecule 55: P-site or E-site fMet-tRNA(fMet)



- Molecule 55: P-site or E-site fMet-tRNA(fMet)



● Molecule 56: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	155440	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	83822	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	458.112, 458.112, 458.112	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.193, 1.193, 1.193	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1MG, OMC, 5MU, MG, 5MC, MA6, MEQ, UR3, 2MG, OMG, OMU, 4OC, ZN, PSU

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/69434	0.71	17/108325 (0.0%)
2	B	0.38	0/2828	0.71	1/4410 (0.0%)
3	C	0.51	0/2121	0.90	1/2852 (0.0%)
4	D	0.55	0/1586	0.90	0/2134
5	E	0.50	0/1571	1.02	4/2113 (0.2%)
6	F	0.56	0/1434	0.98	0/1926
7	G	0.60	0/1343	0.95	1/1816 (0.1%)
8	H	0.57	0/1122	0.93	0/1515
9	J	0.62	0/1046	1.05	3/1410 (0.2%)
10	K	0.51	0/1152	1.00	2/1551 (0.1%)
11	L	0.52	0/955	0.90	3/1279 (0.2%)
12	M	0.54	0/1062	0.92	0/1413
13	N	0.51	0/1093	0.93	1/1460 (0.1%)
14	O	0.57	0/973	1.04	0/1301
15	P	0.49	0/902	1.02	0/1209
16	Q	0.52	0/929	0.84	0/1242
17	R	0.50	0/960	1.10	0/1278
18	S	0.54	0/829	0.83	0/1107
19	T	0.49	0/864	1.03	1/1156 (0.1%)
20	U	0.51	0/744	0.91	0/994
21	V	0.58	0/787	0.88	0/1051
22	W	0.53	0/766	0.95	0/1025
23	X	0.52	0/595	0.85	0/787
24	Y	0.50	0/635	0.95	0/848
25	Z	0.41	0/502	1.08	0/667
26	0	0.57	0/453	1.04	0/605
27	1	0.50	0/450	0.92	0/599
28	2	0.56	0/416	0.77	0/554
29	3	0.49	0/380	1.03	0/498
30	4	0.51	0/513	1.05	0/676
31	5	0.52	0/303	0.88	0/397
32	a	0.38	1/36593 (0.0%)	0.73	9/57081 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.55	0/1784	1.02	2/2403 (0.1%)
34	c	0.52	0/1651	0.95	3/2225 (0.1%)
35	d	0.52	0/1655	1.00	0/2216
36	e	0.53	0/1169	0.98	1/1573 (0.1%)
37	f	0.57	0/835	0.93	0/1128
38	g	0.53	0/1195	1.09	0/1602
39	h	0.53	0/989	0.96	1/1326 (0.1%)
40	i	0.54	0/1034	0.99	0/1375
41	j	0.55	0/796	0.90	0/1077
42	k	0.55	0/893	0.91	0/1205
43	l	0.51	0/969	0.94	0/1300
44	m	0.76	2/892 (0.2%)	1.14	1/1193 (0.1%)
45	n	0.50	0/817	1.06	1/1088 (0.1%)
46	o	0.49	0/722	1.12	0/964
47	p	0.55	0/659	0.93	0/884
48	q	0.57	0/657	0.84	0/881
49	r	0.52	0/548	0.94	0/736
50	s	0.61	0/675	0.93	0/908
51	t	0.51	0/676	1.12	0/895
52	u	0.48	0/472	1.03	0/627
53	v	0.53	0/2865	1.02	4/3858 (0.1%)
54	w	0.45	0/394	0.88	2/519 (0.4%)
55	x	0.39	0/1832	0.75	2/2855 (0.1%)
55	y	0.39	0/1832	0.70	1/2855 (0.0%)
56	z	0.40	0/147	0.70	0/227
All	All	0.43	3/161499 (0.0%)	0.80	61/241199 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	m	90	ARG	CZ-NH1	12.55	1.50	1.32
44	m	90	ARG	CD-NE	6.91	1.55	1.46
32	a	1498	UR3	O3'-P	6.06	1.62	1.56

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1730	C	C2'-C3'-O3'	8.66	122.49	109.50
1	A	2225	A	C4'-C3'-O3'	8.47	122.11	109.40
55	x	17	U	C2'-C3'-O3'	7.96	121.44	109.50
1	A	1344	U	C4'-C3'-O3'	7.67	120.91	109.40
1	A	2193	G	C2'-C3'-O3'	7.42	124.83	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	701	U	C4'-C3'-O3'	7.40	120.50	109.40
55	x	49	G	C2'-C3'-O3'	7.18	124.47	113.70
32	a	1517	G	C2'-C3'-O3'	6.80	123.91	113.70
19	T	29	VAL	N-CA-C	6.80	117.50	110.36
44	m	90	ARG	NE-CZ-NH2	-6.79	113.09	119.20
1	A	896	A	C4'-C3'-O3'	6.58	119.27	109.40
53	v	101	ALA	N-CA-C	6.57	119.26	111.71
53	v	103	LEU	N-CA-C	-6.42	104.37	111.36
32	a	1151	A	C4'-C3'-O3'	6.39	118.99	109.40
1	A	1344	U	C2'-C3'-O3'	6.38	119.07	109.50
53	v	22	ARG	N-CA-C	6.37	118.75	111.11
10	K	112	GLY	CA-C-N	6.30	126.05	119.05
10	K	112	GLY	C-N-CA	6.30	126.05	119.05
1	A	404	A	C4'-C3'-O3'	6.24	118.77	109.40
32	a	1226	C	C4'-C3'-O3'	6.06	118.49	109.40
7	G	11	VAL	N-CA-C	6.02	113.84	107.76
13	N	82	MET	N-CA-C	6.01	119.45	111.75
32	a	1151	A	C2'-C3'-O3'	5.89	118.33	109.50
55	y	17	U	C2'-C3'-O3'	5.88	118.32	109.50
1	A	271	G	C4'-C3'-O3'	5.85	118.17	109.40
1	A	271	G	C2'-C3'-O3'	5.77	118.16	109.50
9	J	21	PRO	N-CA-C	5.71	117.67	110.70
1	A	2286	G	C2'-C3'-O3'	-5.71	105.14	113.70
3	C	165	VAL	N-CA-C	5.67	116.49	111.90
5	E	75	SER	CA-C-N	5.64	125.32	119.56
5	E	75	SER	C-N-CA	5.64	125.32	119.56
9	J	72	THR	CA-C-N	5.64	126.19	120.38
9	J	72	THR	C-N-CA	5.64	126.19	120.38
1	A	1379	U	C4'-C3'-O3'	5.55	121.33	113.00
1	A	100	U	C4'-C3'-O3'	5.54	117.71	109.40
11	L	47	ILE	CA-C-N	5.53	126.75	119.84
11	L	47	ILE	C-N-CA	5.53	126.75	119.84
1	A	675	A	C4'-C3'-O3'	-5.51	104.74	113.00
32	a	1457	G	C3'-C2'-O2'	5.50	118.95	110.70
39	h	111	MET	N-CA-C	5.50	115.50	108.24
32	a	517	G	C4'-C3'-O3'	5.45	121.17	113.00
1	A	1783	A	C4'-C3'-O3'	-5.44	104.84	113.00
34	c	6	HIS	CA-C-N	5.35	124.98	119.05
34	c	6	HIS	C-N-CA	5.35	124.98	119.05
53	v	185	GLY	N-CA-C	5.30	117.17	110.38
1	A	783	A	C4'-C3'-O3'	5.30	120.95	113.00
1	A	1847	A	C4'-C3'-O3'	-5.28	105.08	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	573	A	C4'-C3'-O3'	-5.27	105.10	113.00
5	E	176	ASP	CA-C-N	5.25	124.44	118.97
5	E	176	ASP	C-N-CA	5.25	124.44	118.97
32	a	1493	A	C4'-C3'-O3'	5.23	120.85	113.00
54	w	22	ASP	CA-C-N	5.21	126.35	119.84
54	w	22	ASP	C-N-CA	5.21	126.35	119.84
11	L	116	ILE	N-CA-CB	5.19	118.36	110.58
36	e	60	ILE	N-CA-CB	5.18	117.59	110.54
33	b	70	VAL	N-CA-C	5.16	115.33	108.11
33	b	91	PHE	N-CA-C	5.10	116.60	108.79
34	c	39	VAL	N-CA-CB	5.07	117.44	110.54
1	A	773	U	C4'-C3'-O3'	-5.07	105.40	113.00
45	n	47	LYS	N-CA-C	-5.02	105.08	111.11
2	B	28	C	C4'-C3'-O3'	-5.01	105.49	113.00

There are no chirality outliers.

There are no planarity outliers.

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	62351	0	31373	982	0
2	B	2529	0	1281	33	0
3	C	2082	0	2154	28	0
4	D	1565	0	1616	17	0
5	E	1552	0	1619	18	0
6	F	1410	0	1444	12	0
7	G	1323	0	1371	10	0
8	H	1111	0	1148	8	0
9	J	1032	0	1088	6	0
10	K	1129	0	1162	6	0
11	L	946	0	1023	13	0
12	M	1053	0	1129	13	0
13	N	1074	0	1157	11	0
14	O	960	0	1000	17	0
15	P	892	0	923	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Q	917	0	962	4	0
17	R	947	0	1019	15	0
18	S	816	0	839	12	0
19	T	857	0	922	16	0
20	U	738	0	807	3	0
21	V	779	0	831	8	0
22	W	753	0	780	6	0
23	X	588	0	604	6	0
24	Y	625	0	652	10	0
25	Z	501	0	531	3	0
26	0	449	0	488	2	0
27	1	444	0	458	6	0
28	2	409	0	440	5	0
29	3	377	0	418	4	0
30	4	504	0	572	9	0
31	5	302	0	341	3	0
32	a	32906	0	16575	641	0
33	b	1753	0	1780	16	0
34	c	1624	0	1696	20	0
35	d	1633	0	1694	20	0
36	e	1156	0	1199	21	0
37	f	817	0	808	8	0
38	g	1181	0	1238	16	0
39	h	979	0	1031	9	0
40	i	1022	0	1070	16	0
41	j	786	0	828	9	0
42	k	877	0	887	11	0
43	l	955	0	1016	19	0
44	m	883	0	941	11	0
45	n	805	0	844	14	0
46	o	714	0	734	5	0
47	p	649	0	666	5	0
48	q	648	0	691	5	0
49	r	539	0	553	5	0
50	s	658	0	683	8	0
51	t	670	0	719	15	0
52	u	465	0	491	3	0
53	v	2836	0	2735	42	0
54	w	388	0	400	26	0
55	x	1640	0	837	12	0
55	y	1640	0	837	14	0
56	z	131	0	66	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	A	100	0	0	0	0
57	B	4	0	0	0	0
57	a	20	0	0	0	0
58	5	1	0	0	0	0
All	All	149495	0	101171	2100	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (2100) 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)
32:a:13:U:N3	32:a:915:A:N6	1.69	1.40
1:A:2244:U:N3	1:A:2435:A:N6	1.68	1.35
1:A:2013:A:N6	1:A:2613:U:H3	1.26	1.31
1:A:2067:G:O2'	1:A:2069:G:H8	1.16	1.28
32:a:1358:U:H3	32:a:1363:A:N6	1.31	1.27
1:A:2067:G:O2'	1:A:2069:G:C8	1.88	1.22
1:A:2500:U:O2	1:A:2504:PSU:N1	1.71	1.20
32:a:961:U:N3	32:a:1201:A:N6	1.91	1.15
32:a:551:U:H2'	32:a:552:U:C6	1.80	1.15
1:A:2013:A:N1	1:A:2613:U:O4	1.81	1.14
32:a:961:U:H3	32:a:1201:A:N6	1.41	1.13
1:A:1248:G:H3'	1:A:1249:U:H5''	1.32	1.10
1:A:2244:U:N3	1:A:2435:A:C6	2.23	1.05
32:a:13:U:N3	32:a:915:A:C6	2.22	1.05
1:A:1596:A:H2'	1:A:1597:A:C8	1.93	1.04
32:a:13:U:C2	32:a:915:A:N6	2.25	1.03
1:A:2500:U:C2	1:A:2504:PSU:C2	2.49	1.01
1:A:465:G:H2'	1:A:466:A:C8	1.96	1.00
1:A:2500:U:O2	1:A:2504:PSU:C2	2.14	1.00
1:A:2244:U:C2	1:A:2435:A:N6	2.30	0.99
53:v:135:GLY:HA2	54:w:20:LEU:HD11	1.44	0.98
32:a:506:G:N2	32:a:526:C:O2	1.94	0.98
1:A:234:U:O4	1:A:430:A:N1	2.00	0.95
1:A:2068:U:O4	1:A:2430:A:C8	2.19	0.95
1:A:2244:U:C4	1:A:2435:A:N6	2.34	0.95
32:a:13:U:C4	32:a:915:A:N6	2.33	0.95
1:A:1802:A:H2'	1:A:1803:A:C8	2.01	0.95
1:A:2068:U:N3	1:A:2430:A:N7	2.15	0.94
1:A:814:C:H1'	1:A:1225:G:H21	1.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:U:H2'	1:A:2068:U:C2	2.03	0.93
1:A:2500:U:C2	1:A:2504:PSU:N1	2.36	0.93
32:a:37:U:H3	32:a:397:A:H61	1.07	0.92
1:A:1255:U:OP2	1:A:2502:G:N2	2.02	0.92
1:A:2074:U:H3	1:A:2435:A:H2	1.16	0.92
1:A:172:A:H2'	1:A:173:A:C8	2.05	0.92
55:y:15:C:H3'	55:y:16:C:H5''	1.49	0.92
32:a:1358:U:O4	32:a:1363:A:N1	2.02	0.91
1:A:2500:U:O2	1:A:2504:PSU:C6	2.24	0.91
1:A:2748:A:H5'	1:A:2753:A:H61	1.33	0.91
1:A:653:U:H3'	1:A:654:A:H5''	1.52	0.91
1:A:2060:A:O4'	1:A:2502:G:H1'	1.71	0.90
32:a:528:C:N4	32:a:529:G:C5	2.39	0.90
32:a:1356:G:H2'	32:a:1357:A:C8	2.06	0.90
1:A:234:U:H3	1:A:430:A:H61	1.13	0.90
32:a:1530:G:H2'	32:a:1531:A:C8	2.06	0.90
32:a:961:U:O4	32:a:974:A:N1	2.05	0.89
32:a:32:A:H2'	32:a:33:A:C8	2.06	0.88
1:A:2244:U:O2	1:A:2435:A:N7	2.06	0.88
32:a:974:A:H61	32:a:1201:A:N6	1.72	0.87
1:A:2452:C:H42	1:A:2504:PSU:HN3	1.22	0.85
32:a:842:U:H3'	32:a:843:U:H5''	1.58	0.85
1:A:910:A:H2'	1:A:911:A:C8	2.12	0.84
1:A:1353:A:H2'	1:A:1354:A:C8	2.12	0.84
1:A:1300:G:H4'	1:A:1301:A:H5''	1.58	0.84
32:a:521:G:O6	32:a:528:C:N4	2.11	0.84
53:v:87:ALA:HB2	53:v:95:THR:HB	1.59	0.84
1:A:2756:U:C4	1:A:2758:A:N6	2.45	0.84
1:A:1394:U:H4'	1:A:1603:A:H4'	1.58	0.83
1:A:1405:U:H2'	1:A:1406:U:C6	2.14	0.83
1:A:2788:C:H2'	1:A:2789:C:C6	2.14	0.83
32:a:961:U:H3	32:a:1201:A:H61	0.85	0.83
38:g:150:ALA:HB1	42:k:59:THR:HG21	1.59	0.83
1:A:2646:C:H2'	1:A:2647:U:O4'	1.79	0.82
1:A:2036:C:H2'	1:A:2037:A:C8	2.14	0.82
32:a:974:A:N6	32:a:1201:A:C6	2.47	0.82
1:A:94:A:H2'	1:A:95:A:C8	2.14	0.82
32:a:355:C:H1'	32:a:388:G:H1'	1.61	0.82
1:A:576:U:O2'	1:A:2502:G:O6	1.96	0.82
1:A:2756:U:N3	1:A:2758:A:C6	2.48	0.82
1:A:2452:C:H2'	1:A:2453:A:C8	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:373:A:H4'	32:a:451:A:H62	1.44	0.82
1:A:1433:A:H2'	1:A:1434:A:C8	2.14	0.81
1:A:2036:C:H2'	1:A:2037:A:H8	1.46	0.81
1:A:1326:U:H2'	1:A:1327:A:C8	2.16	0.81
1:A:2500:U:N3	1:A:2504:PSU:O2	2.14	0.80
1:A:675:A:H2'	1:A:676:A:C8	2.17	0.80
8:H:47:PHE:HA	8:H:51:ARG:HB2	1.64	0.80
6:F:105:THR:O	6:F:109:PRO:HD2	1.81	0.80
1:A:2060:A:O4'	1:A:2502:G:C1'	2.30	0.80
32:a:450:G:H1	32:a:483:C:H42	1.30	0.80
1:A:2020:A:H5'	27:1:9:THR:HG23	1.64	0.79
1:A:927:A:H2'	1:A:928:A:C8	2.17	0.79
32:a:946:A:H2'	32:a:947:G:C8	2.18	0.78
1:A:632:A:H2'	1:A:633:A:C8	2.18	0.78
32:a:505:G:H2'	32:a:506:G:C8	2.19	0.78
1:A:1779:U:H5	1:A:1784:A:N7	1.82	0.78
32:a:1071:C:H2'	32:a:1072:G:C8	2.19	0.78
1:A:532:A:H4'	1:A:533:G:C8	2.19	0.78
32:a:37:U:H3	32:a:397:A:N6	1.80	0.78
1:A:2752:C:H3'	1:A:2753:A:H8	1.49	0.78
1:A:2722:G:H2'	1:A:2723:C:C6	2.19	0.77
32:a:1196:A:H5''	54:w:35:GLY:HA3	1.65	0.77
1:A:2557:G:H2'	1:A:2558:C:C6	2.19	0.77
1:A:827:U:H2'	1:A:2068:U:N3	2.00	0.77
1:A:2068:U:O4	1:A:2430:A:H8	1.67	0.77
32:a:1358:U:N3	32:a:1363:A:N6	2.04	0.77
56:z:47:U:H2'	56:z:48:G:C8	2.20	0.77
1:A:1357:C:H2'	1:A:1358:G:O4'	1.85	0.76
1:A:2567:G:H2'	1:A:2568:U:C6	2.21	0.76
1:A:2117:A:H61	1:A:2170:A:H61	1.32	0.76
32:a:1361:G:H2'	32:a:1362:A:C8	2.21	0.76
1:A:1862:G:O6	1:A:1880:U:O2	2.03	0.76
32:a:1366:C:H2'	32:a:1367:C:C6	2.20	0.76
18:S:51:VAL:HB	18:S:52:PRO:HD2	1.66	0.75
32:a:264:C:H2'	32:a:265:G:O4'	1.86	0.75
1:A:581:C:H2'	1:A:582:A:C8	2.21	0.75
1:A:1270:C:H5''	1:A:1271:G:H5'	1.68	0.75
1:A:191:A:H2'	1:A:192:C:C6	2.22	0.75
32:a:1517:G:H2'	32:a:1518:MA6:H8	1.67	0.74
1:A:2093:G:N7	1:A:2225:A:H2'	2.02	0.74
1:A:1432:G:H2'	1:A:1433:A:C8	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:A:H1'	1:A:889:C:H5	1.53	0.74
1:A:1028:A:H2'	1:A:1029:A:C8	2.22	0.74
1:A:2868:A:H2'	1:A:2869:G:C8	2.22	0.74
1:A:1248:G:H3'	1:A:1249:U:C5'	2.13	0.73
1:A:2532:G:O2'	1:A:2665:A:H1'	1.88	0.73
1:A:1548:A:H2'	1:A:1549:A:C8	2.23	0.73
32:a:530:G:N2	54:w:28:ARG:HB3	2.03	0.73
1:A:2882:A:H3'	1:A:2883:A:H5''	1.71	0.73
32:a:868:C:H2'	32:a:869:G:O4'	1.88	0.73
1:A:2756:U:N3	1:A:2758:A:N6	2.36	0.73
32:a:17:U:H2'	32:a:18:C:C6	2.23	0.73
32:a:530:G:H22	54:w:28:ARG:HB3	1.52	0.73
1:A:2836:U:H2'	1:A:2837:A:C8	2.23	0.73
17:R:24:TYR:HB3	17:R:28:ARG:HB3	1.71	0.73
32:a:944:G:O6	32:a:1337:G:H8	1.73	0.72
1:A:172:A:H2'	1:A:173:A:H8	1.54	0.72
1:A:796:C:H2'	1:A:797:G:C8	2.25	0.72
1:A:2086:U:H2'	1:A:2087:G:C8	2.24	0.72
1:A:2273:A:H2'	1:A:2274:A:C8	2.25	0.72
1:A:2006:C:H2'	1:A:2007:U:H6	1.54	0.72
1:A:814:C:H1'	1:A:1225:G:N2	2.04	0.71
1:A:1913:A:O2'	54:w:21:HIS:HB3	1.91	0.71
54:w:20:LEU:O	54:w:20:LEU:HD22	1.91	0.71
1:A:2658:C:H2'	1:A:2659:G:O4'	1.90	0.71
9:J:105:LEU:HD13	9:J:129:GLU:HG2	1.73	0.71
32:a:1071:C:H2'	32:a:1072:G:H8	1.54	0.70
1:A:1434:A:H2'	1:A:1435:G:C8	2.26	0.70
32:a:720:C:H2'	32:a:721:G:C8	2.26	0.70
3:C:144:VAL:HB	3:C:154:LEU:HB2	1.72	0.70
32:a:528:C:C4	32:a:529:G:C8	2.79	0.70
1:A:1326:U:H2'	1:A:1327:A:H8	1.54	0.70
1:A:250:G:H2'	1:A:251:A:C8	2.27	0.70
1:A:1648:U:H2'	1:A:1649:G:O4'	1.92	0.70
1:A:2704:C:H2'	1:A:2705:A:O4'	1.92	0.70
1:A:827:U:C2'	1:A:2068:U:C2	2.75	0.69
32:a:185:U:H3	32:a:192:A:H61	1.39	0.69
1:A:2752:C:H3'	1:A:2753:A:C8	2.28	0.69
1:A:2300:C:H2'	1:A:2301:C:C6	2.27	0.69
1:A:2748:A:H5'	1:A:2753:A:N6	2.06	0.69
1:A:161:A:H2	1:A:2217:G:HO2'	1.39	0.69
1:A:2452:C:N4	1:A:2504:PSU:HN3	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:51:VAL:HB	18:S:52:PRO:CD	2.22	0.69
1:A:851:C:H2'	1:A:852:U:C6	2.29	0.68
1:A:2241:A:H2'	1:A:2242:G:C8	2.28	0.68
32:a:1011:C:H2'	32:a:1012:A:C8	2.29	0.68
1:A:181:A:H2'	1:A:182:A:C8	2.28	0.68
32:a:524:G:H2'	32:a:525:C:C6	2.28	0.68
32:a:399:G:H2'	32:a:400:C:C6	2.28	0.68
32:a:1219:A:H2'	32:a:1220:G:C8	2.29	0.68
53:v:215:THR:HB	54:w:28:ARG:HB2	1.75	0.68
1:A:158:U:H3	1:A:168:G:H1	1.41	0.68
1:A:2500:U:N3	1:A:2504:PSU:C2	2.62	0.68
3:C:84:ASP:HB2	3:C:91:ILE:HG12	1.76	0.68
32:a:589:U:H3	32:a:650:G:H1	1.41	0.68
32:a:784:A:H2'	32:a:785:G:C8	2.29	0.68
32:a:961:U:O4	32:a:974:A:C6	2.47	0.68
1:A:2547:A:H2'	1:A:2548:U:C6	2.29	0.67
1:A:1863:G:H2'	1:A:1864:U:C6	2.28	0.67
1:A:327:G:H1	1:A:335:C:H42	1.41	0.67
53:v:250:GLY:HA3	53:v:254:VAL:HG13	1.76	0.67
1:A:2532:G:H2'	1:A:2533:U:C6	2.30	0.67
1:A:2698:U:H2'	1:A:2699:C:C6	2.30	0.67
32:a:745:G:H2'	32:a:746:A:C8	2.30	0.67
1:A:308:G:H2'	1:A:309:A:C8	2.30	0.67
1:A:2733:A:H3'	1:A:2734:A:H8	1.59	0.67
32:a:37:U:O2	32:a:547:A:H2	1.77	0.67
1:A:576:U:O2'	1:A:2502:G:C6	2.47	0.67
36:e:57:PRO:O	36:e:60:ILE:HG13	1.95	0.67
40:i:120:LYS:HB2	40:i:123:ARG:HB3	1.76	0.67
1:A:56:A:H2'	1:A:57:C:C6	2.29	0.66
1:A:2067:G:C2'	1:A:2069:G:C8	2.77	0.66
53:v:114:GLU:HA	53:v:117:ARG:HE	1.60	0.66
1:A:191:A:H2'	1:A:192:C:H6	1.60	0.66
1:A:12:U:O2	1:A:12:U:H2'	1.95	0.66
32:a:961:U:C2	32:a:1201:A:N6	2.63	0.66
1:A:1899:A:H4'	1:A:1901:A:H5''	1.77	0.66
32:a:483:C:H2'	32:a:484:G:C8	2.30	0.66
1:A:998:C:H2'	1:A:999:U:O4'	1.95	0.66
1:A:1717:A:H2'	1:A:1718:G:O4'	1.94	0.66
32:a:613:C:H2'	32:a:614:C:C6	2.30	0.66
1:A:1805:A:H2'	1:A:1806:C:C6	2.31	0.66
32:a:439:U:H5''	35:d:120:HIS:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:U:H3	1:A:430:A:N6	1.92	0.66
1:A:2006:C:H2'	1:A:2007:U:C6	2.31	0.66
32:a:715:A:H2'	32:a:716:A:C8	2.31	0.66
1:A:234:U:C4	1:A:430:A:N1	2.64	0.66
2:B:80:U:H2'	2:B:81:G:C8	2.31	0.66
1:A:1548:A:H2'	1:A:1549:A:H8	1.60	0.66
1:A:1802:A:H2'	1:A:1803:A:H8	1.57	0.66
1:A:2788:C:H2'	1:A:2789:C:H6	1.61	0.66
53:v:150:ARG:HH22	53:v:154:ARG:HH11	1.42	0.65
1:A:1043:C:H42	1:A:1112:G:H1	1.42	0.65
32:a:39:G:H1'	32:a:498:A:H1'	1.79	0.65
1:A:1736:U:H2'	1:A:1737:G:H8	1.61	0.65
32:a:546:A:H4'	32:a:548:G:H4'	1.79	0.65
32:a:673:A:H2'	32:a:674:G:C8	2.31	0.65
32:a:1106:G:H5''	34:c:172:ARG:HB3	1.78	0.65
33:b:166:ALA:HB3	33:b:191:SER:HB3	1.78	0.65
1:A:2409:G:H2'	1:A:2410:G:O4'	1.97	0.65
32:a:335:C:H2'	32:a:336:A:H8	1.62	0.65
39:h:83:LEU:HD23	43:l:4:VAL:HG21	1.78	0.65
43:l:114:ARG:HB2	43:l:119:VAL:HB	1.79	0.65
32:a:712:A:H2'	32:a:713:G:O4'	1.97	0.65
32:a:915:A:H2'	32:a:916:U:O4'	1.97	0.65
2:B:80:U:H2'	2:B:81:G:H8	1.61	0.64
32:a:13:U:O2	32:a:915:A:N7	2.30	0.64
32:a:1342:C:H2'	32:a:1343:G:C8	2.32	0.64
32:a:32:A:N1	32:a:552:U:O4	2.31	0.64
32:a:660:C:H2'	32:a:661:G:O4'	1.97	0.64
1:A:1709:U:H2'	1:A:1710:G:C8	2.32	0.64
1:A:2514:U:H2'	1:A:2515:C:C6	2.32	0.64
1:A:538:A:H2'	1:A:539:G:O4'	1.97	0.64
1:A:1570:A:H2'	1:A:1571:A:C8	2.32	0.64
7:G:9:VAL:HG23	7:G:69:ARG:HD2	1.78	0.64
32:a:175:C:H2'	32:a:176:C:C6	2.33	0.64
32:a:839:C:H42	32:a:847:G:H1	1.46	0.64
1:A:570:G:H2'	1:A:2030:A:N7	2.13	0.64
1:A:2500:U:H2'	1:A:2504:PSU:HN1	1.61	0.64
32:a:373:A:H4'	32:a:451:A:N6	2.13	0.64
1:A:2399:G:H1	1:A:2417:C:H42	1.46	0.64
3:C:240:PHE:O	3:C:242:LYS:N	2.31	0.64
32:a:713:G:H2'	32:a:714:G:C8	2.32	0.64
1:A:84:A:H62	1:A:101:A:H8	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:G:H22	1:A:555:G:H2'	1.62	0.64
1:A:588:U:H2'	1:A:589:U:C6	2.32	0.64
5:E:97:ASN:HB2	5:E:100:MET:HB2	1.79	0.64
6:F:105:THR:O	6:F:109:PRO:CD	2.45	0.64
32:a:537:G:H2'	32:a:538:G:C8	2.33	0.64
1:A:1201:U:H3	1:A:1244:A:H61	1.45	0.64
32:a:528:C:H3'	32:a:529:G:H5''	1.81	0.63
1:A:2880:C:H2'	1:A:2881:U:C6	2.31	0.63
8:H:132:PHE:H	8:H:140:ALA:HB3	1.63	0.63
18:S:79:ARG:HG2	18:S:80:ARG:HG3	1.78	0.63
32:a:452:A:H2'	32:a:453:G:O4'	1.98	0.63
32:a:911:U:H2'	32:a:912:C:C6	2.32	0.63
32:a:967:5MC:H2'	32:a:968:A:C8	2.34	0.63
32:a:1493:A:H61	53:v:214:HIS:CE1	2.17	0.63
1:A:2811:G:H1	1:A:2889:C:H42	1.47	0.63
1:A:2602:A:H61	53:v:253:HIS:HD2	1.46	0.63
32:a:1004:A:H62	32:a:1025:U:H4'	1.63	0.63
45:n:46:LEU:HD21	50:s:13:LEU:HD13	1.81	0.63
53:v:111:ALA:O	53:v:115:PHE:N	2.28	0.63
1:A:161:A:H2	1:A:2217:G:O2'	1.81	0.63
1:A:2674:G:H4'	11:L:30:ARG:HG3	1.80	0.63
55:y:15:C:H3'	55:y:16:C:C5'	2.27	0.63
1:A:1434:A:H2'	1:A:1435:G:H8	1.62	0.62
32:a:598:U:H2'	32:a:599:C:C6	2.33	0.62
1:A:2500:U:C2	1:A:2504:PSU:O2	2.49	0.62
32:a:337:G:H2'	32:a:338:A:C8	2.34	0.62
32:a:917:G:H2'	32:a:918:A:C8	2.34	0.62
33:b:66:LYS:HB2	33:b:158:PRO:HA	1.82	0.62
1:A:2060:A:H5''	1:A:2502:G:O2'	1.99	0.62
32:a:735:C:H2'	32:a:736:C:C6	2.34	0.62
44:m:89:LEU:HA	44:m:92:ARG:HG2	1.80	0.62
1:A:840:C:H2'	1:A:841:G:H8	1.62	0.62
1:A:2602:A:H61	53:v:253:HIS:CD2	2.17	0.62
32:a:746:A:H2'	32:a:747:A:C8	2.34	0.62
32:a:1088:G:H2'	32:a:1089:G:O4'	1.98	0.62
56:z:44:A:H2'	56:z:45:A:H8	1.63	0.62
1:A:645:C:H2'	1:A:647:G:C8	2.34	0.62
32:a:1308:U:OP1	44:m:96:PRO:HA	1.99	0.62
1:A:992:C:H42	1:A:1162:G:H1	1.47	0.62
1:A:1187:G:H2'	1:A:1188:U:H5	1.65	0.62
32:a:194:C:O2'	51:t:63:ALA:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:U:H3	1:A:350:G:H1	1.47	0.62
1:A:1665:A:H2'	1:A:1666:G:O4'	2.00	0.62
1:A:2013:A:N1	1:A:2613:U:C4	2.66	0.62
32:a:720:C:H2'	32:a:721:G:N7	2.14	0.62
32:a:224:U:H2'	32:a:225:C:C6	2.35	0.62
1:A:2074:U:O4	1:A:2435:A:N1	2.33	0.62
1:A:2079:U:H2'	1:A:2080:A:O4'	1.99	0.62
32:a:1130:A:H61	32:a:1144:G:H1'	1.65	0.61
1:A:796:C:H2'	1:A:797:G:H8	1.64	0.61
1:A:253:C:H2'	1:A:254:G:O4'	1.99	0.61
32:a:303:A:O2'	32:a:555:U:H4'	2.00	0.61
32:a:585:G:H21	32:a:879:C:H4'	1.65	0.61
32:a:860:A:H2'	32:a:861:G:O4'	2.00	0.61
1:A:1599:U:H2'	1:A:1600:C:C6	2.35	0.61
32:a:1328:C:H2'	32:a:1329:A:O4'	2.00	0.61
32:a:463:U:H3	32:a:469:C:H42	1.48	0.61
32:a:660:C:H42	32:a:745:G:H1	1.46	0.61
32:a:878:A:H2'	32:a:879:C:O4'	2.00	0.61
32:a:1240:U:H5'	38:g:42:ILE:HD11	1.83	0.61
1:A:57:C:H42	1:A:70:G:H1	1.49	0.61
1:A:1476:U:H3	1:A:1515:A:H62	1.46	0.61
1:A:2327:A:H2'	1:A:2328:A:C8	2.36	0.61
32:a:32:A:C2	32:a:552:U:N3	2.68	0.61
32:a:1366:C:H2'	32:a:1367:C:H6	1.64	0.61
1:A:850:U:H2'	1:A:851:C:C6	2.36	0.61
32:a:131:A:H2'	32:a:132:C:C6	2.36	0.61
1:A:1284:A:H2'	1:A:1285:A:C8	2.35	0.61
32:a:537:G:H2'	32:a:538:G:H8	1.65	0.61
32:a:664:G:H22	32:a:741:G:H1	1.49	0.61
32:a:769:G:H4'	32:a:1513:A:H4'	1.83	0.61
32:a:842:U:H3'	32:a:843:U:C5'	2.29	0.61
35:d:33:LYS:HD2	35:d:36:GLN:HB2	1.82	0.61
2:B:90:C:H2'	2:B:91:C:O4'	2.00	0.61
3:C:137:VAL:HG21	3:C:167:ARG:HB2	1.83	0.61
32:a:841:C:H2'	32:a:843:U:H5'	1.82	0.61
1:A:589:U:H2'	1:A:590:A:H8	1.66	0.60
2:B:63:C:H2'	2:B:64:G:C8	2.35	0.60
32:a:8:A:H1'	36:e:108:GLY:HA2	1.83	0.60
32:a:70:U:C5	32:a:94:G:H2'	2.36	0.60
34:c:12:LEU:HD13	34:c:18:TRP:HE1	1.66	0.60
35:d:197:GLU:HA	35:d:200:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:G:O6	1:A:349:U:O2	2.19	0.60
1:A:1656:C:H2'	1:A:1657:U:C6	2.36	0.60
32:a:384:G:H2'	32:a:385:C:C6	2.36	0.60
32:a:1287:A:H2'	32:a:1288:A:C8	2.36	0.60
1:A:1783:A:N1	1:A:2587:A:H2'	2.16	0.60
1:A:2187:U:H2'	1:A:2188:U:C6	2.35	0.60
1:A:339:U:H2'	1:A:340:A:H8	1.67	0.60
1:A:743:A:O2'	1:A:1659:G:OP1	2.20	0.60
1:A:1865:U:H2'	1:A:1875:G:N2	2.16	0.60
1:A:1689:A:H2'	1:A:1690:A:C8	2.36	0.60
32:a:179:A:C2	32:a:196:A:N6	2.69	0.60
1:A:581:C:H2'	1:A:582:A:H8	1.67	0.60
1:A:978:G:H1	1:A:985:C:H42	1.48	0.60
1:A:1076:C:H2'	1:A:1077:A:C8	2.36	0.60
1:A:1486:U:H3	1:A:1503:A:H61	1.48	0.60
1:A:1736:U:H2'	1:A:1737:G:C8	2.36	0.60
32:a:528:C:N4	32:a:529:G:C4	2.70	0.60
4:D:116:LYS:HB2	4:D:165:MET:HB3	1.82	0.60
1:A:1361:G:H2'	1:A:1362:C:C6	2.37	0.60
6:F:126:GLY:HA2	6:F:163:ASP:HA	1.83	0.60
32:a:12:U:H4'	32:a:526:C:H4'	1.83	0.60
32:a:555:U:H2'	32:a:556:C:C6	2.36	0.60
1:A:305:C:H2'	1:A:306:U:C6	2.36	0.59
1:A:1744:A:H3'	1:A:1745:A:H8	1.67	0.59
1:A:2532:G:H2'	1:A:2533:U:H6	1.67	0.59
1:A:2836:U:H2'	1:A:2837:A:H8	1.65	0.59
32:a:37:U:O4	32:a:397:A:N1	2.35	0.59
32:a:1047:G:H1	32:a:1210:C:H42	1.49	0.59
1:A:1592:C:H2'	1:A:1593:A:C8	2.37	0.59
1:A:1597:A:H4'	1:A:1598:A:H8	1.65	0.59
1:A:2547:A:H2'	1:A:2548:U:H6	1.67	0.59
32:a:363:A:H5'	43:l:31:ARG:HB3	1.84	0.59
32:a:962:C:C2	32:a:1201:A:N6	2.70	0.59
1:A:1682:G:H2'	1:A:1683:U:C6	2.37	0.59
35:d:102:VAL:HG13	35:d:107:PHE:HB2	1.84	0.59
32:a:225:C:H2'	32:a:226:G:O4'	2.02	0.59
32:a:1517:G:H2'	32:a:1518:MA6:C8	2.33	0.59
1:A:1795:C:H2'	1:A:1796:U:O4'	2.02	0.59
1:A:2013:A:N6	1:A:2613:U:N3	2.05	0.59
1:A:2100:G:H2'	1:A:2101:A:H5'	1.84	0.59
1:A:2244:U:C2	1:A:2435:A:C6	2.88	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1413:A:H2	32:a:1487:G:H22	1.50	0.59
1:A:1746:A:H2'	1:A:1747:U:C6	2.38	0.59
1:A:2403:C:H42	1:A:2414:G:H1	1.49	0.59
1:A:2686:G:H2'	1:A:2687:U:O4'	2.01	0.59
32:a:496:A:H61	32:a:498:A:N6	2.01	0.59
40:i:118:LEU:HA	40:i:125:PRO:HD3	1.85	0.59
1:A:501:A:H2'	1:A:502:A:C8	2.37	0.59
1:A:589:U:H2'	1:A:590:A:C8	2.38	0.59
1:A:2016:U:H2'	1:A:2017:U:C6	2.37	0.59
13:N:33:LEU:HD13	13:N:117:PHE:HB3	1.85	0.59
18:S:27:ILE:HD13	18:S:33:VAL:HG11	1.84	0.59
32:a:200:G:H1	32:a:217:C:H42	1.49	0.59
32:a:335:C:H2'	32:a:336:A:C8	2.37	0.59
54:w:20:LEU:O	54:w:20:LEU:HD13	2.02	0.59
1:A:659:G:H1'	5:E:97:ASN:HD21	1.68	0.58
1:A:1038:G:H2'	1:A:1039:A:C8	2.38	0.58
1:A:1752:C:H2'	1:A:1753:G:C8	2.37	0.58
53:v:338:THR:HG23	53:v:340:VAL:H	1.68	0.58
1:A:184:C:H2'	1:A:185:G:H8	1.68	0.58
1:A:241:A:N1	1:A:255:A:H5''	2.18	0.58
1:A:451:U:H2'	1:A:453:A:N7	2.18	0.58
1:A:753:A:H2'	1:A:754:U:C6	2.38	0.58
1:A:2403:C:H2'	1:A:2404:U:O4'	2.04	0.58
32:a:459:A:H61	32:a:473:U:H3	1.49	0.58
32:a:830:G:H2'	32:a:831:A:C8	2.38	0.58
32:a:1373:G:H5''	38:g:36:LYS:HD3	1.86	0.58
32:a:1426:G:H2'	32:a:1427:C:C6	2.37	0.58
36:e:45:ARG:HG2	36:e:73:ASN:HD22	1.68	0.58
36:e:115:LEU:HD22	36:e:123:VAL:HG11	1.85	0.58
1:A:1423:G:H1	1:A:1575:C:H42	1.52	0.58
1:A:2394:C:H5''	12:M:63:LYS:HE2	1.85	0.58
22:W:72:VAL:HG12	22:W:93:ARG:HA	1.84	0.58
32:a:1097:C:H4'	33:b:139:ARG:HH11	1.68	0.58
32:a:538:G:H2'	32:a:539:A:C8	2.38	0.58
32:a:1221:G:H2'	32:a:1222:G:O4'	2.04	0.58
32:a:1255:G:H1	32:a:1282:C:H42	1.51	0.58
45:n:24:ARG:HH21	45:n:56:SER:HB2	1.69	0.58
53:v:135:GLY:HA2	54:w:20:LEU:CD1	2.26	0.58
1:A:1742:U:H2'	1:A:1743:G:C8	2.39	0.58
32:a:68:G:N2	32:a:152:A:H1'	2.18	0.58
32:a:1309:G:H1	32:a:1328:C:H42	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:C:H2'	1:A:419:U:O4'	2.04	0.58
1:A:754:U:H2'	1:A:755:U:C6	2.38	0.58
17:R:49:ASP:O	17:R:53:ARG:HB3	2.03	0.58
32:a:358:U:H2'	32:a:359:G:C8	2.39	0.58
32:a:961:U:C4	32:a:974:A:N1	2.72	0.58
32:a:1228:C:H5'	44:m:113:ARG:HB3	1.85	0.58
32:a:1323:G:H2'	32:a:1324:A:O4'	2.04	0.58
55:x:34:C:H42	56:z:48:G:H1	1.52	0.58
1:A:1821:A:H2'	1:A:1822:C:C6	2.38	0.58
1:A:1873:G:H2'	1:A:1874:C:C6	2.38	0.58
1:A:2837:A:H2'	1:A:2838:G:C8	2.39	0.58
32:a:1447:A:H3'	32:a:1448:C:C5'	2.33	0.58
1:A:1298:C:H42	1:A:1642:G:H1	1.52	0.58
1:A:2068:U:C4	1:A:2430:A:C8	2.91	0.58
1:A:35:G:H2'	1:A:36:G:O4'	2.04	0.58
1:A:325:G:H1	1:A:337:C:H42	1.52	0.58
1:A:917:A:H5''	1:A:2268:A:H61	1.68	0.58
2:B:45:A:H8	6:F:92:ARG:HD2	1.69	0.58
32:a:24:U:H2'	32:a:25:C:C6	2.39	0.58
32:a:1346:A:N1	32:a:1374:A:H5''	2.18	0.58
1:A:44:A:H2'	1:A:45:G:O4'	2.04	0.57
1:A:1115:G:O2'	1:A:1116:G:H5''	2.04	0.57
32:a:532:A:H2'	32:a:532:A:N3	2.19	0.57
32:a:1172:C:H2'	32:a:1173:U:C6	2.38	0.57
1:A:1019:U:H2'	1:A:1020:A:H8	1.68	0.57
1:A:1726:C:H42	1:A:1734:G:H1	1.50	0.57
1:A:2505:G:O6	1:A:2610:C:O2	2.23	0.57
32:a:982:U:H4'	32:a:983:A:O4'	2.03	0.57
32:a:1061:G:H1	32:a:1195:C:H42	1.51	0.57
1:A:441:U:H2'	1:A:442:G:O4'	2.04	0.57
1:A:1932:A:H2'	1:A:1933:G:O4'	2.04	0.57
1:A:2328:A:H2'	1:A:2329:U:C6	2.38	0.57
1:A:2697:G:H2'	1:A:2698:U:O4'	2.04	0.57
32:a:424:G:HO2'	32:a:425:G:H8	1.50	0.57
32:a:623:C:H2'	32:a:624:C:C6	2.39	0.57
51:t:80:THR:O	51:t:83:ILE:HG13	2.03	0.57
1:A:184:C:H2'	1:A:185:G:C8	2.40	0.57
32:a:784:A:H2'	32:a:785:G:H8	1.68	0.57
32:a:864:A:H5''	36:e:90:THR:HG22	1.86	0.57
1:A:121:G:H4'	1:A:149:A:H5'	1.85	0.57
1:A:580:U:H2'	1:A:581:C:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:G:H1	1:A:634:C:H42	1.52	0.57
1:A:2192:U:H2'	1:A:2193:G:O4'	2.04	0.57
4:D:25:THR:HG21	4:D:193:VAL:HG22	1.86	0.57
19:T:46:LEU:O	19:T:50:VAL:HG23	2.05	0.57
1:A:443:A:H2'	1:A:443:A:N3	2.18	0.57
32:a:946:A:H2'	32:a:947:G:H8	1.65	0.57
32:a:1144:G:H21	32:a:1146:A:H62	1.52	0.57
32:a:1163:A:H2'	32:a:1164:G:C8	2.40	0.57
33:b:131:LYS:O	33:b:135:LEU:N	2.21	0.57
1:A:289:G:H2'	1:A:290:U:C6	2.40	0.57
1:A:1914:C:C1'	54:w:18:ALA:HB2	2.35	0.57
1:A:2061:G:H4'	1:A:2503:A:C2	2.40	0.57
32:a:336:A:H2'	32:a:337:G:C8	2.39	0.57
32:a:662:U:H2'	32:a:663:A:C8	2.40	0.57
32:a:1473:G:H2'	32:a:1474:U:O4'	2.05	0.57
14:O:66:ALA:C	14:O:68:ALA:H	2.13	0.57
32:a:40:C:H2'	32:a:41:G:O4'	2.04	0.57
32:a:450:G:H1	32:a:483:C:N4	2.01	0.57
32:a:855:U:H2'	32:a:856:C:C6	2.40	0.57
32:a:979:C:H1'	32:a:1317:C:N4	2.20	0.57
1:A:1269:A:H2'	1:A:1270:C:C6	2.40	0.57
1:A:1406:U:O4	1:A:1596:A:N1	2.37	0.57
55:y:15:C:C3'	55:y:16:C:H5''	2.30	0.57
1:A:739:A:H1'	1:A:740:C:H5	1.70	0.56
4:D:46:ARG:HB3	4:D:84:LEU:HB2	1.87	0.56
5:E:148:ILE:HB	5:E:169:VAL:HG22	1.85	0.56
1:A:2068:U:C4	1:A:2430:A:N7	2.72	0.56
1:A:2078:C:H2'	1:A:2079:U:C6	2.40	0.56
32:a:613:C:H2'	32:a:614:C:H6	1.70	0.56
43:l:4:VAL:HA	43:l:7:LEU:HD12	1.87	0.56
1:A:1351:C:H2'	1:A:1352:U:C6	2.40	0.56
1:A:2647:U:H2'	1:A:2648:G:C8	2.41	0.56
2:B:45:A:C8	6:F:92:ARG:HD2	2.41	0.56
12:M:62:PRO:HG2	30:4:25:LYS:HB3	1.85	0.56
32:a:253:A:H2'	32:a:254:G:C8	2.41	0.56
32:a:965:U:H4'	32:a:966:2MG:H5'	1.88	0.56
32:a:1367:C:H2'	32:a:1368:A:O4'	2.05	0.56
32:a:1477:U:H2'	32:a:1478:U:C6	2.41	0.56
32:a:1496:C:H2'	32:a:1497:G:O4'	2.05	0.56
1:A:17:G:H2'	1:A:18:U:C6	2.39	0.56
1:A:2783:U:H2'	1:A:2784:U:C6	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:62:U:H2'	32:a:63:C:C6	2.41	0.56
32:a:735:C:H2'	32:a:736:C:H6	1.68	0.56
32:a:192:A:H2'	32:a:193:C:O4'	2.06	0.56
32:a:359:G:H2'	32:a:360:G:O4'	2.05	0.56
32:a:864:A:H2'	32:a:865:A:C8	2.40	0.56
32:a:1346:A:H61	32:a:1374:A:H3'	1.70	0.56
1:A:820:A:H2'	1:A:821:A:C8	2.41	0.56
1:A:893:C:H2'	1:A:894:U:H4'	1.88	0.56
1:A:971:G:H2'	1:A:972:A:O4'	2.05	0.56
1:A:1430:G:H2'	1:A:1431:A:O4'	2.06	0.56
1:A:2037:A:H2'	1:A:2038:G:C8	2.41	0.56
32:a:915:A:H8	32:a:915:A:O5'	1.89	0.56
32:a:1118:U:H1'	32:a:1179:A:C4	2.41	0.56
32:a:1266:G:H2'	32:a:1268:G:N7	2.20	0.56
32:a:1375:A:H2'	32:a:1376:U:O4'	2.06	0.56
44:m:29:ARG:O	44:m:33:ILE:HG12	2.06	0.56
1:A:2732:G:H5''	1:A:2733:A:O4'	2.05	0.56
29:3:24:THR:HG23	29:3:27:GLY:H	1.69	0.56
32:a:45:G:H2'	32:a:46:G:C8	2.41	0.56
32:a:202:G:H2'	32:a:203:G:C8	2.41	0.56
1:A:457:A:N1	1:A:470:A:H5''	2.21	0.56
1:A:621:A:C5	1:A:622:G:H1'	2.41	0.56
1:A:653:U:H3'	1:A:654:A:C5'	2.31	0.56
1:A:957:C:H5'	13:N:75:GLU:HG2	1.87	0.56
1:A:2791:G:H1	1:A:2805:C:H42	1.53	0.56
1:A:329:G:O4'	1:A:477:A:H1'	2.06	0.56
1:A:843:G:H2'	1:A:844:A:C8	2.41	0.56
1:A:1009:A:H2'	1:A:1010:A:C8	2.41	0.56
1:A:1454:C:H5'	14:O:63:ARG:CZ	2.36	0.56
1:A:2400:G:H4'	28:2:18:GLY:HA3	1.87	0.56
32:a:235:C:H2'	32:a:236:A:C8	2.42	0.56
1:A:5:A:H2'	1:A:6:A:C8	2.40	0.55
32:a:450:G:N2	32:a:482:A:N6	2.55	0.55
32:a:1205:U:H2'	32:a:1206:G:C8	2.41	0.55
54:w:20:LEU:HD13	54:w:20:LEU:C	2.31	0.55
55:y:26:G:H1	55:y:44:A:H61	1.52	0.55
1:A:150:U:H2'	1:A:151:C:C6	2.41	0.55
8:H:69:ALA:HA	8:H:72:ILE:HD12	1.87	0.55
32:a:391:G:H2'	32:a:392:C:O4'	2.05	0.55
32:a:399:G:H2'	32:a:400:C:H6	1.69	0.55
32:a:404:G:H2'	32:a:405:U:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1513:A:H2'	32:a:1514:G:C8	2.42	0.55
1:A:1406:U:N3	1:A:1596:A:C2	2.74	0.55
22:W:31:TYR:HE1	22:W:90:ASP:HB3	1.71	0.55
32:a:243:A:H62	32:a:281:G:H1'	1.72	0.55
32:a:1114:C:H2'	32:a:1115:U:C6	2.41	0.55
32:a:1348:U:H2'	32:a:1349:A:C8	2.41	0.55
1:A:1860:G:H2'	1:A:1861:G:C8	2.42	0.55
1:A:2674:G:H2'	1:A:2675:A:C8	2.42	0.55
1:A:443:A:N6	5:E:36:ALA:HB1	2.22	0.55
1:A:1173:U:H2'	1:A:1174:U:H4'	1.89	0.55
1:A:1297:C:OP1	1:A:2710:C:H4'	2.07	0.55
1:A:1864:U:H4'	1:A:2410:G:O2'	2.07	0.55
1:A:2077:A:C6	1:A:2435:A:N6	2.74	0.55
1:A:2675:A:H4'	11:L:29:HIS:HB3	1.89	0.55
32:a:501:C:H2'	32:a:502:A:H8	1.72	0.55
32:a:744:C:H2'	32:a:745:G:C8	2.40	0.55
32:a:926:G:H22	56:z:45:A:H3'	1.72	0.55
32:a:1118:U:H4'	40:i:85:ARG:HH22	1.72	0.55
55:x:53:G:H2'	55:x:54:U:C6	2.40	0.55
1:A:1002:G:H1	1:A:1153:C:H42	1.55	0.55
12:M:57:LEU:HD12	12:M:60:ARG:HH22	1.72	0.55
29:3:12:ARG:HH21	29:3:44:VAL:HB	1.72	0.55
32:a:10:A:H2'	32:a:11:G:H8	1.70	0.55
32:a:102:G:H2'	32:a:103:U:C6	2.42	0.55
1:A:585:G:N7	17:R:6:ARG:NH1	2.55	0.55
1:A:1186:G:H3'	1:A:1187:G:H8	1.72	0.55
1:A:1482:G:H1	1:A:1507:C:H42	1.55	0.55
1:A:1689:A:H2'	1:A:1690:A:H8	1.71	0.55
1:A:840:C:H2'	1:A:841:G:C8	2.41	0.55
1:A:906:U:H4'	13:N:66:ARG:HH21	1.72	0.55
36:e:134:ILE:O	36:e:137:VAL:HG12	2.07	0.55
1:A:2044:C:H42	1:A:2624:G:H1	1.55	0.55
1:A:2645:G:H3'	1:A:2646:C:C5'	2.37	0.55
1:A:2657:A:H61	1:A:2665:A:H3'	1.71	0.55
32:a:215:C:H2'	32:a:216:U:O4'	2.07	0.55
32:a:235:C:H2'	32:a:236:A:H8	1.71	0.55
32:a:256:U:H2'	32:a:257:G:C8	2.42	0.55
45:n:64:CYS:HB3	45:n:68:GLY:H	1.72	0.55
1:A:964:C:O2'	1:A:2273:A:N3	2.39	0.54
1:A:1026:G:H2'	1:A:1027:A:H8	1.72	0.54
1:A:1697:G:H4'	1:A:1978:A:H5''	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2491:U:H5'	1:A:2570:G:H5''	1.88	0.54
1:A:2556:C:H2'	1:A:2557:G:O4'	2.06	0.54
1:A:547:A:H2'	1:A:547:A:N3	2.22	0.54
1:A:576:U:H4'	1:A:2502:G:N7	2.22	0.54
1:A:577:G:H2'	1:A:578:G:C8	2.42	0.54
1:A:2507:C:H2'	1:A:2508:G:O4'	2.07	0.54
1:A:2519:U:H2'	1:A:2541:A:H61	1.72	0.54
24:Y:5:CYS:HA	24:Y:33:LEU:HD21	1.89	0.54
32:a:525:C:C2	32:a:526:C:N3	2.75	0.54
32:a:1155:A:H2'	32:a:1156:G:O4'	2.08	0.54
32:a:1173:U:H2'	32:a:1174:G:O4'	2.06	0.54
1:A:564:C:OP2	18:S:79:ARG:HD3	2.06	0.54
11:L:113:MET:O	11:L:116:ILE:HG13	2.07	0.54
32:a:543:U:H2'	32:a:544:G:O4'	2.07	0.54
32:a:592:G:H2'	32:a:593:U:O4'	2.06	0.54
32:a:1118:U:H2'	32:a:1119:C:C6	2.43	0.54
53:v:135:GLY:CA	54:w:20:LEU:HD11	2.30	0.54
1:A:969:G:H2'	1:A:970:U:C6	2.42	0.54
1:A:1123:C:H2'	1:A:1124:G:O4'	2.07	0.54
1:A:1246:A:H2'	1:A:1247:A:O4'	2.07	0.54
1:A:1280:G:H1	1:A:1290:C:H42	1.55	0.54
32:a:13:U:O4	32:a:21:G:C2	2.60	0.54
32:a:298:A:H2'	32:a:299:G:C8	2.42	0.54
32:a:370:C:H2'	32:a:371:A:O4'	2.08	0.54
1:A:71:A:H5''	1:A:72:U:H3'	1.89	0.54
1:A:825:A:H2'	1:A:826:U:C6	2.43	0.54
19:T:17:VAL:HB	19:T:76:VAL:HG11	1.89	0.54
32:a:12:U:H4'	32:a:526:C:C4'	2.37	0.54
32:a:202:G:O2'	32:a:468:A:C8	2.61	0.54
37:f:10:VAL:HB	37:f:58:HIS:HB3	1.90	0.54
37:f:38:ARG:HH12	37:f:96:VAL:HG12	1.72	0.54
1:A:753:A:H2'	1:A:754:U:H6	1.71	0.54
1:A:2536:G:H2'	1:A:2537:U:O4'	2.06	0.54
1:A:2875:C:H2'	1:A:2876:G:C8	2.43	0.54
32:a:496:A:H61	32:a:498:A:H62	1.56	0.54
32:a:545:C:H5'	35:d:69:GLU:HB2	1.88	0.54
32:a:718:A:H5'	42:k:119:ASN:HD22	1.73	0.54
35:d:19:LEU:HD21	35:d:60:LYS:HG3	1.90	0.54
1:A:1779:U:C5	1:A:1784:A:N7	2.72	0.54
1:A:2067:G:HO2'	1:A:2069:G:H8	0.56	0.54
8:H:84:ALA:HA	8:H:91:PHE:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:32:A:H2	32:a:552:U:H3	1.51	0.54
32:a:580:C:H2'	32:a:581:G:O4'	2.07	0.54
32:a:714:G:H2'	32:a:715:A:C8	2.42	0.54
32:a:974:A:N1	32:a:1201:A:N1	2.56	0.54
1:A:8:C:H2'	1:A:9:G:O4'	2.08	0.54
1:A:347:A:H2'	1:A:348:A:C8	2.43	0.54
1:A:1791:A:N6	1:A:1828:G:O2'	2.39	0.54
32:a:160:A:H2'	32:a:161:A:O4'	2.07	0.54
32:a:528:C:C4	32:a:529:G:N7	2.76	0.54
32:a:1285:A:N6	32:a:1355:G:H4'	2.23	0.54
1:A:1930:G:N2	1:A:1968:G:H2'	2.23	0.54
1:A:2728:U:O2'	1:A:2729:G:H8	1.91	0.54
32:a:109:A:H2'	32:a:109:A:N3	2.21	0.54
32:a:598:U:H2'	32:a:599:C:H6	1.73	0.54
32:a:798:U:H2'	32:a:799:G:O4'	2.08	0.54
32:a:1341:U:H2'	32:a:1342:C:C6	2.43	0.54
32:a:1524:C:H2'	32:a:1525:G:C8	2.43	0.54
33:b:114:LEU:HD13	33:b:148:LEU:HD12	1.90	0.54
32:a:375:U:H2'	32:a:376:G:O4'	2.08	0.54
32:a:551:U:H2'	32:a:552:U:H6	1.63	0.54
32:a:583:A:H3'	32:a:584:G:H8	1.73	0.54
1:A:1592:C:H2'	1:A:1593:A:H8	1.72	0.53
1:A:2050:C:H2'	1:A:2051:A:O4'	2.07	0.53
1:A:2447:G:C6	1:A:2504:PSU:O2	2.61	0.53
32:a:200:G:H2'	32:a:201:G:C8	2.43	0.53
36:e:45:ARG:HD3	36:e:71:MET:HE3	1.90	0.53
41:j:15:HIS:O	41:j:18:ILE:HG22	2.08	0.53
1:A:2244:U:O2	1:A:2435:A:C5	2.60	0.53
1:A:2671:G:H2'	1:A:2672:U:O4'	2.08	0.53
10:K:37:ARG:HA	10:K:118:MET:HE2	1.90	0.53
14:O:51:LEU:HD21	14:O:69:ARG:HG3	1.90	0.53
32:a:949:A:H2'	32:a:950:U:O4'	2.08	0.53
32:a:1228:C:H4'	44:m:115:PRO:HD2	1.89	0.53
32:a:1279:G:H3'	32:a:1279:G:N3	2.22	0.53
1:A:56:A:H2'	1:A:57:C:H6	1.72	0.53
1:A:514:A:H2'	1:A:515:A:C8	2.44	0.53
1:A:639:U:H2'	1:A:640:C:C6	2.43	0.53
1:A:1276:A:H61	1:A:1294:U:H3	1.55	0.53
1:A:1811:G:H2'	1:A:1812:U:C6	2.44	0.53
32:a:442:G:H2'	32:a:443:C:C6	2.44	0.53
32:a:624:C:H2'	32:a:625:U:O4'	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:773:G:H1	32:a:806:C:H42	1.55	0.53
32:a:1428:A:H2'	32:a:1429:A:O4'	2.08	0.53
36:e:82:GLN:H	36:e:147:MET:HE3	1.72	0.53
50:s:50:ALA:HB1	50:s:57:HIS:HB3	1.91	0.53
1:A:1877:A:H2'	1:A:1878:G:O4'	2.07	0.53
1:A:2522:U:O2'	1:A:2647:U:H5'	2.09	0.53
1:A:2740:A:C8	1:A:2763:G:N2	2.76	0.53
1:A:2882:A:C3'	1:A:2883:A:H5''	2.36	0.53
2:B:56:G:H1'	2:B:58:A:N6	2.23	0.53
32:a:790:A:H2'	32:a:791:G:C8	2.43	0.53
56:z:47:U:H2'	56:z:48:G:H8	1.68	0.53
1:A:993:G:H5''	17:R:50:ARG:HD2	1.89	0.53
1:A:1386:C:H2'	1:A:1387:A:H8	1.74	0.53
1:A:1593:A:H2'	1:A:1594:U:O4'	2.08	0.53
1:A:2092:U:H5''	8:H:24:GLY:HA3	1.89	0.53
13:N:69:PRO:HB2	13:N:92:TRP:HB3	1.89	0.53
53:v:133:GLN:HG2	54:w:17:GLU:HG2	1.90	0.53
1:A:489:G:H21	1:A:1320:C:H5''	1.73	0.53
1:A:1511:G:H2'	1:A:1512:C:C6	2.44	0.53
1:A:2273:A:H2'	1:A:2274:A:H8	1.72	0.53
32:a:669:G:H1	32:a:737:C:H42	1.56	0.53
53:v:133:GLN:HG2	54:w:17:GLU:CG	2.37	0.53
1:A:1500:G:H2'	1:A:1501:G:C8	2.43	0.53
1:A:2417:C:H2'	1:A:2418:A:O4'	2.09	0.53
32:a:528:C:C4	32:a:529:G:C5	2.96	0.53
32:a:745:G:H2'	32:a:746:A:H8	1.73	0.53
53:v:219:SER:OG	54:w:16:ILE:HG22	2.09	0.53
32:a:744:C:H2'	32:a:745:G:H8	1.74	0.53
32:a:1434:A:H2'	32:a:1435:G:O4'	2.09	0.53
32:a:1493:A:H62	54:w:29:VAL:HG22	1.74	0.53
1:A:863:A:H4'	2:B:100:G:N2	2.23	0.53
1:A:1071:G:H1'	1:A:1089:A:H2'	1.90	0.53
1:A:1130:U:C2	1:A:2025:C:H5''	2.43	0.53
1:A:1656:C:H2'	1:A:1657:U:H6	1.73	0.53
1:A:1712:U:H2'	1:A:1713:A:C8	2.44	0.53
1:A:2038:G:H2'	1:A:2039:U:O4'	2.09	0.53
1:A:2567:G:H2'	1:A:2568:U:H6	1.71	0.53
1:A:2733:A:H3'	1:A:2734:A:C8	2.43	0.53
32:a:1448:C:H42	32:a:1455:G:H1	1.57	0.53
1:A:947:A:H2'	1:A:948:C:C6	2.44	0.53
1:A:2062:A:C6	1:A:2503:A:N6	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2544:G:H2'	1:A:2545:G:C8	2.44	0.53
1:A:2781:A:H5''	1:A:2782:G:H5'	1.90	0.53
2:B:33:G:H2'	2:B:34:A:O4'	2.08	0.53
11:L:24:VAL:HA	11:L:39:ILE:HG22	1.90	0.53
11:L:58:LEU:HD11	11:L:86:LEU:HD23	1.91	0.53
32:a:67:C:H2'	32:a:68:G:C8	2.44	0.53
32:a:985:C:H2'	32:a:986:U:C6	2.44	0.53
39:h:47:GLU:HG3	39:h:64:LYS:HG3	1.90	0.53
1:A:904:G:H2'	1:A:905:A:O4'	2.09	0.52
32:a:69:G:H2'	32:a:70:U:O4'	2.09	0.52
32:a:1320:C:H2'	32:a:1321:U:C6	2.43	0.52
55:x:43:A:H2'	55:x:44:A:C8	2.44	0.52
1:A:476:G:N2	1:A:478:A:H3'	2.25	0.52
14:O:49:GLU:HG2	14:O:94:TYR:HD2	1.74	0.52
32:a:518:C:H5	32:a:529:G:H3'	1.73	0.52
32:a:597:G:H2'	32:a:598:U:O4'	2.09	0.52
32:a:974:A:N6	32:a:1201:A:N6	2.52	0.52
33:b:70:VAL:HG12	33:b:92:VAL:HB	1.91	0.52
51:t:62:ALA:HB1	51:t:69:LYS:HA	1.92	0.52
1:A:942:G:H2'	1:A:943:A:O4'	2.10	0.52
1:A:2816:G:HO2'	1:A:2883:A:HO2'	1.57	0.52
2:B:89:U:O2	2:B:89:U:O4'	2.28	0.52
3:C:71:LYS:HB3	3:C:74:ILE:HD12	1.91	0.52
9:J:18:ASN:HB2	9:J:38:CYS:HB3	1.89	0.52
43:l:39:THR:HG22	43:l:51:LYS:HA	1.91	0.52
32:a:52:C:H2'	32:a:53:A:C8	2.45	0.52
32:a:528:C:O2	32:a:528:C:H2'	2.08	0.52
32:a:865:A:H2'	32:a:866:C:C6	2.44	0.52
1:A:1675:C:H3'	1:A:1676:A:H8	1.74	0.52
32:a:424:G:O2'	32:a:425:G:H8	1.90	0.52
1:A:377:G:H1	1:A:397:U:H3	1.56	0.52
1:A:560:C:H2'	1:A:561:G:O4'	2.09	0.52
1:A:1301:A:O2'	1:A:1302:A:H3'	2.10	0.52
1:A:1406:U:H2'	1:A:1407:G:O4'	2.10	0.52
1:A:1834:U:H5''	1:A:1835:2MG:H5'	1.91	0.52
1:A:2074:U:H2'	1:A:2075:U:C6	2.44	0.52
1:A:2728:U:HO2'	1:A:2729:G:H8	1.56	0.52
13:N:50:ARG:HA	13:N:53:MET:HE2	1.91	0.52
19:T:24:ILE:HD13	19:T:36:LEU:HD11	1.91	0.52
32:a:943:U:H2'	32:a:944:G:O4'	2.09	0.52
32:a:1424:U:H2'	32:a:1425:U:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:c:169:ARG:HB3	34:c:169:ARG:HH11	1.75	0.52
46:o:64:ARG:HH21	46:o:89:ARG:HH22	1.56	0.52
53:v:333:ILE:HD11	53:v:345:THR:HG23	1.90	0.52
1:A:270:A:H2	1:A:370:G:H5'	1.74	0.52
1:A:1778:U:H3'	1:A:1784:A:N6	2.25	0.52
1:A:2531:A:H61	1:A:2662:A:H61	1.57	0.52
1:A:2717:C:H2'	1:A:2718:G:O4'	2.09	0.52
10:K:17:VAL:HG23	10:K:137:PRO:HB2	1.91	0.52
32:a:7:A:H2'	36:e:124:LEU:HD22	1.91	0.52
32:a:151:A:H2'	32:a:151:A:N3	2.24	0.52
32:a:299:G:H2'	32:a:300:A:C8	2.44	0.52
32:a:1098:C:H2'	32:a:1099:G:O4'	2.09	0.52
32:a:1458:G:H4'	51:t:23:SER:HA	1.92	0.52
41:j:51:VAL:HG11	45:n:85:ARG:HB2	1.92	0.52
1:A:807:U:H2'	1:A:808:G:C8	2.45	0.52
1:A:1653:G:H3'	14:O:2:ARG:HG2	1.92	0.52
1:A:2329:U:H2'	1:A:2330:G:C8	2.45	0.52
19:T:36:LEU:HD13	19:T:48:LYS:HA	1.92	0.52
32:a:788:U:H2'	32:a:789:U:O4'	2.10	0.52
1:A:181:A:H2'	1:A:182:A:H8	1.70	0.52
1:A:2026:U:H2'	1:A:2027:G:O4'	2.09	0.52
1:A:2233:U:H2'	1:A:2234:G:C8	2.44	0.52
2:B:22:U:H3	2:B:61:G:H1	1.57	0.52
2:B:97:C:H2'	2:B:98:G:O4'	2.10	0.52
12:M:109:LYS:HG2	12:M:126:ARG:HB2	1.92	0.52
32:a:884:U:H4'	32:a:885:G:H5''	1.91	0.52
32:a:1432:G:N2	32:a:1467:C:H2'	2.25	0.52
53:v:192:LEU:HB3	53:v:222:VAL:HG11	1.92	0.52
54:w:22:ASP:HB2	54:w:23:PRO:HD2	1.90	0.52
1:A:595:C:H42	1:A:662:G:H1	1.57	0.52
1:A:607:U:H2'	1:A:608:A:H8	1.75	0.52
1:A:833:A:H2'	1:A:834:G:C8	2.45	0.52
1:A:2548:U:H2'	1:A:2549:G:O4'	2.10	0.52
32:a:349:A:H2'	32:a:350:G:O4'	2.10	0.52
32:a:501:C:H1'	32:a:548:G:H21	1.75	0.52
32:a:634:C:H2'	32:a:635:A:C8	2.44	0.52
32:a:981:U:H5''	45:n:63:ARG:HH22	1.74	0.52
32:a:1276:G:H21	32:a:1282:C:H1'	1.75	0.52
32:a:1313:U:H2'	32:a:1314:C:C6	2.45	0.52
50:s:40:ILE:HG21	50:s:66:MET:HB3	1.92	0.52
53:v:196:THR:HG23	53:v:222:VAL:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:G:H1	1:A:2902:C:H42	1.58	0.51
1:A:376:G:H1	1:A:398:C:H42	1.56	0.51
1:A:875:G:C6	1:A:876:C:N4	2.78	0.51
1:A:1126:A:H4'	1:A:1127:A:O5'	2.09	0.51
1:A:272:A:H2'	1:A:273:G:C8	2.45	0.51
1:A:2209:G:H1	1:A:2215:C:H42	1.59	0.51
1:A:2730:C:H2'	1:A:2731:G:C8	2.45	0.51
32:a:13:U:C2	32:a:915:A:C6	2.91	0.51
32:a:155:A:H2	32:a:166:U:H3	1.56	0.51
32:a:234:C:H2'	32:a:235:C:C6	2.44	0.51
32:a:450:G:N2	32:a:482:A:H62	2.08	0.51
32:a:741:G:H2'	32:a:742:G:O4'	2.10	0.51
36:e:115:LEU:HD23	36:e:120:VAL:HG21	1.92	0.51
44:m:16:VAL:HG23	44:m:17:ILE:HD12	1.91	0.51
1:A:2082:A:H2'	1:A:2083:G:O4'	2.10	0.51
3:C:154:LEU:HD22	3:C:176:LEU:HD21	1.92	0.51
23:X:40:GLN:HE22	23:X:45:PHE:HB2	1.76	0.51
24:Y:5:CYS:HB3	24:Y:10:LYS:H	1.75	0.51
32:a:158:G:H2'	32:a:159:G:O4'	2.11	0.51
32:a:184:G:H1	32:a:193:C:H42	1.58	0.51
32:a:573:A:H2'	32:a:574:A:C8	2.46	0.51
32:a:944:G:O6	32:a:1337:G:C8	2.60	0.51
32:a:985:C:H42	32:a:1220:G:H1	1.57	0.51
38:g:24:ALA:O	38:g:27:VAL:HG22	2.10	0.51
1:A:2002:G:O6	1:A:2003:A:N6	2.44	0.51
1:A:2134:A:N6	1:A:2157:G:H1'	2.25	0.51
7:G:145:ALA:HB1	7:G:164:TYR:HE1	1.75	0.51
32:a:78:A:H61	32:a:91:U:H3	1.59	0.51
33:b:91:PHE:H	33:b:150:GLY:HA3	1.75	0.51
1:A:579:G:H2'	1:A:580:U:C6	2.45	0.51
1:A:1027:A:C2	1:A:2488:G:H5'	2.46	0.51
1:A:2071:A:H2'	1:A:2072:C:C6	2.46	0.51
1:A:2314:A:H1'	6:F:155:THR:HG21	1.93	0.51
17:R:40:ILE:HD11	18:S:84:ARG:HE	1.76	0.51
32:a:46:G:O2'	32:a:365:U:H1'	2.09	0.51
53:v:147:MET:O	53:v:150:ARG:HG2	2.09	0.51
1:A:29:U:H2'	1:A:30:G:O4'	2.09	0.51
8:H:94:ILE:HB	8:H:122:LEU:HD12	1.93	0.51
32:a:618:C:H41	32:a:620:C:H3'	1.75	0.51
1:A:150:U:H2'	1:A:151:C:H6	1.75	0.51
1:A:312:G:H2'	1:A:313:G:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:U:O2'	1:A:2068:U:C2	2.64	0.51
1:A:1370:C:H2'	1:A:1371:G:O4'	2.11	0.51
1:A:2267:A:H5''	1:A:2268:A:H5'	1.93	0.51
1:A:2554:U:H2'	1:A:2555:U:C6	2.45	0.51
1:A:2821:A:H2'	1:A:2822:G:O4'	2.10	0.51
32:a:538:G:H2'	32:a:539:A:H8	1.74	0.51
32:a:1507:A:H2'	32:a:1508:A:C8	2.46	0.51
1:A:77:G:H2'	1:A:78:U:C6	2.46	0.51
1:A:1177:G:H2'	1:A:1178:C:O4'	2.11	0.51
1:A:1418:G:H21	1:A:1580:A:H62	1.58	0.51
1:A:1532:A:H61	1:A:1539:U:H3	1.58	0.51
49:r:63:ARG:HB3	49:r:70:TYR:CE1	2.46	0.51
55:x:44:A:H2'	55:x:45:G:C8	2.46	0.51
1:A:1798:U:H2'	1:A:1819:A:N6	2.26	0.51
32:a:190:A:C5	32:a:191:G:H1'	2.45	0.51
32:a:505:G:H2'	32:a:506:G:H8	1.73	0.51
32:a:601:G:H2'	32:a:602:A:C8	2.46	0.51
32:a:601:G:H1	32:a:637:C:H42	1.59	0.51
53:v:221:PHE:HD1	54:w:16:ILE:CD1	2.24	0.51
55:y:43:A:H2'	55:y:44:A:C8	2.45	0.51
1:A:417:C:H2'	1:A:418:C:C6	2.46	0.51
1:A:567:U:H2'	1:A:568:U:O4'	2.11	0.51
1:A:873:C:H2'	1:A:874:G:C8	2.45	0.51
1:A:2523:G:H1	1:A:2540:C:H42	1.59	0.51
32:a:1265:C:H2'	32:a:1266:G:O4'	2.11	0.51
51:t:57:ILE:O	51:t:61:GLN:HG2	2.11	0.51
1:A:817:C:O2'	1:A:839:U:H5''	2.11	0.50
1:A:1659:G:H2'	1:A:1660:G:O4'	2.11	0.50
32:a:427:U:H2'	32:a:428:G:C8	2.46	0.50
1:A:226:A:H5'	1:A:257:C:H4'	1.93	0.50
1:A:339:U:H2'	1:A:340:A:C8	2.47	0.50
1:A:407:G:H2'	1:A:408:G:H8	1.75	0.50
1:A:1599:U:H2'	1:A:1600:C:H6	1.75	0.50
1:A:1687:G:H2'	1:A:1688:U:C6	2.47	0.50
32:a:17:U:H2'	32:a:18:C:H6	1.75	0.50
32:a:372:C:H2'	32:a:387:U:O4	2.11	0.50
34:c:113:ALA:HB1	34:c:200:VAL:HG13	1.93	0.50
53:v:8:ASN:HA	53:v:11:ILE:HD12	1.92	0.50
1:A:266:G:H1	1:A:426:C:H42	1.60	0.50
1:A:855:G:H2'	1:A:856:G:O4'	2.12	0.50
1:A:878:A:H3'	1:A:879:G:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1677:A:H2'	1:A:1678:A:C8	2.47	0.50
3:C:162:VAL:HG12	3:C:174:LEU:HD12	1.92	0.50
4:D:124:ARG:HD2	4:D:165:MET:HB2	1.94	0.50
32:a:259:G:H2'	32:a:260:G:O4'	2.11	0.50
32:a:1087:G:H2'	32:a:1087:G:N3	2.26	0.50
36:e:76:LEU:HD11	36:e:120:VAL:HG13	1.93	0.50
1:A:57:C:H2'	1:A:58:G:O4'	2.11	0.50
1:A:784:G:H5'	1:A:785:G:OP1	2.12	0.50
1:A:1343:G:H1'	1:A:1597:A:C2	2.47	0.50
1:A:2077:A:C5	1:A:2435:A:C6	2.99	0.50
1:A:2241:A:H2'	1:A:2242:G:H8	1.74	0.50
21:V:28:VAL:HG12	21:V:34:VAL:HG12	1.92	0.50
32:a:1521:C:H2'	32:a:1522:U:C6	2.46	0.50
1:A:194:G:H2'	1:A:195:A:O4'	2.11	0.50
1:A:2029:G:O6	1:A:2032:G:H5''	2.12	0.50
1:A:2382:G:H21	30:4:42:ARG:NH1	2.10	0.50
1:A:2623:G:H2'	1:A:2624:G:C8	2.46	0.50
32:a:381:C:H2'	32:a:382:A:O4'	2.12	0.50
32:a:496:A:N6	32:a:498:A:H62	2.09	0.50
32:a:1117:A:H61	32:a:1156:G:H22	1.60	0.50
36:e:156:LYS:HB3	39:h:71:VAL:HG13	1.93	0.50
53:v:246:THR:HG23	53:v:275:GLN:HB2	1.93	0.50
1:A:532:A:H4'	1:A:533:G:H8	1.74	0.50
1:A:579:G:H2'	1:A:580:U:H6	1.77	0.50
1:A:1721:G:H21	1:A:1722:A:H62	1.59	0.50
1:A:2528:U:H5'	31:5:32:LYS:HE3	1.93	0.50
24:Y:33:LEU:HD23	24:Y:50:ARG:HG2	1.93	0.50
1:A:84:A:H4'	1:A:85:G:O5'	2.11	0.50
1:A:236:C:H2'	1:A:237:C:C6	2.47	0.50
1:A:1090:A:H61	1:A:1101:U:H3	1.60	0.50
1:A:2266:A:H1'	1:A:2272:U:H3	1.77	0.50
1:A:2560:A:H2'	1:A:2561:U:O4'	2.12	0.50
1:A:2590:A:H2'	1:A:2591:C:C6	2.45	0.50
32:a:290:C:H42	32:a:310:G:H1	1.59	0.50
32:a:642:A:H2'	32:a:643:C:O4'	2.10	0.50
32:a:1348:U:H2'	32:a:1349:A:H8	1.77	0.50
46:o:36:ILE:HA	46:o:56:LEU:HD11	1.93	0.50
1:A:851:C:H2'	1:A:852:U:H6	1.77	0.50
1:A:2662:A:C5	1:A:2663:G:H1'	2.47	0.50
16:Q:64:ILE:HA	16:Q:69:GLY:HA2	1.93	0.50
32:a:147:G:H2'	32:a:148:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:185:U:H3	32:a:192:A:N6	2.05	0.50
32:a:377:G:H1	32:a:386:C:H42	1.60	0.50
43:l:55:VAL:HG11	43:l:80:ILE:HD11	1.94	0.50
1:A:1054:A:H61	1:A:1105:U:H3	1.60	0.50
1:A:1277:G:H1	1:A:1293:C:H42	1.59	0.50
1:A:2385:C:H2'	1:A:2386:A:C8	2.46	0.50
5:E:149:ILE:HB	5:E:188:MET:HG2	1.92	0.50
12:M:78:ARG:HG2	12:M:113:ALA:HB3	1.93	0.50
20:U:23:ALA:HB1	20:U:29:THR:HB	1.93	0.50
32:a:229:U:H2'	32:a:230:G:C8	2.47	0.50
32:a:1361:G:H2'	32:a:1362:A:H8	1.75	0.50
1:A:219:A:H2'	1:A:220:G:C8	2.47	0.49
1:A:1000:A:H2'	1:A:1001:A:C8	2.47	0.49
1:A:1997:C:H2'	1:A:1998:A:H8	1.76	0.49
1:A:2722:G:H2'	1:A:2723:C:H6	1.71	0.49
12:M:110:VAL:HB	12:M:127:VAL:HG22	1.94	0.49
19:T:20:VAL:HG11	19:T:44:ALA:HA	1.93	0.49
32:a:623:C:H2'	32:a:624:C:H6	1.77	0.49
32:a:666:G:H5'	32:a:726:C:H1'	1.94	0.49
32:a:1151:A:H4'	32:a:1152:A:OP1	2.11	0.49
32:a:1358:U:C4	32:a:1363:A:N1	2.80	0.49
43:l:55:VAL:HG21	43:l:82:ILE:HD11	1.93	0.49
1:A:927:A:H2'	1:A:928:A:H8	1.73	0.49
32:a:620:C:H2'	32:a:621:A:C8	2.47	0.49
32:a:1347:G:H1'	32:a:1348:U:H5	1.77	0.49
32:a:1468:A:H2'	32:a:1469:C:O4'	2.12	0.49
41:j:47:GLU:HB2	41:j:67:ILE:HB	1.94	0.49
1:A:270:A:H5'	1:A:271:G:H5''	1.94	0.49
1:A:327:G:H1	1:A:335:C:N4	2.10	0.49
1:A:673:C:H2'	1:A:674:G:O4'	2.11	0.49
1:A:2217:G:H2'	1:A:2218:G:C8	2.46	0.49
1:A:2364:C:H2'	1:A:2365:G:O4'	2.11	0.49
2:B:70:C:H2'	2:B:71:C:C6	2.47	0.49
7:G:15:VAL:HG22	7:G:79:VAL:HG23	1.94	0.49
17:R:88:VAL:HG11	18:S:49:ILE:HD11	1.93	0.49
23:X:37:ILE:HG22	23:X:38:VAL:HG23	1.95	0.49
1:A:95:A:H2'	1:A:96:C:O4'	2.12	0.49
1:A:697:G:H2'	1:A:698:C:O4'	2.12	0.49
1:A:1922:G:H2'	1:A:1923:U:O4'	2.12	0.49
1:A:2301:C:H2'	1:A:2302:U:C6	2.47	0.49
6:F:108:VAL:HG12	6:F:109:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:69:ALA:O	8:H:72:ILE:HB	2.12	0.49
30:4:38:THR:HA	30:4:41:LYS:HE3	1.93	0.49
32:a:428:G:H4'	32:a:429:U:H5'	1.92	0.49
32:a:528:C:N4	32:a:529:G:C6	2.80	0.49
32:a:1076:U:H2'	32:a:1077:G:O4'	2.12	0.49
33:b:170:HIS:HA	33:b:173:ILE:HD12	1.94	0.49
1:A:1176:U:H2'	1:A:1177:G:C8	2.47	0.49
1:A:1746:A:H2'	1:A:1747:U:H6	1.78	0.49
1:A:2660:A:H3'	1:A:2661:G:H8	1.77	0.49
2:B:51:G:H22	2:B:53:A:H62	1.59	0.49
2:B:110:C:H2'	2:B:111:U:O4'	2.12	0.49
28:2:15:ALA:HB2	28:2:47:VAL:HG11	1.94	0.49
32:a:21:G:N2	32:a:22:G:C6	2.81	0.49
32:a:162:A:C5	32:a:163:C:H1'	2.47	0.49
32:a:1250:A:H2'	32:a:1251:A:C8	2.47	0.49
32:a:1412:C:H2'	32:a:1413:A:C8	2.47	0.49
1:A:475:C:O2	1:A:479:A:N6	2.44	0.49
1:A:1425:G:H2'	1:A:1426:G:C8	2.48	0.49
32:a:336:A:H2'	32:a:337:G:H8	1.77	0.49
32:a:486:U:H2'	32:a:487:A:H8	1.77	0.49
32:a:1005:A:H3'	32:a:1006:G:C8	2.48	0.49
32:a:1342:C:H2'	32:a:1343:G:H8	1.76	0.49
1:A:962:G:H21	1:A:2250:G:H22	1.60	0.49
1:A:1255:U:C6	5:E:68:ALA:HA	2.47	0.49
1:A:2025:C:H2'	1:A:2026:U:C6	2.48	0.49
32:a:229:U:H2'	32:a:230:G:O4'	2.13	0.49
40:i:28:ILE:HG23	40:i:63:LEU:HD11	1.94	0.49
1:A:85:G:H1	1:A:97:C:H42	1.58	0.49
1:A:474:G:H3'	1:A:475:C:C5'	2.42	0.49
1:A:2086:U:H2'	1:A:2087:G:H8	1.73	0.49
1:A:2684:U:H2'	1:A:2685:G:O4'	2.13	0.49
1:A:2814:A:H2'	1:A:2815:C:O4'	2.13	0.49
5:E:112:LEU:HB3	5:E:118:LEU:HB2	1.95	0.49
18:S:38:VAL:HG13	18:S:54:VAL:HG12	1.94	0.49
32:a:34:C:H5'	32:a:363:A:O2'	2.13	0.49
32:a:605:U:O2	32:a:633:G:O6	2.30	0.49
55:y:62:C:H2'	55:y:63:G:C8	2.48	0.49
1:A:77:G:H5'	25:Z:52:ARG:HG2	1.95	0.49
1:A:387:U:H4'	1:A:388:G:O4'	2.12	0.49
1:A:623:C:H2'	1:A:624:C:C6	2.48	0.49
1:A:656:G:H2'	1:A:657:U:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:A:H2'	1:A:960:A:C8	2.47	0.49
1:A:1243:C:H2'	1:A:1244:A:O4'	2.13	0.49
1:A:1964:G:H4'	1:A:1965:C:OP2	2.11	0.49
1:A:2642:G:H1	1:A:2772:C:H42	1.61	0.49
7:G:88:GLN:HG3	7:G:163:ARG:HG3	1.95	0.49
32:a:256:U:H2'	32:a:257:G:H8	1.78	0.49
32:a:337:G:H2'	32:a:338:A:H8	1.76	0.49
32:a:1395:C:H2'	32:a:1396:A:C8	2.47	0.49
32:a:1486:G:H2'	32:a:1487:G:O4'	2.13	0.49
42:k:20:VAL:HA	42:k:83:GLU:HG3	1.95	0.49
53:v:26:ASP:HB3	53:v:29:ALA:HB3	1.93	0.49
53:v:311:GLU:HB3	54:w:15:ALA:HB2	1.93	0.49
1:A:155:A:H2'	1:A:156:A:C8	2.48	0.49
1:A:1028:A:H2'	1:A:1029:A:H8	1.75	0.49
1:A:1030:C:H42	1:A:1124:G:H1	1.59	0.49
1:A:1398:C:H2'	1:A:1399:C:C6	2.47	0.49
1:A:2052:A:H61	1:A:2617:U:H3	1.60	0.49
1:A:2748:A:H2'	1:A:2749:A:C8	2.48	0.49
2:B:10:G:H2'	2:B:11:C:O4'	2.13	0.49
32:a:1476:A:H2'	32:a:1477:U:O4'	2.12	0.49
55:y:71:C:H2'	55:y:72:A:C8	2.48	0.49
1:A:580:U:O3'	17:R:31:VAL:HG13	2.13	0.48
1:A:873:C:H2'	1:A:874:G:H8	1.78	0.48
1:A:1076:C:H2'	1:A:1077:A:H8	1.77	0.48
1:A:1361:G:H2'	1:A:1362:C:H6	1.75	0.48
1:A:1645:G:H5''	1:A:1646:C:H5'	1.95	0.48
1:A:2412:A:H2'	1:A:2413:G:O4'	2.13	0.48
1:A:2819:G:H2'	1:A:2821:A:N7	2.27	0.48
2:B:63:C:H2'	2:B:64:G:H8	1.75	0.48
3:C:221:ARG:HE	3:C:221:ARG:HB2	1.41	0.48
11:L:35:VAL:HG22	11:L:69:VAL:HG11	1.94	0.48
32:a:1048:G:H2'	32:a:1050:G:C8	2.48	0.48
32:a:1064:G:O2'	32:a:1190:G:N2	2.46	0.48
34:c:6:HIS:HB3	45:n:89:MET:SD	2.53	0.48
1:A:1273:U:H4'	1:A:1275:A:OP2	2.13	0.48
1:A:2070:A:H2'	1:A:2071:A:O4'	2.14	0.48
32:a:66:A:HO2'	32:a:172:A:HO2'	1.59	0.48
32:a:253:A:H2'	32:a:254:G:H8	1.78	0.48
32:a:736:C:H2'	32:a:737:C:H6	1.78	0.48
32:a:767:A:H2'	32:a:768:A:O4'	2.13	0.48
32:a:811:C:O2'	32:a:901:A:N1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1268:G:N3	32:a:1326:U:O2'	2.44	0.48
1:A:1138:G:H2'	1:A:1139:G:O4'	2.13	0.48
1:A:1201:U:H3	1:A:1244:A:N6	2.09	0.48
1:A:2395:C:H2'	1:A:2396:G:O4'	2.14	0.48
1:A:2672:U:H2'	1:A:2673:G:C8	2.48	0.48
2:B:6:G:H4'	2:B:28:C:H4'	1.95	0.48
12:M:47:ARG:HG2	12:M:50:PHE:HB2	1.93	0.48
32:a:756:C:H2'	32:a:757:U:C6	2.48	0.48
32:a:777:A:H2'	32:a:778:G:O4'	2.12	0.48
32:a:977:A:H2'	32:a:977:A:N3	2.28	0.48
1:A:1141:U:H4'	1:A:1142:A:O4'	2.12	0.48
1:A:1248:G:C3'	1:A:1249:U:H5''	2.24	0.48
1:A:1386:C:H2'	1:A:1387:A:C8	2.48	0.48
2:B:87:U:H3'	2:B:88:C:H5'	1.95	0.48
3:C:161:TYR:HB3	3:C:194:GLU:HG3	1.95	0.48
3:C:167:ARG:HA	3:C:172:VAL:HG12	1.95	0.48
7:G:156:PRO:HB2	7:G:172:LYS:HG2	1.94	0.48
7:G:163:ARG:HH11	7:G:169:VAL:HB	1.78	0.48
17:R:24:TYR:HB3	17:R:28:ARG:CB	2.42	0.48
32:a:448:A:H3'	32:a:449:G:H8	1.78	0.48
32:a:510:A:N3	32:a:543:U:H1'	2.28	0.48
32:a:839:C:H2'	32:a:840:C:C6	2.49	0.48
32:a:1191:A:H2'	32:a:1192:C:C6	2.48	0.48
36:e:74:VAL:HG21	36:e:144:LEU:HB3	1.94	0.48
39:h:106:THR:HG22	39:h:121:LEU:HD23	1.93	0.48
1:A:1821:A:H2'	1:A:1822:C:H6	1.77	0.48
1:A:2242:G:H2'	1:A:2243:U:O4'	2.14	0.48
1:A:2350:C:H2'	1:A:2351:G:O4'	2.14	0.48
1:A:2524:G:H1	1:A:2539:C:H42	1.60	0.48
9:J:79:LEU:HD12	9:J:108:ILE:HD13	1.94	0.48
32:a:186:C:H42	32:a:191:G:H1	1.61	0.48
32:a:900:A:H2'	32:a:901:A:C8	2.49	0.48
1:A:222:A:N6	1:A:232:G:H1'	2.28	0.48
1:A:699:A:H2'	1:A:700:G:O4'	2.14	0.48
1:A:2354:C:H42	1:A:2363:G:H1	1.61	0.48
2:B:94:A:H2'	2:B:95:U:O4'	2.13	0.48
32:a:302:G:H2'	32:a:303:A:C8	2.49	0.48
32:a:322:C:O2'	51:t:18:ARG:HB2	2.13	0.48
32:a:725:G:H2'	32:a:726:C:C6	2.49	0.48
50:s:40:ILE:HD13	50:s:66:MET:HG2	1.96	0.48
1:A:725:G:C2	1:A:726:G:N2	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1448:G:H2'	1:A:1449:G:O4'	2.13	0.48
1:A:1716:U:H2'	1:A:1717:A:C8	2.49	0.48
1:A:1860:G:H2'	1:A:1861:G:H8	1.77	0.48
1:A:2521:C:H42	1:A:2544:G:H1	1.62	0.48
1:A:2615:U:C2	27:1:4:GLN:HA	2.48	0.48
1:A:2661:G:H2'	1:A:2662:A:C8	2.48	0.48
32:a:66:A:H5'	32:a:173:U:C4	2.49	0.48
32:a:147:G:H21	32:a:1447:A:H1'	1.78	0.48
32:a:358:U:H2'	32:a:359:G:H8	1.78	0.48
32:a:890:G:O2'	32:a:906:A:N6	2.46	0.48
32:a:954:G:H2'	32:a:955:U:C6	2.48	0.48
32:a:1360:A:H2'	32:a:1361:G:H5'	1.96	0.48
32:a:1496:C:O2	32:a:1517:G:N2	2.38	0.48
42:k:64:GLN:HG3	42:k:99:ALA:HB2	1.95	0.48
1:A:771:G:OP1	29:3:14:ARG:HD2	2.14	0.48
1:A:1117:C:O2'	1:A:1118:C:H6	1.96	0.48
1:A:2055:C:C5'	1:A:2056:G:H5''	2.43	0.48
1:A:2557:G:H2'	1:A:2558:C:H6	1.71	0.48
1:A:2756:U:C4	1:A:2758:A:C6	3.00	0.48
18:S:68:ARG:HB3	18:S:90:ARG:HB3	1.96	0.48
23:X:71:VAL:HG22	23:X:78:LYS:HG2	1.96	0.48
32:a:397:A:H2'	32:a:397:A:N3	2.29	0.48
32:a:500:G:H2'	32:a:501:C:C6	2.48	0.48
32:a:523:A:H2	43:l:88:LYS:HG2	1.78	0.48
32:a:861:G:H1	32:a:868:C:H42	1.60	0.48
32:a:974:A:N6	32:a:1201:A:N1	2.61	0.48
32:a:1367:C:H4'	41:j:50:THR:HG21	1.94	0.48
32:a:1390:U:H2'	32:a:1391:U:C6	2.48	0.48
40:i:84:THR:O	40:i:88:MET:HG3	2.13	0.48
1:A:278:A:H2'	1:A:278:A:N3	2.28	0.48
1:A:872:U:H2'	1:A:873:C:C6	2.49	0.48
1:A:1043:C:N4	1:A:1112:G:H1	2.10	0.48
1:A:1137:G:H2'	1:A:1138:G:C8	2.48	0.48
1:A:1805:A:H2'	1:A:1806:C:H6	1.77	0.48
1:A:1935:G:H3'	1:A:1962:5MC:HN41	1.78	0.48
1:A:2024:G:H2'	1:A:2025:C:C6	2.48	0.48
1:A:2225:A:H4'	1:A:2226:C:O5'	2.14	0.48
1:A:2615:U:H2'	1:A:2616:C:C6	2.49	0.48
1:A:2616:C:H2'	1:A:2617:U:C6	2.48	0.48
32:a:262:A:H2'	32:a:263:A:C8	2.48	0.48
32:a:757:U:H2'	32:a:758:C:O4'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:h:30:SER:HB3	39:h:33:LYS:HB2	1.95	0.48
53:v:324:ARG:HA	53:v:335:ASP:HA	1.96	0.48
1:A:1006:C:H42	1:A:1137:G:H1	1.62	0.48
1:A:1444:G:H2'	1:A:1445:G:C8	2.49	0.48
1:A:1521:G:H2'	1:A:1522:A:C8	2.49	0.48
1:A:1725:U:H2'	1:A:1726:C:C6	2.48	0.48
1:A:1967:C:H2'	1:A:1968:G:O4'	2.14	0.48
1:A:2185:U:H2'	1:A:2186:G:C8	2.49	0.48
1:A:2809:A:H2'	1:A:2810:A:C8	2.49	0.48
35:d:64:ILE:O	35:d:111:ARG:HD2	2.14	0.48
49:r:33:ILE:HG22	49:r:39:ILE:HA	1.96	0.48
52:u:17:ARG:O	52:u:21:ARG:HG3	2.14	0.48
55:y:21:A:N6	55:y:46:G:H2'	2.29	0.48
1:A:167:A:H2'	1:A:168:G:O4'	2.14	0.47
1:A:572:A:H2'	1:A:573:U:O4'	2.14	0.47
1:A:807:U:H2'	1:A:808:G:H8	1.79	0.47
1:A:1980:G:HO2'	1:A:1982:U:H6	1.60	0.47
1:A:2885:G:H1	27:1:40:ARG:HH22	1.60	0.47
32:a:32:A:C2'	32:a:33:A:C8	2.90	0.47
32:a:409:U:H2'	32:a:410:G:O4'	2.14	0.47
32:a:815:A:N3	32:a:1527:U:O2'	2.44	0.47
32:a:1348:U:H4'	40:i:122:ARG:HG3	1.96	0.47
32:a:1369:C:H2'	32:a:1370:G:O4'	2.14	0.47
1:A:1278:C:H2'	1:A:1279:G:H8	1.79	0.47
1:A:1510:G:H2'	1:A:1511:G:C8	2.49	0.47
1:A:1713:A:H61	1:A:1745:A:H61	1.62	0.47
1:A:2179:C:H2'	1:A:2180:U:C6	2.49	0.47
1:A:2297:A:N1	1:A:2321:U:H5	2.12	0.47
3:C:232:HIS:NE2	3:C:244:PRO:HA	2.29	0.47
21:V:7:ARG:HB2	21:V:27:ASN:HA	1.96	0.47
32:a:555:U:H2'	32:a:556:C:H6	1.77	0.47
32:a:1060:U:H2'	32:a:1061:G:C8	2.48	0.47
32:a:1106:G:H2'	32:a:1107:C:H6	1.78	0.47
32:a:1225:A:H2'	32:a:1226:C:C6	2.49	0.47
32:a:1338:G:H2'	32:a:1339:A:C8	2.49	0.47
32:a:1356:G:H2'	32:a:1357:A:H8	1.72	0.47
40:i:47:VAL:HA	40:i:50:GLN:HE21	1.79	0.47
1:A:821:A:H3'	1:A:946:C:H6	1.79	0.47
1:A:842:U:H2'	1:A:843:G:C8	2.49	0.47
4:D:110:THR:HB	4:D:202:ILE:HB	1.95	0.47
4:D:141:ARG:HB3	4:D:141:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:96:ARG:HD3	14:O:98:LEU:HD11	1.96	0.47
32:a:186:C:H4'	51:t:76:LYS:HB3	1.97	0.47
32:a:382:A:H2'	32:a:383:A:C8	2.49	0.47
32:a:824:G:H1	32:a:876:C:H42	1.62	0.47
32:a:1426:G:H2'	32:a:1427:C:H6	1.80	0.47
32:a:1490:U:H2'	32:a:1491:G:O4'	2.14	0.47
34:c:3:GLN:O	34:c:4:LYS:HB3	2.15	0.47
35:d:100:ASN:O	35:d:104:ARG:HG2	2.14	0.47
48:q:61:ILE:HA	48:q:75:LEU:HA	1.96	0.47
51:t:55:GLN:N	51:t:56:PRO:HD2	2.29	0.47
1:A:536:G:H2'	1:A:537:G:O4'	2.13	0.47
1:A:2228:G:H2'	1:A:2229:U:C6	2.49	0.47
1:A:2452:C:N3	1:A:2504:PSU:O4	2.47	0.47
2:B:48:U:H2'	2:B:49:C:C6	2.49	0.47
32:a:560:A:H5''	32:a:561:U:H5'	1.97	0.47
53:v:30:LYS:HD3	53:v:63:LEU:HD22	1.97	0.47
53:v:221:PHE:HD1	54:w:16:ILE:HD13	1.79	0.47
1:A:732:C:H2'	1:A:733:G:O4'	2.13	0.47
1:A:1465:G:H2'	1:A:1466:U:O4'	2.15	0.47
1:A:1495:A:H3'	1:A:1496:A:C8	2.49	0.47
1:A:1722:A:H2'	1:A:1723:G:H8	1.79	0.47
1:A:1831:G:H2'	1:A:1832:C:C6	2.49	0.47
1:A:2605:PSU:H2'	1:A:2606:C:C6	2.50	0.47
1:A:2672:U:H2'	1:A:2673:G:H8	1.79	0.47
1:A:2734:A:C4	1:A:2735:G:H1'	2.49	0.47
32:a:37:U:O2	32:a:547:A:C2	2.64	0.47
1:A:805:G:H22	1:A:828:U:H5''	1.79	0.47
1:A:2573:C:OP2	53:v:256:ARG:NH1	2.47	0.47
1:A:2590:A:H2'	1:A:2591:C:H6	1.78	0.47
1:A:2673:G:H2'	1:A:2674:G:C8	2.49	0.47
6:F:65:PRO:HB2	6:F:87:CYS:HB2	1.95	0.47
32:a:67:C:H42	32:a:102:G:H1	1.62	0.47
37:f:29:ILE:HD11	37:f:74:LEU:HD11	1.97	0.47
55:x:62:C:H2'	55:x:63:G:H8	1.79	0.47
1:A:611:C:H2'	1:A:612:G:O4'	2.15	0.47
1:A:813:U:H1'	1:A:1226:A:N3	2.30	0.47
1:A:829:A:H5'	1:A:831:G:N7	2.30	0.47
1:A:1419:A:H2'	1:A:1421:G:N7	2.30	0.47
1:A:1914:C:H1'	54:w:18:ALA:HB2	1.95	0.47
1:A:2013:A:H4'	19:T:96:ILE:HG22	1.97	0.47
1:A:2637:U:H3'	1:A:2638:G:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:4:GLU:HA	20:U:7:LEU:HD12	1.97	0.47
30:4:40:ARG:O	30:4:44:LEU:HG	2.14	0.47
32:a:113:G:H2'	32:a:114:U:C6	2.50	0.47
32:a:317:U:H2'	32:a:318:G:O4'	2.14	0.47
32:a:634:C:H2'	32:a:635:A:H8	1.79	0.47
32:a:830:G:H2'	32:a:831:A:H8	1.80	0.47
32:a:958:A:C8	50:s:55:ARG:HD3	2.49	0.47
36:e:90:THR:HB	36:e:91:GLY:H	1.58	0.47
42:k:25:ALA:HA	42:k:30:THR:HG22	1.97	0.47
43:l:50:ARG:HD2	43:l:66:TYR:HE1	1.80	0.47
53:v:328:LEU:HD13	53:v:345:THR:HG21	1.97	0.47
1:A:2812:G:H2'	1:A:2813:A:O4'	2.15	0.47
3:C:251:GLN:HB3	3:C:255:LYS:HD2	1.97	0.47
17:R:52:GLN:O	17:R:55:ARG:HG2	2.15	0.47
23:X:25:ARG:HB2	23:X:37:ILE:HA	1.97	0.47
53:v:34:LEU:HD11	53:v:64:GLU:HG3	1.97	0.47
1:A:1003:G:H1	1:A:1152:C:H42	1.63	0.47
1:A:1607:C:H4'	1:A:1608:A:O5'	2.15	0.47
1:A:1747:U:H2'	1:A:1748:C:C6	2.49	0.47
1:A:2081:U:H4'	24:Y:25:THR:HG21	1.97	0.47
1:A:2697:G:H1	1:A:2710:C:H42	1.60	0.47
20:U:61:LEU:HG	20:U:82:LYS:HB3	1.96	0.47
32:a:675:A:H2'	32:a:676:A:C8	2.50	0.47
32:a:736:C:H2'	32:a:737:C:C6	2.50	0.47
32:a:1196:A:H5''	54:w:35:GLY:CA	2.40	0.47
32:a:1242:G:H2'	32:a:1243:C:O4'	2.14	0.47
32:a:1352:C:H2'	32:a:1353:G:O4'	2.15	0.47
34:c:62:LYS:HB3	34:c:97:VAL:HG11	1.97	0.47
34:c:110:GLU:HB2	34:c:144:LEU:HG	1.97	0.47
39:h:10:MET:HB2	39:h:33:LYS:HE2	1.97	0.47
1:A:593:U:H1'	30:4:4:ILE:HD11	1.96	0.47
1:A:666:A:H2'	1:A:667:U:C6	2.49	0.47
1:A:724:U:H2'	1:A:725:G:O4'	2.15	0.47
1:A:1722:A:H2'	1:A:1723:G:C8	2.50	0.47
1:A:1749:A:H2'	1:A:1750:G:C8	2.49	0.47
1:A:2657:A:N1	1:A:2665:A:H2'	2.30	0.47
32:a:325:A:H2'	32:a:326:G:C8	2.50	0.47
32:a:1510:C:H42	32:a:1525:G:H1	1.63	0.47
1:A:37:C:H2'	1:A:38:A:O4'	2.15	0.46
1:A:891:G:H2'	1:A:892:A:C8	2.50	0.46
1:A:2616:C:H2'	1:A:2617:U:H6	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2635:A:H2'	1:A:2636:C:O4'	2.15	0.46
1:A:174:U:H2'	1:A:175:G:C8	2.50	0.46
1:A:679:C:H2'	1:A:680:C:C6	2.51	0.46
1:A:755:U:H2'	1:A:756:A:C8	2.50	0.46
1:A:794:A:H2'	1:A:795:C:C6	2.50	0.46
1:A:1478:G:H1	1:A:1513:U:H3	1.63	0.46
26:0:27:LEU:HG	26:0:47:MET:HE2	1.98	0.46
32:a:80:A:H61	32:a:89:U:H3	1.63	0.46
32:a:962:C:H1'	32:a:1201:A:H62	1.80	0.46
38:g:75:VAL:HB	38:g:86:GLN:HG2	1.95	0.46
40:i:13:LYS:HA	40:i:110:GLN:HG2	1.97	0.46
41:j:89:ARG:HG3	41:j:90:LEU:HD12	1.97	0.46
1:A:1020:A:N1	1:A:1141:U:O2'	2.47	0.46
1:A:1993:U:H4'	4:D:133:THR:HG22	1.97	0.46
1:A:2469:A:H2'	1:A:2470:G:O4'	2.16	0.46
3:C:223:THR:HA	3:C:232:HIS:O	2.15	0.46
32:a:604:G:H2'	32:a:605:U:O4'	2.15	0.46
32:a:676:A:H2'	32:a:677:U:H6	1.81	0.46
45:n:46:LEU:HD11	50:s:13:LEU:HB2	1.97	0.46
1:A:934:U:H2'	1:A:935:C:C6	2.51	0.46
1:A:971:G:P	1:A:989:G:H1	2.39	0.46
1:A:2618:G:H2'	1:A:2619:C:O4'	2.14	0.46
2:B:78:A:H62	2:B:98:G:H21	1.62	0.46
11:L:61:VAL:HB	11:L:87:LEU:HD11	1.97	0.46
23:X:43:THR:HB	23:X:46:HIS:CD2	2.50	0.46
28:2:11:LEU:HB3	28:2:49:TYR:HB3	1.98	0.46
32:a:143:A:H5'	32:a:144:G:H8	1.79	0.46
32:a:254:G:H2'	32:a:255:G:C8	2.51	0.46
32:a:309:A:H2'	32:a:310:G:C8	2.50	0.46
32:a:1046:A:H3'	32:a:1047:G:H8	1.80	0.46
32:a:1457:G:O3'	51:t:27:MET:HA	2.15	0.46
41:j:63:ASP:HB3	41:j:65:TYR:HE2	1.81	0.46
55:y:15:C:H1'	55:y:60:U:H4'	1.98	0.46
1:A:121:G:H2'	1:A:122:G:H8	1.80	0.46
1:A:143:C:H2'	1:A:144:A:H8	1.81	0.46
1:A:413:C:H42	1:A:2410:G:H1	1.62	0.46
1:A:477:A:H2'	1:A:478:A:O4'	2.16	0.46
1:A:968:C:O3'	26:0:18:PRO:HD3	2.15	0.46
1:A:1397:U:OP2	1:A:1398:C:N4	2.48	0.46
1:A:1653:G:C6	14:O:9:GLN:HB3	2.50	0.46
1:A:2643:G:H2'	1:A:2644:G:O4'	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:198:G:H1	32:a:219:U:H3	1.64	0.46
32:a:838:G:H2'	32:a:839:C:C6	2.51	0.46
35:d:85:ASN:HB3	35:d:88:GLU:HB2	1.97	0.46
37:f:38:ARG:HD2	37:f:99:ALA:HB2	1.98	0.46
55:x:43:A:H2'	55:x:44:A:H8	1.80	0.46
55:x:62:C:H2'	55:x:63:G:C8	2.50	0.46
1:A:466:A:C2	1:A:796:C:O4'	2.69	0.46
1:A:1266:G:H5''	19:T:15:GLN:HE22	1.79	0.46
1:A:1748:C:H2'	1:A:1749:A:C8	2.50	0.46
1:A:1748:C:H2'	1:A:1749:A:H8	1.81	0.46
1:A:2757:A:C5	1:A:2758:A:N7	2.83	0.46
5:E:48:THR:C	5:E:50:ALA:H	2.24	0.46
32:a:36:C:H2'	32:a:37:U:O4'	2.15	0.46
32:a:979:C:H1'	32:a:1317:C:H42	1.80	0.46
34:c:36:ASP:O	34:c:39:VAL:HG22	2.16	0.46
1:A:348:A:H2'	1:A:349:U:O4'	2.15	0.46
1:A:1289:C:H2'	1:A:1290:C:H6	1.80	0.46
1:A:1843:C:H2'	1:A:1844:C:H6	1.81	0.46
1:A:1930:G:HO2'	1:A:1968:G:H1	1.61	0.46
1:A:2543:G:H2'	1:A:2544:G:C8	2.50	0.46
5:E:5:LEU:HG	5:E:120:VAL:HB	1.98	0.46
5:E:60:TRP:HB2	5:E:65:THR:HG21	1.98	0.46
18:S:66:HIS:HB3	18:S:92:TRP:HZ3	1.80	0.46
28:2:37:LYS:HG2	28:2:46:HIS:HB3	1.98	0.46
32:a:68:G:H22	32:a:101:A:H2	1.64	0.46
32:a:291:U:H3	32:a:309:A:H61	1.63	0.46
32:a:966:2MG:C4	55:x:34:C:H4'	2.51	0.46
32:a:1053:G:N7	32:a:1200:C:H5'	2.31	0.46
32:a:1236:A:H4'	32:a:1304:G:H4'	1.97	0.46
34:c:157:LEU:HD12	34:c:164:ARG:HB3	1.98	0.46
35:d:58:LYS:HD3	35:d:62:ARG:HD2	1.97	0.46
1:A:227:A:H2	1:A:418:C:H1'	1.81	0.46
1:A:407:G:H2'	1:A:408:G:C8	2.50	0.46
1:A:489:G:N2	1:A:1320:C:H5''	2.31	0.46
1:A:672:C:H2'	1:A:673:C:H6	1.81	0.46
1:A:1151:A:H2'	1:A:1152:C:C6	2.50	0.46
1:A:1926:U:O2'	1:A:1928:A:N7	2.41	0.46
1:A:2039:U:H2'	1:A:2040:G:C8	2.51	0.46
1:A:2544:G:H2'	1:A:2545:G:H8	1.81	0.46
1:A:2645:G:H4'	1:A:2732:G:O3'	2.16	0.46
1:A:2800:A:C2	1:A:2895:G:H1'	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:941:G:H5'	38:g:32:VAL:HG21	1.98	0.46
43:l:83:ARG:HB3	43:l:96:HIS:HB2	1.97	0.46
53:v:116:ARG:HA	53:v:119:PHE:HB2	1.98	0.46
1:A:121:G:H2'	1:A:122:G:C8	2.51	0.46
1:A:428:A:H2'	1:A:429:A:C8	2.51	0.46
1:A:672:C:H2'	1:A:673:C:C6	2.50	0.46
1:A:751:A:O4'	19:T:90:LYS:HA	2.16	0.46
1:A:825:A:H2'	1:A:826:U:O4'	2.16	0.46
11:L:21:CYS:HA	11:L:41:ILE:HG22	1.98	0.46
24:Y:5:CYS:HB3	24:Y:9:GLY:H	1.81	0.46
32:a:43:C:H5'	47:p:12:LYS:HB3	1.97	0.46
32:a:1520:C:H2'	32:a:1521:C:C6	2.51	0.46
33:b:151:ILE:HG13	33:b:154:MET:HE3	1.98	0.46
35:d:55:LEU:HD12	35:d:203:LEU:HD21	1.97	0.46
1:A:1002:G:H2'	1:A:1003:G:O4'	2.15	0.46
1:A:1850:G:H2'	1:A:1851:U:O4'	2.16	0.46
32:a:855:U:H2'	32:a:856:C:H6	1.81	0.46
35:d:48:LEU:HD23	35:d:53:VAL:HG12	1.98	0.46
36:e:24:THR:HG23	36:e:29:ARG:HB3	1.97	0.46
38:g:98:ALA:HA	38:g:101:MET:HE3	1.98	0.46
41:j:45:ARG:HB3	41:j:69:THR:HB	1.98	0.46
1:A:489:G:H22	1:A:1320:C:H3'	1.81	0.45
1:A:729:G:C8	3:C:207:LYS:HD2	2.50	0.45
1:A:749:A:H2	1:A:753:A:HO2'	1.57	0.45
1:A:958:U:H2'	2:B:89:U:H1'	1.97	0.45
1:A:2114:A:N6	1:A:2119:A:H62	2.14	0.45
1:A:2146:C:H4'	1:A:2147:A:O5'	2.16	0.45
1:A:2190:G:H2'	1:A:2191:A:O4'	2.15	0.45
3:C:158:ALA:HB1	3:C:197:ASN:HB3	1.98	0.45
32:a:43:C:H42	32:a:399:G:H1	1.64	0.45
32:a:322:C:H41	32:a:328:C:H6	1.63	0.45
32:a:384:G:H2'	32:a:385:C:H6	1.81	0.45
32:a:1067:A:N6	32:a:1109:C:H5'	2.31	0.45
32:a:1433:A:H2'	32:a:1434:A:O4'	2.16	0.45
43:l:110:ARG:HH22	43:l:113:ALA:HB3	1.80	0.45
1:A:821:A:H3'	1:A:946:C:C6	2.50	0.45
1:A:1021:A:H2'	1:A:1023:U:H5''	1.99	0.45
1:A:2623:G:H2'	1:A:2624:G:H8	1.81	0.45
2:B:48:U:H2'	2:B:49:C:H6	1.81	0.45
6:F:92:ARG:HA	6:F:96:MET:HB2	1.96	0.45
17:R:98:ILE:HG22	17:R:106:PHE:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:176:C:H4'	51:t:24:ARG:HH21	1.82	0.45
32:a:1249:C:N4	32:a:1287:A:H3'	2.31	0.45
32:a:1413:A:H2'	32:a:1414:U:O4'	2.16	0.45
48:q:59:VAL:HG21	48:q:75:LEU:HD22	1.98	0.45
1:A:209:C:H4'	1:A:681:G:H4'	1.97	0.45
1:A:351:C:H2'	1:A:352:A:O4'	2.16	0.45
1:A:1018:U:H3	1:A:1144:A:H61	1.65	0.45
1:A:1266:G:O2'	1:A:2012:G:O6	2.29	0.45
1:A:1678:A:H2'	1:A:1679:A:O4'	2.15	0.45
1:A:1847:A:O2'	1:A:1848:A:H5''	2.16	0.45
1:A:2887:A:H2'	1:A:2888:C:H6	1.81	0.45
32:a:113:G:H1'	32:a:354:G:H5'	1.98	0.45
32:a:560:A:H5'	32:a:566:G:N2	2.32	0.45
32:a:600:A:H5'	39:h:122:GLY:H	1.82	0.45
32:a:663:A:H2'	32:a:664:G:O4'	2.16	0.45
32:a:1321:U:H4'	44:m:86:TYR:CE1	2.52	0.45
37:f:38:ARG:HE	37:f:61:LEU:HD21	1.81	0.45
1:A:599:A:H2'	1:A:600:G:O4'	2.16	0.45
1:A:2385:C:H2'	1:A:2386:A:H8	1.81	0.45
1:A:2471:A:H2'	1:A:2472:G:O4'	2.16	0.45
1:A:2837:A:H2'	1:A:2838:G:H8	1.80	0.45
11:L:18:ARG:H	11:L:45:GLU:HB3	1.80	0.45
32:a:1169:A:H2'	32:a:1170:A:C8	2.52	0.45
32:a:1303:C:H2'	32:a:1304:G:C8	2.52	0.45
32:a:1410:A:H2'	32:a:1411:C:C6	2.51	0.45
55:x:60:U:H5'	55:x:61:C:H5	1.81	0.45
1:A:529:A:OP2	10:K:113:PRO:HD3	2.17	0.45
1:A:587:C:C6	1:A:671:C:H1'	2.51	0.45
1:A:752:A:H62	1:A:2609:U:H3	1.64	0.45
1:A:1385:A:H1'	1:A:1386:C:C6	2.52	0.45
10:K:34:ARG:HG3	10:K:39:LYS:HB2	1.97	0.45
32:a:518:C:C5	32:a:529:G:H3'	2.51	0.45
32:a:1313:U:H2'	32:a:1314:C:H6	1.82	0.45
40:i:84:THR:HB	40:i:98:LEU:HD21	1.99	0.45
42:k:67:ALA:HB2	42:k:96:THR:HG22	1.98	0.45
1:A:886:A:H1'	1:A:889:C:C5	2.43	0.45
1:A:991:C:H42	1:A:1163:G:H1	1.64	0.45
1:A:992:C:H2'	1:A:993:G:O4'	2.17	0.45
1:A:1056:G:H5''	1:A:1057:A:O4'	2.17	0.45
1:A:1436:G:H2'	1:A:1437:C:O4'	2.16	0.45
1:A:1700:A:H3'	1:A:1701:A:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2025:C:H42	1:A:2038:G:H1	1.65	0.45
5:E:117:ARG:HD3	12:M:1:MET:HE3	1.99	0.45
10:K:32:LEU:HD22	10:K:54:ILE:HG21	1.98	0.45
21:V:39:ILE:HG22	21:V:40:ASN:HD22	1.80	0.45
32:a:10:A:H2'	32:a:11:G:C8	2.49	0.45
32:a:371:A:O2'	32:a:373:A:N7	2.50	0.45
32:a:696:A:N3	32:a:786:G:O2'	2.48	0.45
32:a:917:G:H2'	32:a:918:A:H8	1.80	0.45
32:a:1049:U:C6	32:a:1201:A:H1'	2.51	0.45
32:a:1341:U:H2'	32:a:1342:C:H6	1.82	0.45
33:b:60:ILE:HD13	33:b:160:ALA:HB2	1.97	0.45
38:g:32:VAL:C	38:g:34:GLY:H	2.24	0.45
38:g:47:LEU:HD23	38:g:58:GLU:HB3	1.99	0.45
40:i:84:THR:HG21	40:i:103:PHE:HB3	1.99	0.45
42:k:23:ILE:HD11	42:k:86:VAL:HG22	1.98	0.45
42:k:116:ILE:HD11	52:u:28:VAL:HG13	1.99	0.45
43:l:73:ASN:HD21	43:l:104:CYS:HA	1.81	0.45
1:A:1859:U:H2'	1:A:1860:G:C8	2.51	0.45
1:A:2396:G:H1	1:A:2420:C:H42	1.64	0.45
1:A:2647:U:H2'	1:A:2648:G:H8	1.79	0.45
1:A:2880:C:H2'	1:A:2881:U:H6	1.75	0.45
32:a:341:C:H2'	32:a:342:C:C6	2.52	0.45
32:a:549:C:H2'	32:a:550:G:C8	2.52	0.45
32:a:559:A:H4'	32:a:560:A:H3'	1.99	0.45
32:a:567:G:H2'	32:a:568:G:O4'	2.17	0.45
32:a:663:A:H2'	32:a:664:G:C8	2.52	0.45
32:a:682:G:H1	32:a:708:C:H42	1.63	0.45
35:d:130:VAL:HG12	35:d:132:ILE:H	1.82	0.45
42:k:24:HIS:HB3	42:k:31:ILE:HB	1.99	0.45
1:A:1722:A:N6	1:A:1737:G:H1	2.14	0.45
1:A:2062:A:N6	1:A:2503:A:N6	2.65	0.45
1:A:2244:U:H2'	1:A:2245:U:C6	2.52	0.45
1:A:2875:C:H2'	1:A:2876:G:H8	1.82	0.45
19:T:86:MET:HA	19:T:87:PRO:HD2	1.85	0.45
32:a:33:A:H2	43:l:29:GLN:HE22	1.65	0.45
32:a:233:C:H2'	32:a:234:C:H6	1.82	0.45
32:a:548:G:H2'	32:a:549:C:O4'	2.17	0.45
34:c:14:ILE:HG13	34:c:178:LEU:HD12	1.99	0.45
1:A:221:A:H61	1:A:428:A:H62	1.65	0.45
1:A:417:C:H2'	1:A:418:C:H6	1.82	0.45
1:A:1806:C:H2'	1:A:1807:G:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2680:U:H2'	1:A:2681:C:C6	2.51	0.45
19:T:83:LYS:HD3	19:T:95:ARG:HD2	1.99	0.45
32:a:52:C:H2'	32:a:53:A:H8	1.81	0.45
32:a:333:U:H2'	32:a:334:C:C6	2.52	0.45
32:a:1322:C:O2	32:a:1322:C:O4'	2.33	0.45
32:a:1443:C:H2'	32:a:1444:U:C6	2.52	0.45
1:A:766:U:H2'	1:A:767:U:C6	2.52	0.45
1:A:1939:5MU:H3'	1:A:1940:U:C5'	2.46	0.45
1:A:1998:A:H2'	1:A:1999:C:C6	2.52	0.45
1:A:2194:U:H2'	1:A:2195:U:C6	2.52	0.45
4:D:142:VAL:HG23	4:D:144:GLY:H	1.82	0.45
11:L:71:ARG:HH22	16:Q:32:VAL:HG12	1.82	0.45
21:V:41:LEU:HB3	21:V:60:GLU:HG2	1.99	0.45
32:a:62:U:H2'	32:a:63:C:H6	1.79	0.45
55:y:0:C:H2'	55:y:1:G:H8	1.82	0.45
1:A:536:G:H1	1:A:557:C:H42	1.65	0.44
1:A:839:U:H2'	1:A:840:C:C6	2.51	0.44
1:A:1815:A:O4'	1:A:1817:G:H1'	2.16	0.44
1:A:1935:G:H1'	1:A:1964:G:N2	2.31	0.44
1:A:2227:A:H2'	1:A:2228:G:O4'	2.17	0.44
1:A:2630:G:H2'	1:A:2631:G:C8	2.52	0.44
4:D:109:VAL:HG22	4:D:203:VAL:HG13	1.97	0.44
8:H:15:LEU:HD21	8:H:56:ALA:HB1	1.97	0.44
19:T:36:LEU:HD22	19:T:47:VAL:HG13	2.00	0.44
32:a:660:C:N4	32:a:745:G:H1	2.14	0.44
32:a:1075:U:H2'	32:a:1076:U:C6	2.52	0.44
34:c:55:ILE:HG22	34:c:68:ILE:HA	1.98	0.44
39:h:13:ARG:HD2	39:h:27:MET:HB3	1.98	0.44
55:y:62:C:H2'	55:y:63:G:H8	1.83	0.44
1:A:373:U:H4'	1:A:423:A:O2'	2.17	0.44
1:A:694:U:H5''	1:A:1569:A:C6	2.52	0.44
1:A:2038:G:H2'	1:A:2039:U:C6	2.52	0.44
1:A:2617:U:H2'	1:A:2618:G:O4'	2.17	0.44
3:C:13:ARG:HG3	3:C:13:ARG:HH11	1.81	0.44
32:a:19:A:H5''	36:e:91:GLY:HA3	1.99	0.44
32:a:233:C:H2'	32:a:234:C:C6	2.51	0.44
35:d:94:LEU:O	35:d:97:ARG:HB2	2.17	0.44
1:A:52:A:H2'	1:A:53:A:C8	2.52	0.44
1:A:207:A:H2'	1:A:208:C:O4'	2.18	0.44
1:A:1077:A:H61	1:A:1088:A:H3'	1.81	0.44
1:A:1149:G:H2'	1:A:1150:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1997:C:H2'	1:A:1998:A:C8	2.53	0.44
1:A:2189:U:H2'	1:A:2190:G:H8	1.80	0.44
1:A:2742:G:H1	1:A:2762:C:H42	1.66	0.44
1:A:2843:G:H1	1:A:2874:C:H42	1.65	0.44
3:C:159:GLY:H	3:C:195:VAL:HB	1.83	0.44
4:D:51:THR:HG21	4:D:68:PHE:HE1	1.81	0.44
7:G:95:ARG:HH12	7:G:129:THR:HG23	1.83	0.44
13:N:41:LEU:HD11	13:N:102:LEU:HD22	1.98	0.44
18:S:38:VAL:HB	18:S:59:ILE:HD11	1.98	0.44
21:V:40:ASN:HB3	21:V:63:ALA:HB3	2.00	0.44
32:a:53:A:H2'	32:a:54:C:O4'	2.18	0.44
32:a:309:A:H2'	32:a:310:G:H8	1.83	0.44
32:a:695:A:H2'	32:a:696:A:C8	2.52	0.44
32:a:838:G:H2'	32:a:839:C:H6	1.82	0.44
32:a:968:A:C8	32:a:1062:U:H4'	2.53	0.44
32:a:1507:A:H2'	32:a:1508:A:H8	1.83	0.44
34:c:26:THR:HG23	45:n:76:LYS:HD2	1.99	0.44
38:g:32:VAL:HG22	38:g:33:ASP:H	1.82	0.44
1:A:694:U:H5''	1:A:1569:A:C5	2.52	0.44
1:A:780:G:H2'	1:A:782:A:N7	2.33	0.44
1:A:934:U:H2'	1:A:935:C:H6	1.82	0.44
1:A:2884:U:H3'	1:A:2885:G:H21	1.82	0.44
3:C:138:GLY:H	3:C:164:ILE:HB	1.82	0.44
21:V:34:VAL:HG13	21:V:67:VAL:HG22	1.99	0.44
32:a:45:G:H2'	32:a:46:G:H8	1.78	0.44
32:a:617:G:H1	32:a:623:C:H42	1.64	0.44
32:a:720:C:OP1	49:r:41:PRO:HG3	2.18	0.44
32:a:974:A:H5''	45:n:71:HIS:HB3	1.99	0.44
32:a:1095:U:H2'	32:a:1096:C:O4'	2.17	0.44
32:a:1170:A:H2'	32:a:1171:A:O4'	2.18	0.44
32:a:1513:A:H2'	32:a:1514:G:H8	1.82	0.44
38:g:150:ALA:CB	42:k:59:THR:HG21	2.41	0.44
1:A:131:A:H2'	1:A:132:G:C8	2.52	0.44
1:A:596:U:H2'	1:A:597:G:C8	2.52	0.44
1:A:1811:G:H2'	1:A:1812:U:H6	1.81	0.44
1:A:2078:C:H2'	1:A:2079:U:H6	1.82	0.44
1:A:2461:A:H2'	1:A:2462:C:C6	2.52	0.44
6:F:100:PHE:O	6:F:104:ILE:HG12	2.17	0.44
9:J:53:PRO:HD2	9:J:77:VAL:HG11	1.99	0.44
32:a:26:A:H61	32:a:558:G:H1'	1.82	0.44
32:a:1511:G:H2'	32:a:1512:U:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:q:21:ILE:HG22	48:q:46:VAL:HB	1.99	0.44
51:t:15:GLU:HG2	51:t:19:LYS:HE2	2.00	0.44
1:A:27:G:C2	1:A:512:G:N3	2.85	0.44
1:A:1137:G:H2'	1:A:1138:G:H8	1.82	0.44
1:A:1518:C:H2'	1:A:1519:G:H8	1.83	0.44
1:A:2645:G:H3'	1:A:2646:C:H5'	1.98	0.44
32:a:459:A:N6	32:a:473:U:H3	2.15	0.44
32:a:923:A:H5'	36:e:26:LYS:HB2	1.98	0.44
32:a:1307:U:H2'	32:a:1308:U:C6	2.53	0.44
32:a:1443:C:H2'	32:a:1444:U:O4'	2.18	0.44
42:k:33:THR:HG23	42:k:44:TRP:HB3	2.00	0.44
43:l:56:ARG:HH22	43:l:62:GLU:HB2	1.83	0.44
47:p:8:ARG:H	47:p:28:ARG:HH22	1.66	0.44
53:v:263:ILE:HG22	53:v:291:MET:HE3	1.99	0.44
1:A:585:G:O2'	5:E:77:ILE:HG22	2.18	0.44
1:A:895:U:H3	1:A:897:C:N4	2.16	0.44
1:A:1055:G:H2'	1:A:1056:G:O4'	2.17	0.44
1:A:1277:G:H2'	1:A:1278:C:C6	2.52	0.44
1:A:1723:G:O6	1:A:1737:G:N2	2.51	0.44
1:A:2024:G:OP2	1:A:2034:U:H4'	2.18	0.44
22:W:25:LYS:HG2	22:W:43:ASP:HA	2.00	0.44
32:a:197:A:N3	32:a:198:G:H1'	2.33	0.44
32:a:405:U:H5''	32:a:495:A:H2	1.81	0.44
32:a:922:G:H2'	32:a:923:A:C8	2.52	0.44
32:a:1001:C:H2'	32:a:1002:G:C8	2.53	0.44
32:a:1036:A:H2'	32:a:1036:A:N3	2.32	0.44
32:a:1106:G:H2'	32:a:1107:C:C6	2.52	0.44
1:A:154:U:H2'	1:A:155:A:C8	2.53	0.44
1:A:297:G:H2'	1:A:298:G:O4'	2.18	0.44
1:A:346:A:H2'	1:A:347:A:O4'	2.17	0.44
1:A:692:C:H2'	1:A:693:A:C8	2.53	0.44
1:A:1278:C:H2'	1:A:1279:G:C8	2.53	0.44
1:A:1849:G:H2'	1:A:1850:G:H8	1.83	0.44
1:A:1959:G:H2'	1:A:1960:A:O4'	2.18	0.44
1:A:2448:A:H3'	1:A:2449:U:H2'	1.99	0.44
1:A:2638:G:H22	1:A:2775:G:H2'	1.83	0.44
27:1:9:THR:HB	27:1:11:SER:H	1.83	0.44
28:2:24:THR:HG23	30:4:34:THR:HG21	2.00	0.44
32:a:440:C:H42	32:a:497:G:H1	1.66	0.44
32:a:918:A:H2'	32:a:919:A:O4'	2.17	0.44
32:a:1097:C:H4'	33:b:139:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:c:12:LEU:HD11	45:n:97:LYS:HA	1.99	0.44
38:g:27:VAL:HG12	38:g:43:VAL:HG21	1.99	0.44
40:i:13:LYS:H	40:i:106:ARG:HH12	1.65	0.44
1:A:588:U:H2'	1:A:589:U:H6	1.78	0.44
1:A:824:U:H3	1:A:833:A:H61	1.64	0.44
1:A:1447:C:H2'	1:A:1448:G:C8	2.53	0.44
1:A:1477:A:C5	1:A:1478:G:H1'	2.53	0.44
1:A:2140:G:H2'	1:A:2141:G:O4'	2.17	0.44
1:A:2270:A:H2'	1:A:2271:G:O4'	2.18	0.44
2:B:30:C:H3'	2:B:31:C:H6	1.83	0.44
5:E:41:GLN:HB3	5:E:43:THR:HG23	1.99	0.44
14:O:103:ARG:HB3	14:O:108:ALA:HB3	2.00	0.44
32:a:385:C:H2'	32:a:386:C:C6	2.53	0.44
32:a:1117:A:N6	32:a:1156:G:H22	2.15	0.44
32:a:1464:U:H2'	32:a:1465:A:C8	2.53	0.44
51:t:4:ILE:HG22	51:t:7:ALA:H	1.83	0.44
1:A:698:C:H5''	1:A:699:A:H5'	2.00	0.43
1:A:780:G:H21	1:A:783:A:H62	1.66	0.43
1:A:863:A:H4'	2:B:100:G:H21	1.82	0.43
1:A:1216:G:H2'	1:A:1217:U:O4'	2.18	0.43
1:A:1773:A:H2'	1:A:1774:C:O4'	2.17	0.43
1:A:2685:G:H4'	11:L:78:ARG:HH22	1.83	0.43
32:a:32:A:H2	32:a:552:U:N3	2.12	0.43
32:a:61:G:H2'	32:a:62:U:O4'	2.18	0.43
32:a:449:G:H1	32:a:484:G:H1	1.66	0.43
32:a:668:G:H2'	32:a:669:G:C8	2.53	0.43
32:a:957:U:H5''	50:s:81:ARG:HH11	1.83	0.43
32:a:1001:C:H2'	32:a:1002:G:H8	1.83	0.43
1:A:1353:A:H2'	1:A:1354:A:H8	1.79	0.43
1:A:1724:G:H2'	1:A:1725:U:C6	2.52	0.43
1:A:1744:A:H3'	1:A:1745:A:C8	2.51	0.43
1:A:2060:A:O4'	1:A:2502:G:O4'	2.36	0.43
1:A:2543:G:H21	1:A:2646:C:H5''	1.83	0.43
4:D:122:VAL:HA	4:D:127:PHE:HB2	2.00	0.43
16:Q:7:GLN:O	16:Q:10:GLN:HG2	2.17	0.43
32:a:129:A:O2'	32:a:130:A:H2'	2.18	0.43
32:a:441:A:H61	32:a:493:A:H61	1.66	0.43
32:a:558:G:C8	32:a:559:A:H2'	2.53	0.43
32:a:601:G:H2'	32:a:602:A:H8	1.83	0.43
32:a:628:G:H2'	32:a:629:A:C8	2.52	0.43
32:a:940:C:H4'	32:a:1374:A:H2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1223:C:OP1	32:a:1225:A:H8	2.01	0.43
32:a:1457:G:O2'	51:t:27:MET:HB2	2.17	0.43
32:a:1458:G:H2'	32:a:1459:G:C8	2.53	0.43
38:g:99:LEU:HA	38:g:102:ARG:HD2	2.00	0.43
39:h:29:SER:HB3	39:h:57:PRO:HB2	2.00	0.43
1:A:609:A:H62	1:A:619:G:H21	1.67	0.43
1:A:754:U:H2'	1:A:755:U:H6	1.81	0.43
1:A:1515:A:H3'	1:A:1516:G:H8	1.84	0.43
1:A:1860:G:H1	1:A:1882:U:H3	1.64	0.43
32:a:390:U:H2'	32:a:391:G:C8	2.53	0.43
32:a:564:C:H5	43:l:12:ARG:HH22	1.66	0.43
32:a:676:A:H2'	32:a:677:U:C6	2.53	0.43
40:i:17:ALA:HB2	40:i:67:VAL:HG23	2.00	0.43
49:r:73:ARG:H	49:r:73:ARG:HG3	1.69	0.43
1:A:838:C:H2'	1:A:839:U:C6	2.53	0.43
1:A:1264:A:OP1	27:1:16:ARG:NH1	2.49	0.43
1:A:2453:A:N6	1:A:2499:C:H42	2.16	0.43
2:B:2:G:H1	2:B:118:C:H42	1.67	0.43
2:B:2:G:H2'	2:B:3:C:C6	2.53	0.43
12:M:107:PHE:HB3	12:M:126:ARG:HH11	1.83	0.43
24:Y:14:THR:HG22	24:Y:28:ARG:HG2	2.00	0.43
32:a:552:U:C2	32:a:553:A:C8	3.07	0.43
32:a:562:U:H1'	43:l:12:ARG:HB3	2.01	0.43
32:a:616:G:H2'	32:a:617:G:C8	2.52	0.43
32:a:802:A:H2'	32:a:803:G:O4'	2.18	0.43
1:A:92:U:H3'	1:A:93:G:H8	1.83	0.43
1:A:173:A:H2'	1:A:174:U:C6	2.53	0.43
1:A:213:A:H2'	1:A:214:G:C8	2.53	0.43
1:A:371:A:H1'	24:Y:61:LYS:HZ1	1.84	0.43
1:A:468:G:H2'	1:A:469:G:O4'	2.18	0.43
1:A:553:G:H2'	1:A:554:U:O4'	2.18	0.43
1:A:734:A:O2'	1:A:1635:A:H4'	2.19	0.43
1:A:749:A:H4'	1:A:1271:G:N3	2.34	0.43
1:A:1408:G:H3'	1:A:1409:U:H5''	2.00	0.43
1:A:1652:A:H3'	1:A:1653:G:H8	1.83	0.43
1:A:2016:U:H2'	1:A:2017:U:H6	1.81	0.43
1:A:2244:U:O4	1:A:2436:G:O6	2.36	0.43
1:A:2584:U:H2'	1:A:2585:U:H2'	2.00	0.43
1:A:2681:C:C4	1:A:2724:U:C4	3.06	0.43
2:B:101:A:H2'	2:B:102:G:O4'	2.18	0.43
5:E:102:ARG:HE	5:E:200:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:552:U:H2'	32:a:553:A:O4'	2.17	0.43
32:a:961:U:O4	32:a:974:A:C2	2.69	0.43
32:a:978:A:O2'	32:a:979:C:H5'	2.18	0.43
32:a:1010:U:H2'	32:a:1011:C:C6	2.54	0.43
32:a:1493:A:H3'	32:a:1493:A:P	2.58	0.43
37:f:71:ILE:HA	37:f:74:LEU:HD12	1.99	0.43
44:m:16:VAL:O	44:m:20:THR:HG23	2.18	0.43
1:A:236:C:H2'	1:A:237:C:H6	1.81	0.43
1:A:728:G:H4'	3:C:13:ARG:HE	1.82	0.43
1:A:1442:U:H2'	1:A:1443:U:O4'	2.18	0.43
1:A:2233:U:H2'	1:A:2234:G:H8	1.83	0.43
32:a:283:U:H2'	32:a:284:C:C6	2.53	0.43
32:a:318:G:H2'	32:a:319:G:O4'	2.18	0.43
32:a:329:A:H2'	32:a:332:G:N7	2.32	0.43
32:a:988:G:H1'	32:a:1014:A:H61	1.84	0.43
32:a:1117:A:O3'	40:i:106:ARG:HD2	2.18	0.43
32:a:1336:C:H4'	32:a:1337:G:H5'	2.01	0.43
40:i:15:SER:HB2	40:i:70:GLY:HA3	2.01	0.43
1:A:1050:A:H2'	1:A:1051:G:O4'	2.18	0.43
1:A:1585:C:O2	1:A:1585:C:H2'	2.18	0.43
1:A:1654:A:C8	1:A:2823:A:O4'	2.72	0.43
1:A:1708:C:H2'	1:A:1709:U:C6	2.53	0.43
1:A:1790:C:H3'	1:A:1828:G:N2	2.34	0.43
1:A:2099:U:H2'	1:A:2100:G:H8	1.83	0.43
1:A:2835:A:N6	1:A:2878:U:H2'	2.33	0.43
11:L:23:LYS:HB3	11:L:40:LYS:HB3	2.01	0.43
32:a:461:A:H2'	32:a:462:G:C8	2.53	0.43
32:a:703:G:H4'	32:a:704:A:H8	1.84	0.43
35:d:92:ALA:HA	35:d:186:PRO:HG2	1.99	0.43
44:m:9:ILE:HD11	44:m:22:ILE:HD11	2.00	0.43
1:A:16:C:H2'	1:A:17:G:H8	1.83	0.43
1:A:271:G:H4'	1:A:272:A:OP1	2.18	0.43
1:A:511:U:H5'	1:A:1236:G:OP1	2.18	0.43
1:A:586:A:N1	1:A:809:G:O2'	2.49	0.43
1:A:859:G:N2	1:A:916:G:H2'	2.34	0.43
1:A:1199:U:H2'	1:A:1200:C:C6	2.54	0.43
1:A:1946:U:H2'	1:A:1947:C:C6	2.53	0.43
1:A:2811:G:H1	1:A:2889:C:N4	2.15	0.43
32:a:526:C:H3'	32:a:526:C:H6	1.83	0.43
32:a:689:C:H2'	32:a:690:G:C8	2.54	0.43
32:a:866:C:H2'	32:a:867:G:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:c:174:PRO:HD2	34:c:182:ILE:HD11	2.01	0.43
51:t:27:MET:HE3	51:t:57:ILE:HG12	1.99	0.43
1:A:1993:U:H4'	4:D:133:THR:CG2	2.49	0.43
1:A:2070:A:C6	1:A:2442:C:N3	2.86	0.43
1:A:2110:G:H5'	1:A:2118:U:O2'	2.19	0.43
1:A:2633:G:H2'	1:A:2634:A:O4'	2.18	0.43
9:J:24:GLY:HA3	9:J:25:PRO:HD3	1.81	0.43
32:a:32:A:N1	32:a:552:U:C4	2.87	0.43
32:a:102:G:H2'	32:a:103:U:H6	1.82	0.43
32:a:200:G:H1	32:a:217:C:N4	2.17	0.43
32:a:1069:C:H42	32:a:1106:G:H1	1.66	0.43
32:a:1308:U:H2'	32:a:1309:G:C8	2.53	0.43
36:e:16:ILE:HD12	36:e:36:LEU:HG	2.00	0.43
37:f:88:MET:HE1	49:r:61:ARG:HA	2.01	0.43
41:j:80:THR:HB	41:j:83:THR:HG22	2.01	0.43
44:m:7:ILE:HD11	44:m:22:ILE:HA	2.00	0.43
50:s:18:LYS:HB3	50:s:31:LEU:HD21	2.00	0.43
52:u:43:THR:O	52:u:47:ARG:HG3	2.19	0.43
1:A:676:A:H2	1:A:2069:G:O2'	2.02	0.43
1:A:1379:U:H4'	1:A:1380:G:OP1	2.19	0.43
1:A:2361:G:H2'	1:A:2362:C:O4'	2.19	0.43
1:A:2386:A:H4'	23:X:56:ASP:HA	2.00	0.43
1:A:2591:C:H2'	1:A:2592:G:C8	2.54	0.43
1:A:2639:A:H2'	1:A:2640:G:O4'	2.19	0.43
1:A:2784:U:H2'	1:A:2785:C:H6	1.84	0.43
4:D:107:VAL:HG12	4:D:205:PRO:HA	2.00	0.43
17:R:62:ILE:HG12	17:R:76:TYR:OH	2.19	0.43
32:a:644:U:H2'	32:a:645:G:O4'	2.18	0.43
34:c:85:GLU:HA	34:c:88:ARG:HD3	2.00	0.43
1:A:118:A:H2'	1:A:120:U:O4	2.18	0.42
1:A:676:A:C2	1:A:2070:A:O4'	2.72	0.42
1:A:984:A:H2'	1:A:984:A:N3	2.33	0.42
1:A:1182:G:H2'	1:A:1183:U:O4'	2.19	0.42
7:G:73:ASN:O	7:G:77:ILE:HG12	2.19	0.42
14:O:21:PHE:CZ	14:O:43:GLU:HB3	2.54	0.42
32:a:203:G:H1'	32:a:466:A:C2	2.54	0.42
32:a:530:G:C6	54:w:30:GLU:HA	2.54	0.42
32:a:961:U:H2'	32:a:962:C:O4'	2.19	0.42
38:g:115:SER:HB3	38:g:118:LEU:HB2	2.00	0.42
40:i:11:ARG:HB2	40:i:106:ARG:HG3	2.00	0.42
43:l:33:VAL:HG22	43:l:79:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:G:H1	1:A:427:U:H3'	1.84	0.42
1:A:493:G:H2'	1:A:494:G:O4'	2.19	0.42
1:A:1531:C:H2'	1:A:1532:A:C8	2.54	0.42
1:A:1789:A:H2'	1:A:1790:C:O4'	2.18	0.42
1:A:1914:C:O4'	54:w:18:ALA:HB2	2.19	0.42
1:A:2051:A:H4'	4:D:146:ILE:HG12	2.01	0.42
1:A:2247:A:H2'	1:A:2248:C:C6	2.54	0.42
1:A:2286:G:H4'	1:A:2287:A:O5'	2.19	0.42
1:A:2435:A:H2'	1:A:2436:G:O4'	2.19	0.42
1:A:2650:U:H2'	1:A:2651:C:C6	2.53	0.42
9:J:73:PRO:HA	9:J:74:PRO:HD3	1.92	0.42
25:Z:18:LEU:HB2	25:Z:53:VAL:HG11	2.01	0.42
30:4:33:LEU:HD22	30:4:41:LYS:HD3	2.01	0.42
32:a:200:G:H2'	32:a:201:G:H8	1.85	0.42
32:a:254:G:H2'	32:a:255:G:H8	1.83	0.42
32:a:526:C:O5'	32:a:526:C:C6	2.72	0.42
32:a:786:G:H2'	32:a:787:A:O4'	2.19	0.42
32:a:1237:C:H42	32:a:1337:G:H1	1.66	0.42
32:a:1526:G:H2'	32:a:1527:U:C6	2.54	0.42
38:g:91:VAL:HG13	38:g:96:ARG:HE	1.84	0.42
47:p:54:LEU:HA	47:p:57:ILE:HD12	2.01	0.42
1:A:414:C:H1'	1:A:1864:U:O2	2.19	0.42
1:A:1662:U:H2'	1:A:1663:G:O4'	2.19	0.42
1:A:1719:G:H2'	1:A:1720:U:O4'	2.19	0.42
1:A:2439:A:H5'	1:A:2441:U:O5'	2.19	0.42
1:A:2646:C:H42	1:A:2674:G:H1	1.66	0.42
1:A:2786:U:H2'	1:A:2787:C:C6	2.54	0.42
32:a:340:U:H2'	32:a:341:C:O4'	2.19	0.42
35:d:61:VAL:HA	35:d:64:ILE:HD12	2.01	0.42
55:x:53:G:H2'	55:x:54:U:H6	1.83	0.42
1:A:452:G:H2'	1:A:453:A:C8	2.54	0.42
1:A:826:U:O2'	12:M:53:GLY:HA3	2.19	0.42
1:A:1199:U:H2'	1:A:1200:C:O4'	2.19	0.42
1:A:1265:A:O3'	1:A:1266:G:H4'	2.19	0.42
1:A:1669:A:H2'	1:A:1669:A:N3	2.34	0.42
1:A:1726:C:N4	1:A:1734:G:H1	2.17	0.42
1:A:1849:G:H2'	1:A:1850:G:C8	2.55	0.42
1:A:2679:A:H2'	1:A:2680:U:O4'	2.20	0.42
2:B:42:C:H2'	2:B:43:C:C6	2.55	0.42
32:a:473:U:H2'	32:a:474:G:O4'	2.20	0.42
32:a:764:C:H5''	46:o:50:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:775:G:H2'	32:a:776:G:O4'	2.19	0.42
32:a:928:G:H2'	32:a:929:G:O4'	2.19	0.42
32:a:1114:C:H2'	32:a:1115:U:H6	1.83	0.42
32:a:1329:A:H5'	44:m:29:ARG:HG3	2.02	0.42
36:e:133:PRO:O	36:e:136:VAL:HG12	2.19	0.42
1:A:610:C:H2'	1:A:611:C:C6	2.55	0.42
1:A:918:A:H2'	1:A:919:U:O4'	2.20	0.42
1:A:2856:A:H2'	1:A:2857:G:O4'	2.20	0.42
32:a:310:G:H2'	32:a:311:C:C6	2.54	0.42
32:a:556:C:H2'	32:a:557:G:O4'	2.19	0.42
32:a:925:G:H1'	32:a:1502:A:C4	2.54	0.42
32:a:1372:U:H2'	32:a:1373:G:O4'	2.20	0.42
33:b:46:THR:HG23	33:b:201:PRO:HD2	1.99	0.42
48:q:19:LYS:HE3	48:q:50:ASN:H	1.84	0.42
1:A:1463:C:H2'	1:A:1464:G:C8	2.55	0.42
1:A:2724:U:H2'	1:A:2725:A:C8	2.55	0.42
1:A:2741:A:H2'	1:A:2742:G:O4'	2.19	0.42
6:F:29:PRO:HB2	6:F:169:LEU:HD22	2.00	0.42
32:a:765:G:H3'	32:a:812:G:H22	1.84	0.42
32:a:1360:A:C2'	32:a:1361:G:H5'	2.50	0.42
53:v:324:ARG:HH21	53:v:356:PHE:HB3	1.84	0.42
1:A:610:C:H42	1:A:618:G:H1	1.68	0.42
1:A:1388:G:H1	1:A:1399:C:H42	1.66	0.42
1:A:1995:U:H3'	1:A:1996:C:H2'	2.02	0.42
32:a:625:U:H2'	32:a:626:G:C8	2.55	0.42
32:a:1068:G:N7	32:a:1094:G:H2'	2.35	0.42
34:c:57:ILE:HG12	34:c:66:VAL:HG22	2.01	0.42
37:f:51:ILE:HG22	37:f:52:ASN:HD22	1.84	0.42
1:A:76:C:H2'	1:A:77:G:C8	2.54	0.42
1:A:215:G:O3'	1:A:216:A:H4'	2.19	0.42
1:A:289:G:H2'	1:A:290:U:H6	1.84	0.42
1:A:409:G:H2'	1:A:410:G:C8	2.55	0.42
1:A:700:G:H1	1:A:732:C:H42	1.66	0.42
1:A:1816:C:H3'	3:C:62:TYR:HE1	1.84	0.42
1:A:2407:A:N3	1:A:2407:A:H2'	2.34	0.42
1:A:2861:U:H2'	1:A:2862:G:C8	2.55	0.42
3:C:44:ASN:HD21	3:C:46:ASN:HB2	1.85	0.42
19:T:10:ALA:HB3	19:T:101:SER:HB2	2.01	0.42
46:o:32:LEU:HD13	46:o:63:ARG:HB2	2.00	0.42
1:A:64:A:H2'	1:A:65:U:C6	2.55	0.42
1:A:514:A:N3	1:A:581:C:O2'	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:U:H6	1:A:788:A:N1	2.18	0.42
1:A:802:A:H2'	1:A:803:U:O4'	2.19	0.42
1:A:1117:C:O2'	1:A:1118:C:C6	2.73	0.42
1:A:1406:U:C4	1:A:1596:A:N1	2.88	0.42
1:A:1418:G:C2	1:A:1579:A:N7	2.88	0.42
1:A:1741:C:H2'	1:A:1742:U:O4'	2.20	0.42
1:A:2013:A:C2	1:A:2613:U:O4	2.64	0.42
1:A:2637:U:H3'	1:A:2638:G:H8	1.85	0.42
1:A:2638:G:N2	1:A:2775:G:H2'	2.35	0.42
3:C:147:LYS:HD2	3:C:150:LYS:HD2	2.02	0.42
4:D:14:ILE:HG12	4:D:24:VAL:HG21	2.01	0.42
14:O:28:LEU:HD23	14:O:48:VAL:HG21	2.01	0.42
17:R:62:ILE:HG23	17:R:76:TYR:CZ	2.55	0.42
21:V:26:LYS:HD3	21:V:37:GLU:HB3	2.01	0.42
32:a:151:A:H3'	32:a:152:A:H8	1.84	0.42
32:a:202:G:O2'	32:a:468:A:H8	2.00	0.42
32:a:840:C:H3'	32:a:841:C:C5'	2.50	0.42
32:a:1187:G:H1'	45:n:100:SER:OG	2.19	0.42
32:a:1484:C:H2'	32:a:1485:U:O4'	2.20	0.42
34:c:7:PRO:HD2	34:c:184:TYR:CD2	2.55	0.42
1:A:2002:G:OP1	14:O:13:ASN:HA	2.19	0.42
1:A:2061:G:C4'	1:A:2503:A:C2	3.03	0.42
1:A:2600:A:H2'	1:A:2601:C:C6	2.55	0.42
2:B:104:A:H1'	22:W:31:TYR:HE2	1.85	0.42
14:O:66:ALA:C	14:O:68:ALA:N	2.78	0.42
30:4:62:LEU:HB3	30:4:65:ALA:HB3	2.02	0.42
31:5:2:LYS:HB2	31:5:35:GLN:HG2	2.01	0.42
32:a:450:G:N2	32:a:483:C:N3	2.64	0.42
32:a:715:A:H2'	32:a:716:A:H8	1.81	0.42
45:n:82:ILE:H	45:n:82:ILE:HG13	1.62	0.42
55:y:29:G:H1	55:y:41:C:H42	1.68	0.42
1:A:327:G:H2'	1:A:328:U:C6	2.55	0.41
1:A:677:A:H4'	1:A:2070:A:O2'	2.20	0.41
1:A:1515:A:H2'	1:A:1516:G:O4'	2.20	0.41
1:A:1518:C:H2'	1:A:1519:G:C8	2.55	0.41
1:A:1835:2MG:H2'	1:A:1836:C:C6	2.55	0.41
1:A:2813:A:H2'	1:A:2814:A:C8	2.55	0.41
21:V:47:LYS:HA	21:V:48:PRO:HD3	1.94	0.41
24:Y:15:GLY:HA3	24:Y:29:PHE:HE1	1.85	0.41
32:a:46:G:H1	32:a:395:C:H42	1.68	0.41
32:a:419:C:H2'	32:a:420:U:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1011:C:H2'	32:a:1012:A:H8	1.84	0.41
53:v:150:ARG:O	53:v:154:ARG:HG2	2.20	0.41
1:A:272:A:H2'	1:A:273:G:H8	1.84	0.41
1:A:1266:G:O6	19:T:13:SER:HB3	2.21	0.41
1:A:1446:C:H42	1:A:1465:G:H1	1.67	0.41
1:A:1511:G:H2'	1:A:1512:C:H6	1.85	0.41
1:A:1973:G:H2'	1:A:1974:C:O4'	2.20	0.41
1:A:2527:C:H5'	31:5:34:LYS:HE2	2.02	0.41
1:A:2564:A:OP1	1:A:2648:G:O2'	2.38	0.41
1:A:2615:U:H2'	1:A:2616:C:H6	1.85	0.41
1:A:2821:A:H2'	1:A:2822:G:C8	2.55	0.41
13:N:35:ALA:HA	13:N:128:THR:HG22	2.01	0.41
32:a:294:U:H2'	32:a:295:C:C6	2.55	0.41
32:a:861:G:H2'	32:a:862:C:O4'	2.20	0.41
32:a:1304:G:C6	32:a:1305:G:N2	2.89	0.41
33:b:39:HIS:HB3	33:b:189:THR:HG21	2.01	0.41
1:A:16:C:H2'	1:A:17:G:C8	2.55	0.41
1:A:20:C:H2'	1:A:21:A:C8	2.55	0.41
1:A:56:A:N1	1:A:114:U:O4	2.53	0.41
1:A:471:A:H2'	1:A:472:A:O4'	2.19	0.41
1:A:1818:U:H2'	3:C:156:ARG:HD2	2.03	0.41
1:A:2453:A:H61	1:A:2499:C:H42	1.67	0.41
1:A:2774:C:H2'	1:A:2775:G:O4'	2.21	0.41
6:F:8:TYR:HA	6:F:12:VAL:HB	2.02	0.41
15:P:68:LYS:HA	15:P:102:ARG:HG2	2.02	0.41
32:a:64:G:N2	32:a:69:G:C6	2.88	0.41
32:a:549:C:H2'	32:a:550:G:H8	1.85	0.41
32:a:632:U:H5''	32:a:633:G:H8	1.86	0.41
32:a:994:A:N1	32:a:1047:G:H4'	2.35	0.41
1:A:153:U:C2	1:A:173:A:N1	2.88	0.41
1:A:828:U:H4'	1:A:831:G:C6	2.55	0.41
1:A:1598:A:H3'	1:A:1599:U:H6	1.85	0.41
1:A:2660:A:H2'	1:A:2661:G:O4'	2.20	0.41
2:B:10:G:H1	2:B:110:C:H42	1.68	0.41
11:L:40:LYS:HE3	11:L:57:VAL:HB	2.02	0.41
32:a:778:G:H2'	32:a:779:C:O4'	2.20	0.41
32:a:1225:A:H2'	32:a:1226:C:C5	2.55	0.41
33:b:15:HIS:HB2	33:b:40:ILE:HG23	2.03	0.41
36:e:13:GLU:HB2	36:e:39:VAL:HG12	2.02	0.41
1:A:45:G:H5''	1:A:46:G:OP1	2.20	0.41
1:A:145:C:H2'	1:A:146:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:A:N6	1:A:555:G:O2'	2.54	0.41
1:A:1490:A:H2'	1:A:1490:A:N3	2.35	0.41
1:A:2045:C:H2'	1:A:2046:G:O4'	2.20	0.41
1:A:2730:C:H2'	1:A:2731:G:H8	1.85	0.41
3:C:44:ASN:ND2	3:C:46:ASN:H	2.18	0.41
32:a:1255:G:H1	32:a:1282:C:N4	2.18	0.41
53:v:322:GLN:HB2	54:w:25:PHE:CE1	2.56	0.41
1:A:163:C:H2'	1:A:164:C:C6	2.56	0.41
1:A:668:A:H2'	1:A:670:A:H62	1.84	0.41
1:A:1248:G:C5	17:R:3:ARG:HB2	2.56	0.41
1:A:1317:G:H2'	1:A:1318:U:O4'	2.21	0.41
1:A:1426:G:C8	1:A:1427:A:H2'	2.54	0.41
1:A:1787:A:O4'	1:A:2589:A:H4'	2.21	0.41
1:A:2024:G:H2'	1:A:2025:C:H6	1.84	0.41
1:A:2358:A:H2'	1:A:2359:C:O4'	2.20	0.41
3:C:53:HIS:HA	3:C:217:ARG:HB2	2.03	0.41
5:E:46:GLN:HB2	5:E:86:ALA:HB1	2.02	0.41
14:O:2:ARG:HA	14:O:5:LYS:HD2	2.03	0.41
14:O:98:LEU:HD22	27:1:54:VAL:HG21	2.03	0.41
32:a:254:G:H5''	48:q:71:LYS:HD2	2.02	0.41
32:a:372:C:N4	32:a:387:U:H2'	2.36	0.41
32:a:551:U:C2'	32:a:552:U:C6	2.75	0.41
32:a:609:A:H2'	32:a:610:U:O4'	2.20	0.41
32:a:827:U:H2'	32:a:870:U:O4	2.21	0.41
32:a:839:C:N4	32:a:847:G:H1	2.13	0.41
32:a:1234:C:H2'	32:a:1235:U:C6	2.55	0.41
32:a:1235:U:H2'	32:a:1236:A:O4'	2.21	0.41
32:a:1239:A:H61	32:a:1296:C:H2'	1.85	0.41
1:A:182:A:H2'	1:A:183:C:C6	2.56	0.41
1:A:910:A:H62	13:N:12:MET:HA	1.86	0.41
1:A:932:U:OP2	1:A:932:U:H6	2.04	0.41
1:A:1023:U:H4'	1:A:1123:C:OP1	2.20	0.41
1:A:1036:G:H2'	1:A:1037:G:C8	2.56	0.41
1:A:1170:C:H2'	1:A:1171:G:C8	2.56	0.41
1:A:1266:G:N2	1:A:2012:G:H2'	2.36	0.41
1:A:1314:C:H42	1:A:1338:G:H1	1.68	0.41
1:A:1327:A:H2'	1:A:1328:A:O4'	2.21	0.41
1:A:1435:G:H2'	1:A:1436:G:O4'	2.21	0.41
1:A:2411:A:H2'	1:A:2412:A:C8	2.56	0.41
1:A:2415:G:H2'	1:A:2416:C:O4'	2.21	0.41
1:A:2505:G:C8	1:A:2576:G:N1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2848:G:O2'	1:A:2867:G:N2	2.51	0.41
14:O:31:HIS:C	14:O:33:ILE:H	2.29	0.41
15:P:5:SER:O	15:P:9:ARG:HG3	2.21	0.41
32:a:160:A:H2'	32:a:161:A:C8	2.56	0.41
32:a:234:C:H2'	32:a:235:C:H6	1.84	0.41
32:a:653:U:O2'	32:a:654:G:H8	2.03	0.41
32:a:722:G:H1	32:a:733:G:H1	1.68	0.41
32:a:1172:C:H2'	32:a:1173:U:H6	1.85	0.41
32:a:1222:G:OP1	32:a:1321:U:H2'	2.21	0.41
32:a:1288:A:C2	32:a:1352:C:O2	2.73	0.41
32:a:1417:G:C6	32:a:1482:G:C6	3.08	0.41
33:b:114:LEU:HD12	33:b:144:LEU:HB3	2.03	0.41
35:d:13:ARG:HG2	35:d:34:ILE:HA	2.01	0.41
35:d:61:VAL:HG21	35:d:200:ILE:HD11	2.03	0.41
40:i:19:VAL:HA	40:i:65:ILE:HG22	2.02	0.41
1:A:741:U:H2'	1:A:742:A:C8	2.56	0.41
1:A:1007:C:H4'	10:K:110:PRO:HD3	2.03	0.41
1:A:1117:C:HO2'	1:A:1118:C:H6	1.68	0.41
1:A:1266:G:H5''	19:T:15:GLN:NE2	2.36	0.41
1:A:1432:G:H2'	1:A:1433:A:H8	1.79	0.41
1:A:1739:A:H2'	1:A:1740:G:O4'	2.21	0.41
1:A:1790:C:H2'	1:A:1791:A:C5	2.56	0.41
1:A:2084:C:H2'	1:A:2085:U:O4'	2.21	0.41
1:A:2737:G:H2'	1:A:2738:A:C8	2.56	0.41
3:C:243:HIS:HA	3:C:244:PRO:HD3	1.85	0.41
22:W:30:ILE:HG23	22:W:72:VAL:HG11	2.02	0.41
24:Y:71:LEU:HD21	24:Y:78:TYR:HB3	2.02	0.41
32:a:104:G:H1'	32:a:172:A:H2	1.85	0.41
32:a:202:G:HO2'	32:a:468:A:H8	1.60	0.41
32:a:525:C:N3	32:a:526:C:N3	2.68	0.41
32:a:939:G:N3	32:a:1375:A:H2	2.18	0.41
1:A:118:A:H5''	29:3:22:MET:HE2	2.03	0.41
1:A:175:G:H2'	1:A:176:A:C8	2.56	0.41
1:A:355:U:H2'	1:A:356:G:C8	2.56	0.41
1:A:406:G:H2'	1:A:407:G:C8	2.55	0.41
1:A:418:C:H2'	1:A:419:U:C6	2.56	0.41
1:A:600:G:H1	1:A:657:U:H3	1.67	0.41
1:A:676:A:C2	1:A:2069:G:O2'	2.74	0.41
1:A:783:A:H3'	1:A:783:A:C8	2.56	0.41
1:A:822:G:H2'	1:A:823:C:C6	2.56	0.41
1:A:872:U:H2'	1:A:873:C:H6	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:C:H2'	1:A:986:C:C6	2.56	0.41
1:A:1170:C:H42	1:A:1178:C:N4	2.19	0.41
1:A:1249:U:H3'	12:M:18:ARG:HH22	1.86	0.41
1:A:1478:G:N2	1:A:1514:G:H1'	2.36	0.41
1:A:1801:A:C8	1:A:2203:U:H2'	2.55	0.41
1:A:1843:C:H2'	1:A:1844:C:C6	2.56	0.41
1:A:2025:C:H2'	1:A:2026:U:H6	1.86	0.41
1:A:2037:A:H2'	1:A:2038:G:H8	1.86	0.41
1:A:2236:U:H2'	1:A:2237:G:O4'	2.21	0.41
1:A:2447:G:O6	1:A:2504:PSU:O2	2.38	0.41
1:A:2494:G:O2'	13:N:79:ALA:HA	2.21	0.41
1:A:2533:U:H2'	1:A:2534:A:O4'	2.21	0.41
1:A:2633:G:H1	1:A:2785:C:H42	1.68	0.41
7:G:170:ARG:NH2	7:G:170:ARG:HB3	2.35	0.41
12:M:79:LEU:HD11	12:M:112:LEU:HD12	2.03	0.41
32:a:68:G:O2'	32:a:170:U:H1'	2.21	0.41
32:a:294:U:H2'	32:a:295:C:H6	1.86	0.41
32:a:505:G:OP2	32:a:535:A:H5'	2.21	0.41
32:a:527:A:N6	43:l:89:ASP:OD1	2.54	0.41
32:a:674:G:H2'	32:a:675:A:C8	2.56	0.41
32:a:687:A:N3	32:a:688:G:H1'	2.36	0.41
32:a:903:G:H2'	32:a:904:U:O4'	2.21	0.41
32:a:930:C:O2	32:a:930:C:H2'	2.21	0.41
32:a:1102:A:H2'	32:a:1103:C:C6	2.56	0.41
32:a:1171:A:H2'	32:a:1172:C:C6	2.55	0.41
32:a:1339:A:H2'	32:a:1340:A:O4'	2.21	0.41
36:e:141:ILE:HA	36:e:144:LEU:HD12	2.02	0.41
45:n:69:ARG:HA	45:n:70:PRO:HD3	1.90	0.41
47:p:4:ILE:HG12	47:p:21:VAL:HG22	2.03	0.41
53:v:250:GLY:HA3	53:v:254:VAL:CG1	2.47	0.41
55:y:43:A:H2'	55:y:44:A:H8	1.84	0.41
1:A:693:A:H1'	1:A:1354:A:H1'	2.02	0.41
1:A:1664:A:H61	1:A:1996:C:H42	1.69	0.41
1:A:2061:G:H4'	1:A:2061:G:OP1	2.20	0.41
1:A:2185:U:H2'	1:A:2186:G:H8	1.86	0.41
1:A:2230:G:H2'	1:A:2231:U:C6	2.56	0.41
1:A:2594:C:H2'	1:A:2595:G:O4'	2.21	0.41
4:D:13:ARG:HH11	16:Q:56:HIS:HA	1.86	0.41
5:E:5:LEU:HD11	5:E:12:LEU:HD12	2.01	0.41
13:N:30:SER:HA	13:N:133:LYS:HB2	2.02	0.41
32:a:73:C:H2'	32:a:74:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:109:A:O2'	32:a:326:G:N2	2.54	0.41
32:a:154:U:H2'	32:a:155:A:C8	2.56	0.41
32:a:442:G:H1	32:a:492:C:H42	1.69	0.41
32:a:825:A:H2'	32:a:826:C:C6	2.56	0.41
32:a:1255:G:H3'	32:a:1279:G:O6	2.21	0.41
34:c:23:PHE:HB3	41:j:97:ASP:HB2	2.03	0.41
34:c:87:LEU:O	34:c:90:VAL:HG23	2.21	0.41
53:v:196:THR:HG22	54:w:16:ILE:HD13	2.02	0.41
55:y:66:C:H2'	55:y:67:C:C6	2.55	0.41
1:A:151:C:H2'	1:A:152:A:O4'	2.21	0.40
1:A:202:U:O2	1:A:202:U:H2'	2.20	0.40
1:A:1130:U:N3	1:A:2025:C:H5''	2.36	0.40
1:A:1880:U:H2'	1:A:1881:C:C6	2.56	0.40
1:A:1991:U:H2'	1:A:1992:G:H5'	2.02	0.40
1:A:2649:C:H2'	1:A:2650:U:C6	2.56	0.40
1:A:2664:G:O2'	1:A:2665:A:O4'	2.39	0.40
1:A:2786:U:H2'	1:A:2787:C:H6	1.86	0.40
1:A:2864:G:H2'	1:A:2865:U:O4'	2.21	0.40
13:N:126:ILE:H	13:N:126:ILE:HG13	1.81	0.40
25:Z:39:GLN:HE21	25:Z:41:HIS:HE1	1.69	0.40
32:a:376:G:H5''	47:p:5:ARG:HD2	2.01	0.40
32:a:532:A:N3	32:a:532:A:C2'	2.84	0.40
32:a:536:C:H2'	32:a:537:G:C8	2.56	0.40
32:a:1317:C:H4'	45:n:48:LEU:HG	2.03	0.40
1:A:296:U:H2'	1:A:297:G:C8	2.56	0.40
1:A:299:A:N6	1:A:322:A:O2'	2.54	0.40
1:A:715:A:C8	46:o:60:VAL:HG11	2.56	0.40
1:A:858:G:N3	1:A:2268:A:H2'	2.36	0.40
1:A:1128:G:H21	1:A:2517:C:H1'	1.85	0.40
1:A:1502:A:H3'	1:A:1503:A:H5''	2.03	0.40
1:A:1804:C:N4	1:A:1814:G:N2	2.68	0.40
1:A:2519:U:H2'	1:A:2541:A:N6	2.36	0.40
1:A:2889:C:H2'	1:A:2890:G:O4'	2.22	0.40
7:G:11:VAL:HA	7:G:12:PRO:HD3	1.92	0.40
14:O:69:ARG:H	14:O:69:ARG:HG2	1.71	0.40
14:O:79:LEU:HA	14:O:83:LEU:HB2	2.03	0.40
32:a:20:U:H3'	32:a:21:G:H8	1.87	0.40
32:a:66:A:N1	32:a:103:U:O4	2.55	0.40
32:a:645:G:C2	32:a:646:G:C8	3.09	0.40
32:a:648:A:H2'	32:a:649:A:O4'	2.21	0.40
32:a:812:G:OP1	32:a:902:G:N2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:x:0:C:H2'	55:x:1:G:H8	1.86	0.40
1:A:863:A:H2'	1:A:864:G:C8	2.56	0.40
1:A:978:G:H1	1:A:985:C:N4	2.16	0.40
1:A:992:C:N4	1:A:1162:G:H1	2.15	0.40
1:A:1023:U:H1'	1:A:1122:G:H5''	2.03	0.40
1:A:1186:G:H2'	1:A:1187:G:O4'	2.22	0.40
1:A:1462:C:H2'	1:A:1463:C:C6	2.56	0.40
1:A:2376:A:H2'	1:A:2377:A:O4'	2.21	0.40
1:A:2525:G:H1'	1:A:2741:A:H2	1.86	0.40
1:A:2813:A:H3'	1:A:2814:A:H8	1.86	0.40
4:D:5:VAL:HG21	4:D:80:TRP:CG	2.57	0.40
30:4:6:THR:HG23	30:4:63:PRO:HD2	2.04	0.40
32:a:44:A:H2'	32:a:45:G:O4'	2.21	0.40
32:a:375:U:H3	32:a:389:A:H61	1.68	0.40
32:a:974:A:C6	32:a:1201:A:N1	2.90	0.40
32:a:1011:C:H42	32:a:1018:G:H1	1.69	0.40
32:a:1349:A:H3'	32:a:1350:A:H8	1.87	0.40
32:a:1464:U:H2'	32:a:1465:A:H8	1.85	0.40
35:d:36:GLN:HG2	35:d:42:GLY:C	2.46	0.40
51:t:60:ARG:HB3	51:t:64:LYS:NZ	2.37	0.40
1:A:372:G:C8	24:Y:61:LYS:HD2	2.57	0.40
1:A:528:A:C2	1:A:2042:A:H2'	2.55	0.40
1:A:1060:U:C2	1:A:1062:G:H5'	2.56	0.40
1:A:1788:C:H2'	1:A:1789:A:O4'	2.21	0.40
1:A:2008:C:H2'	1:A:2009:A:C8	2.57	0.40
1:A:2128:G:H2'	1:A:2129:C:O4'	2.22	0.40
1:A:2403:C:N4	1:A:2414:G:H1	2.17	0.40
1:A:2506:U:H4'	53:v:256:ARG:HH21	1.87	0.40
2:B:56:G:H1'	2:B:58:A:H62	1.87	0.40
3:C:122:ALA:HB1	3:C:128:ASN:HD22	1.86	0.40
5:E:76:PRO:HG2	5:E:84:THR:HB	2.03	0.40
17:R:66:ASN:HD21	17:R:70:ARG:HE	1.70	0.40
19:T:66:ILE:HA	19:T:69:LEU:HD12	2.04	0.40
22:W:5:ASN:HA	22:W:64:VAL:HG12	2.03	0.40
32:a:145:G:H2'	32:a:146:G:C8	2.57	0.40
32:a:300:A:H2'	32:a:564:C:H42	1.86	0.40
32:a:938:A:H2'	32:a:939:G:O4'	2.22	0.40
32:a:952:U:H2'	32:a:953:G:O4'	2.20	0.40
33:b:32:PHE:HB2	33:b:42:ASN:HA	2.04	0.40
35:d:118:VAL:HG11	35:d:133:ALA:HA	2.03	0.40
53:v:272:THR:HG21	53:v:290:GLN:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:x:61:C:H2'	55:x:62:C:C6	2.56	0.40
1:A:169:G:H2'	1:A:170:U:C6	2.57	0.40
1:A:448:U:H5''	1:A:449:A:C8	2.57	0.40
1:A:484:C:H42	1:A:496:G:H1	1.69	0.40
1:A:866:A:H61	1:A:913:U:H1'	1.86	0.40
1:A:1248:G:C4	17:R:3:ARG:HB2	2.55	0.40
1:A:1932:A:H3'	1:A:1933:G:H8	1.87	0.40
1:A:2043:C:H1'	1:A:2779:U:O4	2.21	0.40
1:A:2505:G:C6	1:A:2610:C:O2	2.75	0.40
1:A:2840:C:H2'	1:A:2841:C:C6	2.57	0.40
3:C:210:ALA:HA	3:C:213:TRP:CE3	2.57	0.40
5:E:178:VAL:HG23	12:M:3:LEU:HD21	2.03	0.40
18:S:35:PHE:HB2	18:S:59:ILE:HB	2.04	0.40
19:T:66:ILE:H	19:T:66:ILE:HG13	1.76	0.40
32:a:39:G:C1'	32:a:498:A:H1'	2.50	0.40
32:a:614:C:H2'	32:a:615:G:O4'	2.21	0.40
32:a:909:A:H2'	32:a:910:C:O4'	2.22	0.40
38:g:46:ALA:HA	38:g:121:ALA:HB2	2.03	0.40
43:l:10:LYS:HA	43:l:11:PRO:HD3	1.90	0.40
53:v:22:ARG:HG2	53:v:27:TYR:HB2	2.02	0.40
53:v:326:TYR:HA	53:v:333:ILE:HG12	2.04	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	269/273 (98%)	246 (91%)	20 (7%)	3 (1%)	11	43
4	D	207/209 (99%)	193 (93%)	13 (6%)	1 (0%)	24	57
5	E	199/201 (99%)	183 (92%)	14 (7%)	2 (1%)	12	44
6	F	175/179 (98%)	155 (89%)	16 (9%)	4 (2%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
8	H	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	9	38
9	J	139/142 (98%)	117 (84%)	16 (12%)	6 (4%)	2	18
10	K	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	18	51
11	L	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
12	M	142/144 (99%)	130 (92%)	11 (8%)	1 (1%)	18	51
13	N	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
14	O	118/127 (93%)	105 (89%)	12 (10%)	1 (1%)	16	49
15	P	114/117 (97%)	103 (90%)	10 (9%)	1 (1%)	14	47
16	Q	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
17	R	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
18	S	101/103 (98%)	90 (89%)	8 (8%)	3 (3%)	3	25
19	T	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	14	47
20	U	91/100 (91%)	83 (91%)	6 (7%)	2 (2%)	5	30
21	V	100/104 (96%)	82 (82%)	17 (17%)	1 (1%)	12	44
22	W	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
23	X	75/85 (88%)	68 (91%)	6 (8%)	1 (1%)	9	39
24	Y	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
25	Z	60/63 (95%)	56 (93%)	3 (5%)	1 (2%)	7	35
26	0	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	6	34
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	48/55 (87%)	44 (92%)	3 (6%)	1 (2%)	5	31
29	3	44/46 (96%)	44 (100%)	0	0	100	100
30	4	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	5	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
33	b	222/241 (92%)	207 (93%)	14 (6%)	1 (0%)	24	57
34	c	204/233 (88%)	192 (94%)	10 (5%)	2 (1%)	12	44
35	d	202/206 (98%)	192 (95%)	10 (5%)	0	100	100
36	e	155/167 (93%)	145 (94%)	8 (5%)	2 (1%)	9	39
37	f	98/135 (73%)	93 (95%)	4 (4%)	1 (1%)	12	44
38	g	149/179 (83%)	141 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	h	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
40	i	125/130 (96%)	112 (90%)	10 (8%)	3 (2%)	4	29
41	j	96/103 (93%)	87 (91%)	6 (6%)	3 (3%)	3	25
42	k	115/117 (98%)	103 (90%)	11 (10%)	1 (1%)	14	47
43	l	121/123 (98%)	112 (93%)	8 (7%)	1 (1%)	16	49
44	m	112/118 (95%)	105 (94%)	7 (6%)	0	100	100
45	n	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
46	o	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	10	41
47	p	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
48	q	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
49	r	63/75 (84%)	62 (98%)	1 (2%)	0	100	100
50	s	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	9	39
51	t	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
52	u	54/71 (76%)	54 (100%)	0	0	100	100
53	v	354/383 (92%)	334 (94%)	19 (5%)	1 (0%)	36	67
54	w	45/57 (79%)	39 (87%)	5 (11%)	1 (2%)	5	30
All	All	6056/6398 (95%)	5615 (93%)	390 (6%)	51 (1%)	18	49

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	241	GLY
5	E	64	GLY
18	S	82	HIS
6	F	174	ASP
9	J	20	SER
10	K	81	ILE
14	O	67	PHE
18	S	51	VAL
34	c	4	LYS
37	f	52	ASN
41	j	36	VAL
41	j	57	VAL
3	C	255	LYS
9	J	92	PRO
19	T	72	THR

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Mol	Chain	Res	Type
21	V	90	GLY
26	0	4	THR
33	b	126	PHE
36	e	78	ASN
40	i	13	LYS
40	i	111	VAL
41	j	94	ALA
4	D	206	ALA
6	F	21	ASN
8	H	15	LEU
8	H	72	ILE
12	M	86	GLU
40	i	109	ARG
53	v	250	GLY
3	C	69	ARG
6	F	176	PRO
6	F	177	PHE
18	S	80	ARG
23	X	76	ASN
25	Z	37	LEU
42	k	39	GLY
46	o	19	ALA
9	J	18	ASN
15	P	34	HIS
20	U	10	VAL
28	2	5	ILE
43	l	42	PRO
36	e	44	GLY
54	w	23	PRO
9	J	22	PRO
9	J	31	GLY
34	c	108	LYS
5	E	77	ILE
9	J	12	VAL
50	s	29	LYS
20	U	14	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	216/218 (99%)	198 (92%)	18 (8%)	10	34
4	D	164/164 (100%)	154 (94%)	10 (6%)	17	43
5	E	165/165 (100%)	153 (93%)	12 (7%)	13	38
6	F	148/150 (99%)	135 (91%)	13 (9%)	9	32
7	G	137/138 (99%)	130 (95%)	7 (5%)	21	48
8	H	114/114 (100%)	108 (95%)	6 (5%)	20	47
9	J	109/110 (99%)	103 (94%)	6 (6%)	19	46
10	K	116/116 (100%)	111 (96%)	5 (4%)	26	51
11	L	104/104 (100%)	92 (88%)	12 (12%)	5	24
12	M	103/103 (100%)	96 (93%)	7 (7%)	14	40
13	N	109/109 (100%)	101 (93%)	8 (7%)	13	38
14	O	100/103 (97%)	95 (95%)	5 (5%)	22	48
15	P	86/87 (99%)	77 (90%)	9 (10%)	6	27
16	Q	99/100 (99%)	93 (94%)	6 (6%)	17	43
17	R	89/90 (99%)	81 (91%)	8 (9%)	9	32
18	S	84/84 (100%)	76 (90%)	8 (10%)	8	31
19	T	93/93 (100%)	91 (98%)	2 (2%)	45	65
20	U	80/84 (95%)	76 (95%)	4 (5%)	22	48
21	V	83/85 (98%)	79 (95%)	4 (5%)	23	49
22	W	78/78 (100%)	66 (85%)	12 (15%)	2	16
23	X	59/63 (94%)	54 (92%)	5 (8%)	10	34
24	Y	67/68 (98%)	59 (88%)	8 (12%)	5	23
25	Z	54/55 (98%)	51 (94%)	3 (6%)	19	46
26	0	48/49 (98%)	48 (100%)	0	100	100
27	1	47/48 (98%)	45 (96%)	2 (4%)	26	51
28	2	45/49 (92%)	44 (98%)	1 (2%)	45	65
29	3	38/38 (100%)	38 (100%)	0	100	100
30	4	51/52 (98%)	49 (96%)	2 (4%)	28	54
31	5	34/34 (100%)	32 (94%)	2 (6%)	18	44
33	b	186/199 (94%)	167 (90%)	19 (10%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	c	170/190 (90%)	149 (88%)	21 (12%)	4	22
35	d	171/173 (99%)	157 (92%)	14 (8%)	10	34
36	e	119/126 (94%)	101 (85%)	18 (15%)	3	16
37	f	87/116 (75%)	80 (92%)	7 (8%)	11	35
38	g	124/147 (84%)	115 (93%)	9 (7%)	13	38
39	h	104/104 (100%)	95 (91%)	9 (9%)	9	33
40	i	105/107 (98%)	96 (91%)	9 (9%)	10	33
41	j	86/90 (96%)	74 (86%)	12 (14%)	3	19
42	k	90/90 (100%)	87 (97%)	3 (3%)	33	58
43	l	103/103 (100%)	96 (93%)	7 (7%)	14	40
44	m	92/96 (96%)	84 (91%)	8 (9%)	9	33
45	n	83/83 (100%)	77 (93%)	6 (7%)	13	38
46	o	76/76 (100%)	66 (87%)	10 (13%)	4	20
47	p	65/65 (100%)	56 (86%)	9 (14%)	3	19
48	q	74/78 (95%)	66 (89%)	8 (11%)	6	26
49	r	57/66 (86%)	50 (88%)	7 (12%)	4	22
50	s	72/72 (100%)	64 (89%)	8 (11%)	6	25
51	t	65/65 (100%)	60 (92%)	5 (8%)	12	37
52	u	48/61 (79%)	46 (96%)	2 (4%)	26	52
53	v	304/324 (94%)	276 (91%)	28 (9%)	8	32
54	w	40/46 (87%)	31 (78%)	9 (22%)	1	5
All	All	5041/5228 (96%)	4628 (92%)	413 (8%)	13	34

All (413) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	13	ARG
3	C	33	LEU
3	C	51	THR
3	C	63	ARG
3	C	64	ILE
3	C	74	ILE
3	C	95	LEU
3	C	135	ILE
3	C	142	HIS

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Mol	Chain	Res	Type
3	C	156	ARG
3	C	164	ILE
3	C	174	LEU
3	C	175	ARG
3	C	176	LEU
3	C	182	ARG
3	C	184	VAL
3	C	199	GLU
3	C	221	ARG
4	D	5	VAL
4	D	12	THR
4	D	50	VAL
4	D	77	ARG
4	D	121	THR
4	D	141	ARG
4	D	142	VAL
4	D	159	LYS
4	D	179	ARG
4	D	200	ASP
5	E	4	VAL
5	E	21	ARG
5	E	27	LEU
5	E	28	VAL
5	E	58	LYS
5	E	100	MET
5	E	108	ILE
5	E	120	VAL
5	E	138	LEU
5	E	139	LYS
5	E	189	THR
5	E	193	VAL
6	F	6	ASP
6	F	12	VAL
6	F	16	LEU
6	F	22	TYR
6	F	74	VAL
6	F	108	VAL
6	F	135	GLN
6	F	136	ILE
6	F	146	VAL
6	F	150	ARG
6	F	152	LEU

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Mol	Chain	Res	Type
6	F	155	THR
6	F	170	LEU
7	G	45	HIS
7	G	50	LEU
7	G	72	LEU
7	G	89	LEU
7	G	98	VAL
7	G	132	VAL
7	G	148	LEU
8	H	1	MET
8	H	2	GLN
8	H	9	VAL
8	H	27	ARG
8	H	96	THR
8	H	124	THR
9	J	8	VAL
9	J	37	PHE
9	J	60	VAL
9	J	79	LEU
9	J	133	ARG
9	J	137	LEU
10	K	28	LEU
10	K	81	ILE
10	K	95	ARG
10	K	101	ILE
10	K	140	LEU
11	L	24	VAL
11	L	25	LEU
11	L	29	HIS
11	L	31	ARG
11	L	47	ILE
11	L	57	VAL
11	L	63	VAL
11	L	71	ARG
11	L	78	ARG
11	L	84	CYS
11	L	85	VAL
11	L	116	ILE
12	M	23	ILE
12	M	27	LEU
12	M	46	VAL
12	M	48	ARG

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Mol	Chain	Res	Type
12	M	110	VAL
12	M	126	ARG
12	M	132	ARG
13	N	44	ARG
13	N	63	ILE
13	N	66	ARG
13	N	74	THR
13	N	86	LYS
13	N	101	VAL
13	N	119	LEU
13	N	126	ILE
14	O	15	SER
14	O	37	THR
14	O	70	THR
14	O	79	LEU
14	O	90	ARG
15	P	7	ARG
15	P	21	LEU
15	P	30	ARG
15	P	36	TYR
15	P	53	THR
15	P	74	VAL
15	P	83	LEU
15	P	84	GLU
15	P	106	LEU
16	Q	33	VAL
16	Q	88	ARG
16	Q	93	ARG
16	Q	97	LEU
16	Q	100	LEU
16	Q	109	ARG
17	R	9	ILE
17	R	11	ARG
17	R	30	ARG
17	R	40	ILE
17	R	51	ARG
17	R	53	ARG
17	R	74	ILE
17	R	83	LEU
18	S	23	GLU
18	S	29	THR
18	S	40	MET

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Mol	Chain	Res	Type
18	S	47	VAL
18	S	54	VAL
18	S	75	VAL
18	S	80	ARG
18	S	98	ILE
19	T	46	LEU
19	T	66	ILE
20	U	8	LEU
20	U	53	VAL
20	U	55	VAL
20	U	60	THR
21	V	9	ASP
21	V	49	VAL
21	V	72	ILE
21	V	81	ASP
22	W	4	ILE
22	W	9	ARG
22	W	12	GLN
22	W	18	ARG
22	W	29	ILE
22	W	40	ILE
22	W	43	ASP
22	W	47	VAL
22	W	51	GLN
22	W	61	LEU
22	W	64	VAL
22	W	82	TYR
23	X	25	ARG
23	X	43	THR
23	X	51	VAL
23	X	56	ASP
23	X	69	PHE
24	Y	18	ARG
24	Y	23	ASN
24	Y	33	LEU
24	Y	37	ARG
24	Y	40	VAL
24	Y	46	PHE
24	Y	60	ASP
24	Y	78	TYR
25	Z	18	LEU
25	Z	43	LEU

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Mol	Chain	Res	Type
25	Z	56	LEU
27	1	9	THR
27	1	39	LEU
28	2	47	VAL
30	4	4	ILE
30	4	38	THR
31	5	7	VAL
31	5	15	LYS
33	b	18	HIS
33	b	19	GLN
33	b	35	ARG
33	b	39	HIS
33	b	47	VAL
33	b	87	CYS
33	b	97	LEU
33	b	102	THR
33	b	106	THR
33	b	109	GLN
33	b	114	LEU
33	b	125	THR
33	b	137	ARG
33	b	139	ARG
33	b	157	LEU
33	b	179	LEU
33	b	204	ASP
33	b	207	ILE
33	b	221	VAL
34	c	3	GLN
34	c	19	ASN
34	c	43	LEU
34	c	59	ARG
34	c	64	ILE
34	c	65	ARG
34	c	66	VAL
34	c	75	ILE
34	c	76	VAL
34	c	87	LEU
34	c	90	VAL
34	c	93	ASP
34	c	103	ILE
34	c	106	VAL
34	c	110	GLU

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Mol	Chain	Res	Type
34	c	128	VAL
34	c	134	MET
34	c	140	ASN
34	c	169	ARG
34	c	176	HIS
34	c	178	LEU
35	d	3	ARG
35	d	28	ILE
35	d	35	GLU
35	d	44	ARG
35	d	48	LEU
35	d	55	LEU
35	d	88	GLU
35	d	91	LEU
35	d	93	LEU
35	d	116	GLN
35	d	159	LEU
35	d	187	GLU
35	d	191	LEU
35	d	195	ILE
36	e	16	ILE
36	e	30	ILE
36	e	31	PHE
36	e	34	THR
36	e	45	ARG
36	e	56	VAL
36	e	69	ARG
36	e	76	LEU
36	e	90	THR
36	e	93	ARG
36	e	120	VAL
36	e	123	VAL
36	e	131	THR
36	e	134	ILE
36	e	136	VAL
36	e	141	ILE
36	e	153	VAL
36	e	165	LEU
37	f	16	GLU
37	f	18	VAL
37	f	24	ARG
37	f	64	VAL

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Mol	Chain	Res	Type
37	f	70	VAL
37	f	86	ARG
37	f	92	THR
38	g	21	GLU
38	g	23	LEU
38	g	40	GLU
38	g	73	VAL
38	g	92	ARG
38	g	95	ARG
38	g	99	LEU
38	g	102	ARG
38	g	105	VAL
39	h	32	LEU
39	h	40	LEU
39	h	61	LEU
39	h	76	GLN
39	h	83	LEU
39	h	106	THR
39	h	110	VAL
39	h	113	ASP
39	h	121	LEU
40	i	18	ARG
40	i	104	VAL
40	i	113	ARG
40	i	115	LYS
40	i	119	ARG
40	i	120	LYS
40	i	124	ARG
40	i	129	LYS
40	i	130	ARG
41	j	7	ARG
41	j	9	ARG
41	j	10	LEU
41	j	16	ARG
41	j	31	ARG
41	j	50	THR
41	j	53	ILE
41	j	73	LEU
41	j	74	VAL
41	j	77	VAL
41	j	82	LYS
41	j	102	LEU

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Mol	Chain	Res	Type
42	k	37	ARG
42	k	53	ARG
42	k	96	THR
43	l	31	ARG
43	l	56	ARG
43	l	74	LEU
43	l	107	VAL
43	l	110	ARG
43	l	112	GLN
43	l	115	SER
44	m	16	VAL
44	m	22	ILE
44	m	29	ARG
44	m	39	ILE
44	m	52	GLN
44	m	56	LEU
44	m	102	THR
44	m	113	ARG
45	n	20	TYR
45	n	24	ARG
45	n	33	ASP
45	n	41	ARG
45	n	74	LEU
45	n	82	ILE
46	o	37	ASN
46	o	39	LEU
46	o	56	LEU
46	o	57	LEU
46	o	67	LEU
46	o	73	LYS
46	o	75	VAL
46	o	84	ARG
46	o	88	ARG
46	o	89	ARG
47	p	9	HIS
47	p	14	ARG
47	p	24	SER
47	p	25	ARG
47	p	31	ARG
47	p	36	VAL
47	p	50	THR
47	p	59	HIS

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Mol	Chain	Res	Type
47	p	66	THR
48	q	6	ARG
48	q	16	LYS
48	q	21	ILE
48	q	23	VAL
48	q	42	THR
48	q	57	ASP
48	q	67	LEU
48	q	79	VAL
49	r	18	VAL
49	r	26	ILE
49	r	39	ILE
49	r	47	THR
49	r	67	LEU
49	r	72	ASP
49	r	73	ARG
50	s	11	ILE
50	s	24	GLU
50	s	36	ARG
50	s	40	ILE
50	s	49	ILE
50	s	55	ARG
50	s	63	THR
50	s	66	MET
51	t	18	ARG
51	t	27	MET
51	t	28	MET
51	t	57	ILE
51	t	79	LEU
52	u	17	ARG
52	u	44	GLU
53	v	12	GLN
53	v	28	ASP
53	v	49	GLU
53	v	69	THR
53	v	70	LEU
53	v	80	VAL
53	v	83	LEU
53	v	95	THR
53	v	142	GLN
53	v	150	ARG
53	v	159	ARG

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Mol	Chain	Res	Type
53	v	163	THR
53	v	167	GLU
53	v	202	VAL
53	v	238	ASP
53	v	254	VAL
53	v	262	ARG
53	v	273	GLN
53	v	285	ASP
53	v	295	LEU
53	v	299	GLU
53	v	310	MET
53	v	315	SER
53	v	323	ILE
53	v	337	ARG
53	v	338	THR
53	v	354	ASP
53	v	361	LEU
54	w	8	LYS
54	w	13	ASP
54	w	17	GLU
54	w	19	LEU
54	w	20	LEU
54	w	22	ASP
54	w	29	VAL
54	w	30	GLU
54	w	41	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	37	ASN
3	C	44	ASN
3	C	226	ASN
3	C	239	ASN
4	D	36	GLN
4	D	94	GLN
4	D	173	GLN
5	E	30	GLN
5	E	62	GLN
5	E	90	GLN
5	E	94	GLN
5	E	115	GLN

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Mol	Chain	Res	Type
5	E	163	ASN
7	G	20	ASN
7	G	22	GLN
7	G	30	ASN
7	G	38	ASN
7	G	101	ASN
8	H	11	ASN
8	H	20	ASN
8	H	119	ASN
8	H	135	HIS
9	J	5	GLN
9	J	18	ASN
10	K	47	HIS
10	K	80	HIS
11	L	5	GLN
11	L	29	HIS
12	M	38	GLN
13	N	13	HIS
14	O	13	ASN
14	O	16	HIS
14	O	23	ASN
14	O	62	ASN
14	O	73	ASN
14	O	81	ASN
15	P	38	GLN
15	P	104	GLN
16	Q	3	ASN
16	Q	15	GLN
17	R	20	GLN
17	R	72	ASN
18	S	12	HIS
18	S	18	GLN
18	S	43	ASN
18	S	82	HIS
18	S	86	GLN
18	S	91	GLN
19	T	15	GLN
19	T	40	ASN
19	T	61	ASN
20	U	91	GLN
21	V	27	ASN
21	V	54	GLN

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Mol	Chain	Res	Type
21	V	66	GLN
22	W	44	HIS
22	W	49	ASN
22	W	78	GLN
23	X	50	ASN
24	Y	20	HIS
25	Z	31	GLN
25	Z	39	GLN
33	b	42	ASN
33	b	168	HIS
33	b	177	ASN
33	b	178	ASN
34	c	8	ASN
34	c	139	GLN
34	c	190	HIS
35	d	36	GLN
35	d	40	GLN
35	d	74	ASN
35	d	196	ASN
35	d	198	HIS
36	e	73	ASN
36	e	97	GLN
36	e	122	ASN
36	e	146	ASN
36	e	148	ASN
37	f	52	ASN
37	f	58	HIS
37	f	81	ASN
38	g	86	GLN
38	g	122	ASN
39	h	21	ASN
39	h	76	GLN
40	i	4	ASN
40	i	110	GLN
40	i	126	GLN
41	j	15	HIS
41	j	35	GLN
41	j	58	ASN
42	k	40	ASN
42	k	109	ASN
42	k	119	ASN
43	l	29	GLN

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Mol	Chain	Res	Type
43	l	96	HIS
43	l	112	GLN
44	m	14	HIS
44	m	52	GLN
47	p	59	HIS
47	p	63	GLN
47	p	79	ASN
48	q	9	GLN
48	q	51	ASN
49	r	31	ASN
50	s	43	ASN
51	t	52	ASN
51	t	55	GLN
53	v	43	GLN
53	v	72	GLN
53	v	97	ASN
53	v	253	HIS
53	v	280	GLN
53	v	283	ASN
53	v	308	GLN
54	w	5	GLN
54	w	6	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2903/2904 (99%)	869 (29%)	82 (2%)
2	B	117/118 (99%)	35 (29%)	1 (0%)
32	a	1532/1533 (99%)	493 (32%)	0
55	x	76/77 (98%)	22 (28%)	0
55	y	76/77 (98%)	18 (23%)	0
56	z	5/18 (27%)	1 (20%)	0
All	All	4709/4727 (99%)	1438 (30%)	83 (1%)

All (1438) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	13	A
1	A	14	A
1	A	23	G

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Mol	Chain	Res	Type
1	A	27	G
1	A	34	U
1	A	35	G
1	A	39	G
1	A	43	G
1	A	45	G
1	A	46	G
1	A	49	A
1	A	51	G
1	A	55	G
1	A	60	G
1	A	61	C
1	A	63	A
1	A	69	C
1	A	71	A
1	A	73	A
1	A	74	A
1	A	75	G
1	A	83	A
1	A	84	A
1	A	86	G
1	A	88	G
1	A	92	U
1	A	93	G
1	A	96	C
1	A	101	A
1	A	102	U
1	A	103	A
1	A	110	G
1	A	114	U
1	A	118	A
1	A	119	A
1	A	120	U
1	A	122	G
1	A	125	A
1	A	127	A
1	A	131	A
1	A	137	U
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G

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Mol	Chain	Res	Type
1	A	142	A
1	A	150	U
1	A	157	C
1	A	163	C
1	A	177	G
1	A	178	G
1	A	179	C
1	A	181	A
1	A	184	C
1	A	196	A
1	A	199	A
1	A	204	A
1	A	205	G
1	A	215	G
1	A	216	A
1	A	222	A
1	A	224	U
1	A	228	C
1	A	230	G
1	A	233	A
1	A	239	C
1	A	241	A
1	A	248	G
1	A	249	C
1	A	252	G
1	A	261	G
1	A	264	C
1	A	265	A
1	A	266	G
1	A	271	G
1	A	272	A
1	A	276	U
1	A	278	A
1	A	279	A
1	A	285	G
1	A	291	G
1	A	295	G
1	A	302	C
1	A	311	A
1	A	312	G
1	A	313	G
1	A	318	C

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Mol	Chain	Res	Type
1	A	322	A
1	A	323	C
1	A	329	G
1	A	330	A
1	A	331	C
1	A	346	A
1	A	352	A
1	A	353	C
1	A	356	G
1	A	361	G
1	A	362	A
1	A	367	G
1	A	370	G
1	A	371	A
1	A	372	G
1	A	373	U
1	A	386	G
1	A	387	U
1	A	399	U
1	A	402	A
1	A	403	U
1	A	404	A
1	A	405	U
1	A	408	G
1	A	411	G
1	A	421	C
1	A	424	G
1	A	425	G
1	A	427	U
1	A	431	U
1	A	435	C
1	A	442	G
1	A	443	A
1	A	444	C
1	A	446	G
1	A	447	A
1	A	451	U
1	A	454	A
1	A	455	C
1	A	457	A
1	A	467	G
1	A	474	G

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Mol	Chain	Res	Type
1	A	475	C
1	A	476	G
1	A	479	A
1	A	481	G
1	A	490	C
1	A	491	G
1	A	501	A
1	A	504	A
1	A	505	A
1	A	506	G
1	A	507	A
1	A	512	G
1	A	513	A
1	A	516	C
1	A	518	G
1	A	519	U
1	A	527	C
1	A	528	A
1	A	529	A
1	A	531	C
1	A	532	A
1	A	544	C
1	A	546	U
1	A	547	A
1	A	548	G
1	A	549	G
1	A	551	G
1	A	555	G
1	A	562	U
1	A	563	A
1	A	565	C
1	A	566	U
1	A	568	U
1	A	573	U
1	A	575	A
1	A	577	G
1	A	580	U
1	A	588	U
1	A	592	A
1	A	593	U
1	A	601	C
1	A	603	A

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Mol	Chain	Res	Type
1	A	610	C
1	A	613	A
1	A	614	A
1	A	615	U
1	A	621	A
1	A	627	A
1	A	637	A
1	A	638	G
1	A	645	C
1	A	647	G
1	A	651	G
1	A	653	U
1	A	654	A
1	A	655	A
1	A	659	G
1	A	664	G
1	A	668	A
1	A	670	A
1	A	675	A
1	A	676	A
1	A	677	A
1	A	684	G
1	A	686	U
1	A	691	C
1	A	694	U
1	A	702	U
1	A	710	U
1	A	717	C
1	A	726	G
1	A	728	G
1	A	729	G
1	A	730	A
1	A	731	C
1	A	734	A
1	A	738	G
1	A	742	A
1	A	743	A
1	A	746	PSU
1	A	747	5MU
1	A	757	G
1	A	763	G
1	A	764	A

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Mol	Chain	Res	Type
1	A	765	C
1	A	775	G
1	A	776	G
1	A	777	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	788	A
1	A	792	A
1	A	799	G
1	A	800	A
1	A	805	G
1	A	811	U
1	A	812	C
1	A	819	A
1	A	821	A
1	A	827	U
1	A	828	U
1	A	831	G
1	A	845	A
1	A	846	U
1	A	847	U
1	A	850	U
1	A	856	G
1	A	858	G
1	A	859	G
1	A	869	G
1	A	877	A
1	A	878	A
1	A	881	G
1	A	882	G
1	A	883	G
1	A	886	A
1	A	887	A
1	A	888	C
1	A	889	C
1	A	890	C
1	A	894	U
1	A	895	U
1	A	896	A
1	A	897	C
1	A	907	G

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Mol	Chain	Res	Type
1	A	910	A
1	A	914	G
1	A	915	C
1	A	918	A
1	A	926	G
1	A	931	U
1	A	932	U
1	A	941	A
1	A	946	C
1	A	953	G
1	A	957	C
1	A	958	U
1	A	961	C
1	A	964	C
1	A	965	C
1	A	968	C
1	A	973	A
1	A	974	G
1	A	983	A
1	A	984	A
1	A	988	A
1	A	989	G
1	A	990	A
1	A	995	C
1	A	996	A
1	A	997	G
1	A	1007	C
1	A	1008	A
1	A	1009	A
1	A	1012	U
1	A	1013	C
1	A	1017	G
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1024	G
1	A	1025	G
1	A	1026	G
1	A	1033	U
1	A	1034	G
1	A	1045	C
1	A	1046	A

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Mol	Chain	Res	Type
1	A	1047	G
1	A	1051	G
1	A	1052	C
1	A	1054	A
1	A	1059	G
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	1075	C
1	A	1076	C
1	A	1077	A
1	A	1078	U
1	A	1080	A
1	A	1083	U
1	A	1085	A
1	A	1087	G
1	A	1088	A
1	A	1089	A
1	A	1096	A
1	A	1097	U
1	A	1098	A
1	A	1101	U
1	A	1102	C
1	A	1106	G
1	A	1111	A
1	A	1112	G
1	A	1118	C
1	A	1119	U
1	A	1121	C
1	A	1126	A
1	A	1127	A
1	A	1131	G
1	A	1132	U
1	A	1133	A
1	A	1134	A
1	A	1135	C
1	A	1136	G

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Mol	Chain	Res	Type
1	A	1142	A
1	A	1143	A
1	A	1144	A
1	A	1151	A
1	A	1155	A
1	A	1156	A
1	A	1165	A
1	A	1170	C
1	A	1173	U
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1179	G
1	A	1180	U
1	A	1182	G
1	A	1186	G
1	A	1187	G
1	A	1188	U
1	A	1195	G
1	A	1205	A
1	A	1206	G
1	A	1210	G
1	A	1212	G
1	A	1218	G
1	A	1223	G
1	A	1227	G
1	A	1236	G
1	A	1238	G
1	A	1240	U
1	A	1244	A
1	A	1247	A
1	A	1248	G
1	A	1249	U
1	A	1252	G
1	A	1253	A
1	A	1256	G
1	A	1263	U
1	A	1265	A
1	A	1266	G
1	A	1271	G
1	A	1272	A
1	A	1273	U

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Mol	Chain	Res	Type
1	A	1277	G
1	A	1278	C
1	A	1288	G
1	A	1289	C
1	A	1294	U
1	A	1300	G
1	A	1301	A
1	A	1302	A
1	A	1306	C
1	A	1311	G
1	A	1312	U
1	A	1313	U
1	A	1314	C
1	A	1315	C
1	A	1320	C
1	A	1321	A
1	A	1326	U
1	A	1329	U
1	A	1341	G
1	A	1344	U
1	A	1345	C
1	A	1352	U
1	A	1360	G
1	A	1365	A
1	A	1368	G
1	A	1371	G
1	A	1379	U
1	A	1380	G
1	A	1383	A
1	A	1395	A
1	A	1398	C
1	A	1403	A
1	A	1404	C
1	A	1407	G
1	A	1408	G
1	A	1409	U
1	A	1416	G
1	A	1417	C
1	A	1419	A
1	A	1420	A
1	A	1421	G
1	A	1427	A

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Mol	Chain	Res	Type
1	A	1428	C
1	A	1429	G
1	A	1433	A
1	A	1434	A
1	A	1437	C
1	A	1438	U
1	A	1444	G
1	A	1449	G
1	A	1451	C
1	A	1453	A
1	A	1455	G
1	A	1456	G
1	A	1458	U
1	A	1460	U
1	A	1461	C
1	A	1466	U
1	A	1468	U
1	A	1471	G
1	A	1478	G
1	A	1482	G
1	A	1486	U
1	A	1488	C
1	A	1490	A
1	A	1492	G
1	A	1493	C
1	A	1494	A
1	A	1497	U
1	A	1502	A
1	A	1503	A
1	A	1508	A
1	A	1515	A
1	A	1522	A
1	A	1523	U
1	A	1531	C
1	A	1532	A
1	A	1533	C
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1550	C
1	A	1555	G

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Mol	Chain	Res	Type
1	A	1558	C
1	A	1566	A
1	A	1567	G
1	A	1569	A
1	A	1578	U
1	A	1580	A
1	A	1581	G
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1586	A
1	A	1592	C
1	A	1597	A
1	A	1599	U
1	A	1602	U
1	A	1603	A
1	A	1607	C
1	A	1608	A
1	A	1610	A
1	A	1613	G
1	A	1619	G
1	A	1627	G
1	A	1634	A
1	A	1638	C
1	A	1639	C
1	A	1643	G
1	A	1644	C
1	A	1646	C
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1652	A
1	A	1654	A
1	A	1660	G
1	A	1664	A
1	A	1666	G
1	A	1667	G
1	A	1669	A
1	A	1674	G
1	A	1675	C
1	A	1695	G
1	A	1713	A

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Mol	Chain	Res	Type
1	A	1715	G
1	A	1721	G
1	A	1724	G
1	A	1729	U
1	A	1730	C
1	A	1731	G
1	A	1732	C
1	A	1733	G
1	A	1742	U
1	A	1758	U
1	A	1759	A
1	A	1764	C
1	A	1773	A
1	A	1782	U
1	A	1786	A
1	A	1791	A
1	A	1794	A
1	A	1800	C
1	A	1801	A
1	A	1808	A
1	A	1816	C
1	A	1821	A
1	A	1829	A
1	A	1835	2MG
1	A	1848	A
1	A	1864	U
1	A	1865	U
1	A	1866	A
1	A	1869	G
1	A	1870	C
1	A	1871	A
1	A	1872	A
1	A	1873	G
1	A	1875	G
1	A	1876	A
1	A	1882	U
1	A	1884	G
1	A	1885	A
1	A	1900	A
1	A	1901	A
1	A	1906	G
1	A	1907	G

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Mol	Chain	Res	Type
1	A	1913	A
1	A	1914	C
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1936	A
1	A	1937	A
1	A	1938	A
1	A	1939	5MU
1	A	1940	U
1	A	1944	U
1	A	1955	U
1	A	1964	G
1	A	1965	C
1	A	1966	A
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1981	A
1	A	1982	U
1	A	1991	U
1	A	1992	G
1	A	1993	U
1	A	1997	C
1	A	2000	C
1	A	2002	G
1	A	2004	G
1	A	2006	C
1	A	2016	U
1	A	2018	G
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2027	G
1	A	2030	A
1	A	2031	A
1	A	2034	U
1	A	2036	C
1	A	2043	C
1	A	2046	G
1	A	2049	G

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Mol	Chain	Res	Type
1	A	2050	C
1	A	2052	A
1	A	2055	C
1	A	2056	G
1	A	2057	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2068	U
1	A	2069	G
1	A	2070	A
1	A	2072	C
1	A	2074	U
1	A	2075	U
1	A	2077	A
1	A	2080	A
1	A	2087	G
1	A	2093	G
1	A	2095	A
1	A	2101	A
1	A	2102	G
1	A	2107	G
1	A	2110	G
1	A	2111	U
1	A	2113	U
1	A	2115	G
1	A	2116	G
1	A	2117	A
1	A	2118	U
1	A	2121	G
1	A	2122	U
1	A	2125	G
1	A	2130	U
1	A	2131	U
1	A	2132	U
1	A	2134	A
1	A	2139	U
1	A	2142	A
1	A	2146	C
1	A	2147	A
1	A	2148	G

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Mol	Chain	Res	Type
1	A	2150	C
1	A	2154	A
1	A	2157	G
1	A	2158	A
1	A	2159	G
1	A	2160	C
1	A	2162	G
1	A	2164	C
1	A	2165	C
1	A	2171	A
1	A	2172	U
1	A	2173	A
1	A	2178	C
1	A	2182	U
1	A	2183	A
1	A	2189	U
1	A	2193	G
1	A	2194	U
1	A	2198	A
1	A	2203	U
1	A	2204	G
1	A	2211	A
1	A	2212	A
1	A	2213	U
1	A	2214	C
1	A	2216	G
1	A	2221	G
1	A	2223	G
1	A	2225	A
1	A	2226	C
1	A	2234	G
1	A	2238	G
1	A	2243	U
1	A	2249	U
1	A	2250	G
1	A	2266	A
1	A	2278	A
1	A	2279	G
1	A	2280	G
1	A	2282	G
1	A	2283	C
1	A	2286	G

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Mol	Chain	Res	Type
1	A	2287	A
1	A	2288	A
1	A	2292	U
1	A	2297	A
1	A	2301	C
1	A	2305	U
1	A	2307	G
1	A	2309	A
1	A	2311	A
1	A	2319	G
1	A	2322	A
1	A	2324	U
1	A	2325	G
1	A	2326	C
1	A	2327	A
1	A	2331	G
1	A	2333	A
1	A	2335	A
1	A	2336	A
1	A	2339	C
1	A	2345	G
1	A	2347	C
1	A	2350	C
1	A	2353	G
1	A	2354	C
1	A	2355	G
1	A	2357	G
1	A	2361	G
1	A	2376	A
1	A	2383	G
1	A	2384	U
1	A	2385	C
1	A	2388	A
1	A	2391	G
1	A	2400	G
1	A	2402	U
1	A	2403	C
1	A	2406	A
1	A	2408	U
1	A	2409	G
1	A	2410	G
1	A	2419	U

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Mol	Chain	Res	Type
1	A	2423	U
1	A	2424	C
1	A	2425	A
1	A	2427	C
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2432	A
1	A	2434	A
1	A	2435	A
1	A	2436	G
1	A	2441	U
1	A	2445	2MG
1	A	2447	G
1	A	2448	A
1	A	2457	PSU
1	A	2464	G
1	A	2468	A
1	A	2469	A
1	A	2470	G
1	A	2476	A
1	A	2480	C
1	A	2484	G
1	A	2487	G
1	A	2490	G
1	A	2491	U
1	A	2492	U
1	A	2494	G
1	A	2498	OMC
1	A	2500	U
1	A	2502	G
1	A	2503	A
1	A	2504	PSU
1	A	2505	G
1	A	2506	U
1	A	2511	U
1	A	2513	A
1	A	2517	C
1	A	2518	A
1	A	2519	U
1	A	2520	C

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Mol	Chain	Res	Type
1	A	2528	U
1	A	2531	A
1	A	2535	G
1	A	2549	G
1	A	2554	U
1	A	2561	U
1	A	2562	U
1	A	2566	A
1	A	2567	G
1	A	2569	G
1	A	2573	C
1	A	2574	G
1	A	2578	G
1	A	2581	G
1	A	2582	G
1	A	2585	U
1	A	2602	A
1	A	2603	G
1	A	2608	G
1	A	2609	U
1	A	2613	U
1	A	2614	A
1	A	2615	U
1	A	2621	G
1	A	2623	G
1	A	2629	U
1	A	2632	A
1	A	2634	A
1	A	2636	C
1	A	2639	A
1	A	2645	G
1	A	2646	C
1	A	2647	U
1	A	2656	U
1	A	2658	C
1	A	2663	G
1	A	2665	A
1	A	2673	G
1	A	2682	A
1	A	2685	G
1	A	2689	U
1	A	2690	U

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Mol	Chain	Res	Type
1	A	2713	U
1	A	2714	G
1	A	2716	C
1	A	2718	G
1	A	2723	C
1	A	2725	A
1	A	2726	A
1	A	2728	U
1	A	2731	G
1	A	2732	G
1	A	2733	A
1	A	2735	G
1	A	2739	U
1	A	2744	G
1	A	2748	A
1	A	2750	A
1	A	2751	G
1	A	2752	C
1	A	2754	U
1	A	2756	U
1	A	2761	A
1	A	2762	C
1	A	2763	G
1	A	2765	A
1	A	2776	A
1	A	2777	G
1	A	2778	A
1	A	2780	G
1	A	2784	U
1	A	2791	G
1	A	2792	A
1	A	2793	C
1	A	2794	C
1	A	2797	U
1	A	2800	A
1	A	2803	G
1	A	2805	C
1	A	2808	G
1	A	2809	A
1	A	2813	A
1	A	2816	G
1	A	2818	U

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Mol	Chain	Res	Type
1	A	2820	A
1	A	2821	A
1	A	2823	A
1	A	2824	C
1	A	2830	C
1	A	2833	U
1	A	2835	A
1	A	2836	U
1	A	2848	G
1	A	2849	U
1	A	2854	G
1	A	2867	G
1	A	2873	A
1	A	2880	C
1	A	2883	A
1	A	2884	U
1	A	2885	G
1	A	2886	A
1	A	2891	U
1	A	2892	G
1	A	2898	U
1	A	2899	A
1	A	2902	C
1	A	2903	U
1	A	2904	U
2	B	7	G
2	B	9	G
2	B	12	C
2	B	14	U
2	B	15	A
2	B	17	C
2	B	22	U
2	B	24	G
2	B	29	A
2	B	30	C
2	B	34	A
2	B	35	C
2	B	40	U
2	B	41	G
2	B	42	C
2	B	44	G
2	B	47	C

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Mol	Chain	Res	Type
2	B	56	G
2	B	58	A
2	B	64	G
2	B	66	A
2	B	68	C
2	B	83	G
2	B	86	G
2	B	88	C
2	B	89	U
2	B	90	C
2	B	91	C
2	B	99	A
2	B	105	G
2	B	108	A
2	B	109	A
2	B	117	G
2	B	118	C
2	B	119	A
32	a	3	A
32	a	4	U
32	a	6	G
32	a	9	G
32	a	11	G
32	a	13	U
32	a	18	C
32	a	22	G
32	a	25	C
32	a	32	A
32	a	33	A
32	a	43	C
32	a	47	C
32	a	48	C
32	a	50	A
32	a	51	A
32	a	54	C
32	a	58	C
32	a	60	A
32	a	65	A
32	a	66	A
32	a	70	U
32	a	71	A
32	a	72	A

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Mol	Chain	Res	Type
32	a	82	G
32	a	83	C
32	a	84	U
32	a	86	G
32	a	87	C
32	a	88	U
32	a	92	U
32	a	93	U
32	a	94	G
32	a	95	C
32	a	99	C
32	a	100	G
32	a	101	A
32	a	104	G
32	a	105	G
32	a	108	G
32	a	109	A
32	a	110	C
32	a	114	U
32	a	119	A
32	a	120	A
32	a	122	G
32	a	126	G
32	a	127	G
32	a	128	G
32	a	129	A
32	a	130	A
32	a	131	A
32	a	132	C
32	a	133	U
32	a	134	G
32	a	137	U
32	a	141	G
32	a	142	G
32	a	144	G
32	a	145	G
32	a	146	G
32	a	149	A
32	a	158	G
32	a	161	A
32	a	163	C
32	a	164	G

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Mol	Chain	Res	Type
32	a	165	G
32	a	168	G
32	a	169	C
32	a	171	A
32	a	173	U
32	a	182	A
32	a	184	G
32	a	187	G
32	a	191	G
32	a	195	A
32	a	197	A
32	a	202	G
32	a	203	G
32	a	204	G
32	a	205	A
32	a	207	C
32	a	209	U
32	a	210	C
32	a	211	G
32	a	212	G
32	a	213	G
32	a	214	C
32	a	217	C
32	a	219	U
32	a	226	G
32	a	231	U
32	a	232	G
32	a	235	C
32	a	240	G
32	a	245	U
32	a	247	G
32	a	251	G
32	a	253	A
32	a	256	U
32	a	260	G
32	a	261	U
32	a	264	C
32	a	266	G
32	a	267	C
32	a	279	A
32	a	280	C
32	a	281	G

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Mol	Chain	Res	Type
32	a	289	G
32	a	298	A
32	a	300	A
32	a	301	G
32	a	306	A
32	a	308	C
32	a	315	A
32	a	316	C
32	a	321	A
32	a	322	C
32	a	328	C
32	a	329	A
32	a	332	G
32	a	346	G
32	a	350	G
32	a	351	G
32	a	352	C
32	a	354	G
32	a	356	A
32	a	362	G
32	a	367	U
32	a	368	U
32	a	369	G
32	a	370	C
32	a	371	A
32	a	372	C
32	a	373	A
32	a	377	G
32	a	378	G
32	a	380	G
32	a	382	A
32	a	390	U
32	a	392	C
32	a	397	A
32	a	398	U
32	a	406	G
32	a	408	A
32	a	412	A
32	a	413	G
32	a	414	A
32	a	421	U
32	a	422	C

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Mol	Chain	Res	Type
32	a	423	G
32	a	424	G
32	a	425	G
32	a	426	U
32	a	429	U
32	a	434	U
32	a	436	C
32	a	437	U
32	a	439	U
32	a	449	G
32	a	451	A
32	a	454	G
32	a	456	A
32	a	458	U
32	a	463	U
32	a	464	U
32	a	465	A
32	a	467	U
32	a	469	C
32	a	474	G
32	a	476	U
32	a	478	A
32	a	481	G
32	a	482	A
32	a	484	G
32	a	485	U
32	a	488	C
32	a	495	A
32	a	497	G
32	a	499	A
32	a	503	C
32	a	507	C
32	a	508	U
32	a	509	A
32	a	511	C
32	a	514	C
32	a	517	G
32	a	518	C
32	a	521	G
32	a	527	A
32	a	529	G
32	a	531	U

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Mol	Chain	Res	Type
32	a	532	A
32	a	533	A
32	a	536	C
32	a	542	G
32	a	547	A
32	a	549	C
32	a	555	U
32	a	559	A
32	a	561	U
32	a	562	U
32	a	563	A
32	a	564	C
32	a	572	A
32	a	573	A
32	a	575	G
32	a	576	C
32	a	577	G
32	a	579	A
32	a	585	G
32	a	588	G
32	a	596	A
32	a	605	U
32	a	606	G
32	a	607	A
32	a	615	G
32	a	619	U
32	a	620	C
32	a	625	U
32	a	626	G
32	a	632	U
32	a	633	G
32	a	641	U
32	a	642	A
32	a	647	C
32	a	653	U
32	a	654	G
32	a	656	G
32	a	661	G
32	a	665	A
32	a	667	G
32	a	671	G
32	a	672	U

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Mol	Chain	Res	Type
32	a	687	A
32	a	688	G
32	a	701	U
32	a	702	A
32	a	703	G
32	a	707	U
32	a	712	A
32	a	713	G
32	a	720	C
32	a	721	G
32	a	723	U
32	a	724	G
32	a	729	A
32	a	731	G
32	a	733	G
32	a	734	G
32	a	744	C
32	a	747	A
32	a	748	G
32	a	752	G
32	a	753	A
32	a	755	G
32	a	760	G
32	a	772	U
32	a	774	G
32	a	787	A
32	a	790	A
32	a	793	U
32	a	794	A
32	a	799	G
32	a	809	G
32	a	812	G
32	a	813	U
32	a	814	A
32	a	815	A
32	a	817	C
32	a	818	G
32	a	820	U
32	a	821	G
32	a	827	U
32	a	828	U
32	a	829	G

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Mol	Chain	Res	Type
32	a	832	G
32	a	841	C
32	a	844	G
32	a	845	A
32	a	846	G
32	a	849	G
32	a	851	G
32	a	854	U
32	a	862	C
32	a	873	A
32	a	874	G
32	a	880	C
32	a	884	U
32	a	899	C
32	a	902	G
32	a	913	A
32	a	914	A
32	a	919	A
32	a	922	G
32	a	931	C
32	a	934	C
32	a	935	A
32	a	939	G
32	a	941	G
32	a	943	U
32	a	960	U
32	a	961	U
32	a	965	U
32	a	966	2MG
32	a	967	5MC
32	a	968	A
32	a	969	A
32	a	971	G
32	a	974	A
32	a	975	A
32	a	976	G
32	a	977	A
32	a	983	A
32	a	986	U
32	a	990	C
32	a	992	U
32	a	993	G

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Mol	Chain	Res	Type
32	a	994	A
32	a	996	A
32	a	999	C
32	a	1001	C
32	a	1004	A
32	a	1009	U
32	a	1017	U
32	a	1018	G
32	a	1023	U
32	a	1024	G
32	a	1026	G
32	a	1028	C
32	a	1029	U
32	a	1030	U
32	a	1031	C
32	a	1032	G
32	a	1033	G
32	a	1034	G
32	a	1036	A
32	a	1037	C
32	a	1043	G
32	a	1044	A
32	a	1046	A
32	a	1053	G
32	a	1054	C
32	a	1056	U
32	a	1061	G
32	a	1065	U
32	a	1070	U
32	a	1081	A
32	a	1082	A
32	a	1085	U
32	a	1087	G
32	a	1088	G
32	a	1089	G
32	a	1094	G
32	a	1095	U
32	a	1100	C
32	a	1101	A
32	a	1110	A
32	a	1118	U
32	a	1119	C

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Mol	Chain	Res	Type
32	a	1123	U
32	a	1124	G
32	a	1125	U
32	a	1127	G
32	a	1132	C
32	a	1136	C
32	a	1137	C
32	a	1138	G
32	a	1139	G
32	a	1140	C
32	a	1141	C
32	a	1142	G
32	a	1143	G
32	a	1145	A
32	a	1146	A
32	a	1148	U
32	a	1150	A
32	a	1151	A
32	a	1152	A
32	a	1157	A
32	a	1159	U
32	a	1160	G
32	a	1168	U
32	a	1169	A
32	a	1171	A
32	a	1174	G
32	a	1181	G
32	a	1184	G
32	a	1190	G
32	a	1191	A
32	a	1193	G
32	a	1194	U
32	a	1195	C
32	a	1196	A
32	a	1197	A
32	a	1200	C
32	a	1201	A
32	a	1204	A
32	a	1207	2MG
32	a	1212	U
32	a	1213	A
32	a	1220	G

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Mol	Chain	Res	Type
32	a	1221	G
32	a	1224	U
32	a	1225	A
32	a	1226	C
32	a	1227	A
32	a	1229	A
32	a	1236	A
32	a	1238	A
32	a	1239	A
32	a	1240	U
32	a	1256	A
32	a	1257	A
32	a	1258	G
32	a	1260	G
32	a	1261	A
32	a	1266	G
32	a	1267	C
32	a	1271	A
32	a	1275	A
32	a	1278	G
32	a	1280	A
32	a	1281	C
32	a	1282	C
32	a	1283	U
32	a	1286	U
32	a	1287	A
32	a	1298	U
32	a	1299	A
32	a	1300	G
32	a	1302	C
32	a	1305	G
32	a	1309	G
32	a	1314	C
32	a	1317	C
32	a	1318	A
32	a	1322	C
32	a	1324	A
32	a	1327	C
32	a	1331	G
32	a	1332	A
32	a	1336	C
32	a	1346	A

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Mol	Chain	Res	Type
32	a	1347	G
32	a	1348	U
32	a	1351	U
32	a	1359	C
32	a	1361	G
32	a	1362	A
32	a	1363	A
32	a	1366	C
32	a	1370	G
32	a	1374	A
32	a	1375	A
32	a	1379	G
32	a	1381	U
32	a	1389	C
32	a	1394	A
32	a	1395	C
32	a	1397	C
32	a	1402	4OC
32	a	1404	C
32	a	1419	G
32	a	1422	G
32	a	1427	C
32	a	1428	A
32	a	1429	A
32	a	1432	G
32	a	1433	A
32	a	1436	U
32	a	1441	A
32	a	1446	A
32	a	1447	A
32	a	1448	C
32	a	1452	C
32	a	1453	G
32	a	1455	G
32	a	1458	G
32	a	1491	G
32	a	1492	A
32	a	1493	A
32	a	1494	G
32	a	1499	A
32	a	1502	A
32	a	1503	A

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Mol	Chain	Res	Type
32	a	1506	U
32	a	1517	G
32	a	1518	MA6
32	a	1529	G
32	a	1530	G
32	a	1533	C
32	a	1534	A
55	x	5	G
55	x	7	U
55	x	8	G
55	x	12	C
55	x	15	C
55	x	17	U
55	x	18	G
55	x	19	G
55	x	20	U
55	x	21	A
55	x	22	G
55	x	26	G
55	x	35	A
55	x	36	U
55	x	47	U
55	x	48	C
55	x	49	G
55	x	50	U
55	x	52	G
55	x	59	A
55	x	60	U
55	x	76	A
55	y	4	G
55	y	5	G
55	y	15	C
55	y	16	C
55	y	18	G
55	y	20	U
55	y	21	A
55	y	22	G
55	y	35	A
55	y	37	A
55	y	46	G
55	y	47	U
55	y	48	C

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Mol	Chain	Res	Type
55	y	49	G
55	y	55	U
55	y	60	U
55	y	61	C
55	y	76	A
56	z	45	A

All (83) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	62	U
1	A	100	U
1	A	119	A
1	A	137	U
1	A	177	G
1	A	181	A
1	A	196	A
1	A	197	A
1	A	212	G
1	A	249	C
1	A	264	C
1	A	271	G
1	A	279	A
1	A	310	A
1	A	322	A
1	A	404	A
1	A	412	A
1	A	446	G
1	A	455	C
1	A	463	G
1	A	481	G
1	A	506	G
1	A	512	G
1	A	620	G
1	A	675	A
1	A	728	G
1	A	733	G
1	A	762	U
1	A	764	A
1	A	784	G
1	A	830	G

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Mol	Chain	Res	Type
1	A	884	U
1	A	896	A
1	A	913	U
1	A	974	G
1	A	984	A
1	A	1088	A
1	A	1126	A
1	A	1140	C
1	A	1141	U
1	A	1151	A
1	A	1190	G
1	A	1200	C
1	A	1224	U
1	A	1288	G
1	A	1311	G
1	A	1320	C
1	A	1344	U
1	A	1379	U
1	A	1602	U
1	A	1608	A
1	A	1730	C
1	A	1786	A
1	A	1857	G
1	A	1884	G
1	A	1918	A
1	A	1937	A
1	A	1939	5MU
1	A	2074	U
1	A	2146	C
1	A	2157	G
1	A	2182	U
1	A	2193	G
1	A	2225	A
1	A	2286	G
1	A	2324	U
1	A	2326	C
1	A	2427	C
1	A	2458	G
1	A	2504	PSU
1	A	2517	C
1	A	2519	U
1	A	2581	G

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Mol	Chain	Res	Type
1	A	2595	G
1	A	2602	A
1	A	2638	G
1	A	2645	G
1	A	2681	C
1	A	2790	U
1	A	2808	G
1	A	2893	A
2	B	40	U

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

28 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	A	2251	1,55	23,26,27	1.27	3 (13%)	32,38,41	2.06	7 (21%)
32	2MG	a	1207	32	23,26,27	1.34	3 (13%)	33,38,41	2.25	6 (18%)
32	4OC	a	1402	32	20,23,24	0.84	0	25,32,35	1.27	3 (12%)
1	OMC	A	2498	1,57	19,22,23	0.89	1 (5%)	25,31,34	1.28	3 (12%)
32	PSU	a	516	32	18,21,22	1.43	3 (16%)	21,30,33	2.07	5 (23%)
1	PSU	A	2580	1	18,21,22	1.46	3 (16%)	21,30,33	2.27	6 (28%)
1	PSU	A	2504	1	18,21,22	1.33	2 (11%)	21,30,33	2.29	6 (28%)
53	MEQ	v	252	53	8,9,10	0.46	0	5,10,12	0.46	0
1	OMU	A	2552	1	19,22,23	1.22	3 (15%)	25,31,34	1.86	6 (24%)
1	5MU	A	1939	1	19,22,23	1.48	5 (26%)	27,32,35	2.08	7 (25%)
32	2MG	a	966	32	23,26,27	1.33	4 (17%)	33,38,41	2.29	7 (21%)
1	PSU	A	746	1,57	18,21,22	1.39	2 (11%)	21,30,33	2.11	4 (19%)
1	2MG	A	2445	1	23,26,27	1.25	5 (21%)	33,38,41	2.27	8 (24%)
1	5MU	A	747	1	19,22,23	1.54	4 (21%)	27,32,35	2.17	11 (40%)
32	UR3	a	1498	32	19,22,23	1.20	1 (5%)	26,32,35	2.04	7 (26%)
1	PSU	A	955	1	18,21,22	1.43	3 (16%)	21,30,33	2.05	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	2457	1	18,21,22	1.48	3 (16%)	21,30,33	2.15	5 (23%)
32	5MC	a	967	32	19,22,23	1.98	2 (10%)	26,32,35	1.36	5 (19%)
1	5MC	A	1962	1	19,22,23	1.89	2 (10%)	26,32,35	1.42	4 (15%)
32	MA6	a	1518	32	23,26,27	1.57	3 (13%)	33,38,41	2.58	15 (45%)
32	2MG	a	1516	32	23,26,27	1.25	4 (17%)	33,38,41	2.25	8 (24%)
1	1MG	A	745	1	23,26,27	1.29	3 (13%)	33,39,42	1.88	7 (21%)
1	PSU	A	1917	1	18,21,22	1.39	3 (16%)	21,30,33	2.07	5 (23%)
1	PSU	A	2605	1	18,21,22	1.44	2 (11%)	21,30,33	2.24	4 (19%)
1	2MG	A	1835	1	23,26,27	1.32	4 (17%)	33,38,41	2.24	8 (24%)
32	5MC	a	1407	32	19,22,23	1.83	2 (10%)	26,32,35	1.35	4 (15%)
1	PSU	A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	2.02	4 (19%)
32	MA6	a	1519	32	23,26,27	1.68	4 (17%)	33,38,41	2.49	15 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A	2251	1,55	-	0/9/27/28	0/3/3/3
32	2MG	a	1207	32	-	3/9/27/28	0/3/3/3
32	4OC	a	1402	32	-	2/9/29/30	0/2/2/2
1	OMC	A	2498	1,57	-	0/9/27/28	0/2/2/2
32	PSU	a	516	32	-	0/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	0/7/25/26	0/2/2/2
53	MEQ	v	252	53	-	1/8/9/11	-
1	OMU	A	2552	1	-	0/9/27/28	0/2/2/2
1	5MU	A	1939	1	-	2/7/25/26	0/2/2/2
32	2MG	a	966	32	-	2/9/27/28	0/3/3/3
1	PSU	A	746	1,57	-	3/7/25/26	0/2/2/2
1	2MG	A	2445	1	-	2/9/27/28	0/3/3/3
1	5MU	A	747	1	-	0/7/25/26	0/2/2/2
32	UR3	a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2457	1	-	2/7/25/26	0/2/2/2
32	5MC	a	967	32	-	0/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	a	1518	32	-	4/11/29/30	0/3/3/3
32	2MG	a	1516	32	-	0/9/27/28	0/3/3/3
1	1MG	A	745	1	-	0/7/25/26	0/3/3/3
1	PSU	A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	2/9/27/28	0/3/3/3
32	5MC	a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	a	1519	32	-	4/11/29/30	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	967	5MC	C5-C4	7.39	1.49	1.44
1	A	1962	5MC	C5-C4	7.06	1.49	1.44
32	a	1407	5MC	C5-C4	6.99	1.49	1.44
32	a	1519	MA6	C5-C4	4.89	1.47	1.39
32	a	1518	MA6	C5-C4	4.63	1.47	1.39
32	a	516	PSU	C6-C5	4.56	1.40	1.35
1	A	955	PSU	C6-C5	4.43	1.40	1.35
1	A	2457	PSU	C6-C5	4.38	1.40	1.35
1	A	1911	PSU	C6-C5	4.18	1.39	1.35
1	A	746	PSU	C6-C5	4.12	1.39	1.35
1	A	1917	PSU	C6-C5	4.01	1.39	1.35
1	A	2605	PSU	C6-C5	3.96	1.39	1.35
1	A	2580	PSU	C6-C5	3.70	1.39	1.35
32	a	1207	2MG	C5-C4	3.42	1.48	1.38
1	A	2504	PSU	C6-C5	3.40	1.39	1.35
32	a	1519	MA6	C5-C6	3.39	1.50	1.41
32	a	966	2MG	C5-C4	3.38	1.48	1.38
1	A	747	5MU	C2-N1	3.36	1.43	1.38
32	a	967	5MC	C6-C5	3.22	1.39	1.34
1	A	2251	OMG	C5-C4	3.17	1.47	1.38
1	A	745	1MG	C5-C4	3.11	1.47	1.38
1	A	1835	2MG	C5-C4	3.10	1.47	1.38
32	a	1498	UR3	C2-N1	3.09	1.42	1.38
32	a	1516	2MG	C5-C4	3.06	1.47	1.38
1	A	747	5MU	C4-C5	2.98	1.49	1.44
1	A	2445	2MG	C5-C4	2.93	1.46	1.38
1	A	745	1MG	C2-N1	2.92	1.42	1.37
32	a	1207	2MG	C2-N3	2.91	1.37	1.32
1	A	1939	5MU	C4-N3	-2.89	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2605	PSU	C4-N3	-2.84	1.33	1.38
32	a	966	2MG	C2-N3	2.80	1.37	1.32
1	A	2580	PSU	C4-N3	-2.79	1.33	1.38
1	A	1962	5MC	C6-C5	2.74	1.39	1.34
32	a	1518	MA6	C5-C6	2.73	1.48	1.41
1	A	747	5MU	C6-C5	2.72	1.39	1.34
1	A	2552	OMU	C2-N1	2.71	1.42	1.38
1	A	1939	5MU	C6-C5	2.70	1.39	1.34
1	A	2457	PSU	C4-N3	-2.66	1.33	1.38
32	a	1518	MA6	C5-N7	-2.61	1.34	1.39
1	A	2504	PSU	C4-N3	-2.57	1.34	1.38
1	A	1835	2MG	C6-N1	-2.56	1.34	1.38
1	A	1939	5MU	C2-N1	2.53	1.42	1.38
1	A	2251	OMG	C6-N1	-2.52	1.34	1.38
32	a	1519	MA6	C8-N7	2.50	1.36	1.31
1	A	745	1MG	C5-N7	-2.47	1.34	1.39
1	A	2251	OMG	C5-N7	-2.47	1.34	1.39
1	A	1835	2MG	C2-N3	2.46	1.36	1.32
32	a	1407	5MC	C6-C5	2.44	1.38	1.34
1	A	747	5MU	C4-N3	-2.40	1.34	1.38
1	A	2552	OMU	C4-N3	-2.36	1.34	1.38
32	a	1519	MA6	C5-N7	-2.36	1.34	1.39
1	A	1911	PSU	C4-N3	-2.35	1.34	1.38
1	A	746	PSU	C4-N3	-2.30	1.34	1.38
1	A	2445	2MG	C5-N7	-2.25	1.34	1.39
1	A	955	PSU	C4-N3	-2.23	1.34	1.38
32	a	966	2MG	C5-N7	-2.21	1.34	1.39
1	A	1939	5MU	C2-N3	-2.21	1.34	1.38
1	A	1835	2MG	C5-N7	-2.20	1.34	1.39
1	A	2445	2MG	C4-N9	-2.18	1.32	1.38
1	A	1917	PSU	C4-N3	-2.17	1.34	1.38
32	a	1516	2MG	C6-N1	-2.16	1.34	1.38
1	A	2580	PSU	C2-N3	-2.13	1.34	1.37
32	a	1207	2MG	C5-N7	-2.12	1.34	1.39
1	A	2552	OMU	C6-C5	2.12	1.40	1.35
32	a	516	PSU	C4-C5	2.11	1.50	1.44
1	A	955	PSU	C4-C5	2.11	1.50	1.44
1	A	1939	5MU	C6-N1	-2.09	1.34	1.38
32	a	1516	2MG	C5-N7	-2.08	1.34	1.39
1	A	2445	2MG	C6-N1	-2.07	1.35	1.38
32	a	966	2MG	C6-N1	-2.06	1.35	1.38
1	A	2457	PSU	C4-C5	2.04	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	1516	2MG	C4-N9	-2.04	1.32	1.38
32	a	516	PSU	C4-N3	-2.04	1.35	1.38
1	A	2498	OMC	C6-C5	2.03	1.39	1.35
1	A	2445	2MG	C2-N3	2.03	1.35	1.32
1	A	1917	PSU	C4-C5	2.03	1.50	1.44

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	966	2MG	C2-N3-C4	7.90	121.89	112.00
32	a	1207	2MG	C2-N3-C4	7.80	121.76	112.00
1	A	1835	2MG	C2-N3-C4	7.63	121.54	112.00
32	a	1498	UR3	C4-N3-C2	-7.54	118.51	124.58
1	A	2445	2MG	C2-N3-C4	7.51	121.39	112.00
32	a	1516	2MG	C2-N3-C4	7.44	121.31	112.00
1	A	2580	PSU	N1-C2-N3	6.74	122.28	115.17
1	A	2251	OMG	C5-C4-N3	-6.63	117.84	128.39
1	A	2605	PSU	N1-C2-N3	6.61	122.14	115.17
1	A	2457	PSU	N1-C2-N3	6.53	122.06	115.17
32	a	966	2MG	C5-C4-N3	-6.45	118.13	128.39
1	A	2504	PSU	N1-C2-N3	6.39	121.91	115.17
1	A	746	PSU	N1-C2-N3	6.39	121.91	115.17
1	A	955	PSU	N1-C2-N3	6.31	121.83	115.17
32	a	1207	2MG	C5-C4-N3	-6.28	118.40	128.39
1	A	1835	2MG	C5-C4-N3	-6.16	118.58	128.39
32	a	1518	MA6	N1-C6-N6	6.04	124.21	116.86
32	a	516	PSU	N1-C2-N3	5.96	121.45	115.17
1	A	1917	PSU	N1-C2-N3	5.83	121.32	115.17
1	A	1911	PSU	N1-C2-N3	5.82	121.31	115.17
1	A	2445	2MG	C5-C4-N3	-5.65	119.39	128.39
32	a	1516	2MG	C5-C4-N3	-5.62	119.44	128.39
32	a	1519	MA6	C5-C4-N3	-5.47	119.18	126.72
32	a	1518	MA6	C5-C4-N3	-5.39	119.29	126.72
1	A	2251	OMG	C2-N3-C4	5.27	121.38	112.30
1	A	745	1MG	C5-C4-N3	-5.25	120.03	128.39
1	A	747	5MU	N3-C2-N1	5.14	121.58	114.89
1	A	1939	5MU	N3-C2-N1	4.88	121.25	114.89
1	A	2251	OMG	N9-C4-N3	4.86	135.66	125.95
1	A	2605	PSU	C4-N3-C2	-4.77	119.81	126.37
32	a	966	2MG	N9-C4-N3	4.71	135.37	125.95
32	a	1207	2MG	N9-C4-N3	4.68	135.31	125.95
1	A	2552	OMU	N3-C2-N1	4.68	120.98	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1835	2MG	N9-C4-N3	4.67	135.29	125.95
1	A	1939	5MU	C4-N3-C2	-4.58	121.33	127.34
32	a	1518	MA6	N3-C4-N9	4.55	134.91	127.17
1	A	747	5MU	C4-N3-C2	-4.52	121.41	127.34
32	a	1519	MA6	C2-N1-C6	4.48	122.78	111.83
1	A	745	1MG	C2-N3-C4	4.47	122.03	111.98
32	a	1519	MA6	C4-C5-N7	-4.47	105.47	110.58
1	A	2552	OMU	C4-N3-C2	-4.47	121.06	126.61
32	a	1518	MA6	C2-N1-C6	4.35	122.44	111.83
1	A	746	PSU	C4-N3-C2	-4.18	120.61	126.37
1	A	2504	PSU	C4-N3-C2	-4.16	120.64	126.37
1	A	2580	PSU	C4-N3-C2	-4.05	120.79	126.37
32	a	1518	MA6	C5-C6-N6	-4.05	118.93	125.33
1	A	745	1MG	N9-C4-N3	4.04	134.02	125.95
1	A	2445	2MG	N9-C4-N3	3.99	133.93	125.95
1	A	955	PSU	C4-N3-C2	-3.99	120.88	126.37
1	A	2457	PSU	C4-N3-C2	-3.94	120.94	126.37
1	A	1911	PSU	C4-N3-C2	-3.94	120.95	126.37
1	A	955	PSU	O2-C2-N1	-3.82	118.84	122.79
32	a	1516	2MG	C6-C5-N7	3.82	137.25	130.29
32	a	516	PSU	C4-N3-C2	-3.81	121.12	126.37
1	A	1939	5MU	C5-C4-N3	3.81	118.64	115.32
1	A	1917	PSU	O2-C2-N1	-3.80	118.86	122.79
1	A	2504	PSU	C3'-C2'-C1'	3.74	106.10	101.69
32	a	1516	2MG	N9-C4-N3	3.72	133.40	125.95
32	a	1498	UR3	C5-C4-N3	3.71	119.93	115.04
1	A	1917	PSU	C4-N3-C2	-3.68	121.30	126.37
32	a	1519	MA6	N3-C4-N9	3.68	133.43	127.17
32	a	1519	MA6	C2-N3-C4	3.64	120.72	111.83
1	A	2504	PSU	O2-C2-N1	-3.64	119.04	122.79
32	a	1518	MA6	C2'-C1'-N9	-3.62	104.30	113.30
1	A	746	PSU	O2-C2-N1	-3.62	119.05	122.79
1	A	747	5MU	C5M-C5-C4	3.57	122.59	118.78
1	A	2457	PSU	O2-C2-N1	-3.56	119.12	122.79
1	A	2552	OMU	C5-C4-N3	3.54	119.76	114.80
1	A	747	5MU	C5-C4-N3	3.54	118.40	115.32
1	A	1911	PSU	O2-C2-N1	-3.52	119.16	122.79
1	A	2445	2MG	C6-C5-N7	3.52	136.69	130.29
1	A	1939	5MU	C5-C6-N1	-3.51	119.50	123.31
32	a	516	PSU	O2-C2-N1	-3.49	119.19	122.79
32	a	1518	MA6	C2-N3-C4	3.49	120.35	111.83
32	a	1519	MA6	C9-N6-C6	-3.47	111.69	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2605	PSU	O2-C2-N1	-3.42	119.26	122.79
32	a	1519	MA6	C10-N6-C6	-3.41	111.83	120.52
32	a	1518	MA6	C9-N6-C6	-3.39	111.90	120.52
1	A	1835	2MG	C6-C5-N7	3.36	136.41	130.29
1	A	1962	5MC	O2-C2-N3	-3.35	117.04	122.33
32	a	1518	MA6	N1-C2-N3	-3.35	123.52	128.58
32	a	1519	MA6	N1-C2-N3	-3.27	123.62	128.58
32	a	967	5MC	O2-C2-N3	-3.24	117.22	122.33
1	A	2445	2MG	N1-C2-N2	3.22	119.85	116.56
32	a	1207	2MG	C6-C5-N7	3.21	136.13	130.29
1	A	1939	5MU	O4-C4-C5	-3.18	121.27	124.92
32	a	1519	MA6	C10-N6-C9	-3.18	105.97	116.18
32	a	1519	MA6	C2'-C1'-N9	-3.17	105.42	113.30
32	a	967	5MC	C5-C4-N3	-3.14	118.54	121.75
1	A	2580	PSU	O2-C2-N1	-3.12	119.57	122.79
32	a	1407	5MC	O2-C2-N3	-3.12	117.42	122.33
1	A	1962	5MC	C5-C4-N3	-3.05	118.63	121.75
32	a	966	2MG	C6-C5-N7	3.02	135.79	130.29
32	a	516	PSU	C3'-C2'-C1'	3.01	105.24	101.69
1	A	1917	PSU	C6-C5-C4	-3.00	116.15	118.17
1	A	2498	OMC	O2-C2-N3	-3.00	117.61	122.33
1	A	747	5MU	C5M-C5-C6	-2.98	118.82	122.85
32	a	1518	MA6	C4-C5-N7	-2.96	107.20	110.58
32	a	1519	MA6	C5-N7-C8	2.94	108.07	103.45
1	A	2552	OMU	O4-C4-C5	-2.92	120.12	125.16
1	A	1917	PSU	C3'-C2'-C1'	2.90	105.11	101.69
32	a	1519	MA6	N1-C6-N6	2.89	120.38	116.86
1	A	2251	OMG	C6-C5-N7	2.89	135.54	130.29
1	A	2457	PSU	C3'-C2'-C1'	2.84	105.04	101.69
32	a	1402	4OC	O2-C2-N3	-2.78	117.95	122.33
32	a	1407	5MC	C5-C4-N3	-2.76	118.92	121.75
32	a	1516	2MG	N1-C2-N2	2.75	119.36	116.56
32	a	1518	MA6	C10-N6-C6	-2.74	113.54	120.52
32	a	1516	2MG	C4-C5-N7	-2.73	106.34	110.67
1	A	1962	5MC	CM5-C5-C6	-2.71	119.19	122.85
1	A	1911	PSU	C6-C5-C4	-2.70	116.35	118.17
32	a	1407	5MC	C5-C6-N1	-2.70	120.38	123.31
32	a	1519	MA6	O4'-C1'-N9	2.68	113.24	108.09
1	A	2580	PSU	C3'-C2'-C1'	2.65	104.82	101.69
32	a	1407	5MC	CM5-C5-C6	-2.59	119.34	122.85
1	A	747	5MU	O4-C4-C5	-2.57	121.97	124.92
1	A	2552	OMU	C6-N1-C2	-2.50	117.95	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	747	5MU	O2-C2-N3	-2.48	116.91	121.49
1	A	1939	5MU	O4'-C1'-N1	2.48	113.97	108.36
1	A	747	5MU	C1'-N1-C2	2.47	122.02	117.59
32	a	1518	MA6	C4-N9-C8	2.46	108.33	105.74
1	A	2445	2MG	C4-C5-N7	-2.46	106.77	110.67
1	A	2445	2MG	O6-C6-C5	-2.45	120.07	126.53
32	a	1207	2MG	C4-C5-N7	-2.44	106.80	110.67
32	a	516	PSU	C6-C5-C4	-2.43	116.54	118.17
1	A	2251	OMG	C4-C5-N7	-2.39	106.89	110.67
32	a	1519	MA6	C6-C5-N7	2.38	137.24	133.43
1	A	745	1MG	C6-C5-N7	2.36	134.61	129.36
32	a	1402	4OC	C6-C5-C4	2.36	119.84	117.00
1	A	2605	PSU	C5-C6-N1	-2.34	118.89	122.14
1	A	2445	2MG	C2'-C1'-N9	-2.34	106.74	113.25
1	A	1835	2MG	C2'-C1'-N9	-2.33	106.75	113.25
32	a	966	2MG	C3'-C2'-C1'	2.32	105.86	101.46
1	A	2580	PSU	O4'-C1'-C2'	2.32	108.36	105.15
32	a	966	2MG	C4-C5-N7	-2.29	107.04	110.67
1	A	1962	5MC	C5-C6-N1	-2.29	120.83	123.31
1	A	745	1MG	C4-C5-N7	-2.29	107.05	110.67
1	A	2251	OMG	O6-C6-C5	-2.28	120.53	126.53
1	A	747	5MU	C5-C6-N1	-2.27	120.85	123.31
1	A	1835	2MG	C4-C5-N7	-2.26	107.08	110.67
32	a	1402	4OC	O4'-C1'-N1	2.25	113.47	108.36
1	A	745	1MG	O6-C6-C5	-2.25	118.78	124.59
1	A	747	5MU	C3'-C2'-C1'	2.25	105.72	101.46
32	a	966	2MG	O6-C6-C5	-2.25	120.59	126.53
32	a	1207	2MG	O6-C6-C5	-2.24	120.62	126.53
1	A	745	1MG	C2'-C1'-N9	-2.22	107.06	113.25
1	A	1939	5MU	O2-C2-N3	-2.22	117.39	121.49
1	A	2498	OMC	O4'-C1'-N1	2.21	113.36	108.36
1	A	1835	2MG	C5-C6-N1	2.20	118.85	113.25
1	A	2504	PSU	C5-C6-N1	-2.19	119.10	122.14
32	a	967	5MC	CM5-C5-C6	-2.16	119.93	122.85
32	a	1516	2MG	O6-C6-C5	-2.16	120.84	126.53
32	a	1518	MA6	C5-N7-C8	2.15	106.83	103.45
1	A	747	5MU	C6-N1-C2	-2.14	119.17	121.30
1	A	1835	2MG	O6-C6-C5	-2.13	120.91	126.53
1	A	746	PSU	C5-C6-N1	-2.13	119.19	122.14
32	a	1516	2MG	C2'-C1'-N9	-2.10	107.39	113.25
32	a	967	5MC	C3'-C2'-C1'	2.10	105.44	101.46
32	a	1498	UR3	C3U-N3-C4	2.10	120.78	117.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2580	PSU	O2-C2-N3	-2.09	118.16	121.86
1	A	2251	OMG	C5-C6-N1	2.08	118.54	113.25
32	a	1498	UR3	O4-C4-C5	-2.07	118.47	124.35
1	A	2498	OMC	C1'-N1-C2	2.06	123.00	118.44
32	a	1498	UR3	O3'-C3'-C4'	2.05	116.98	111.08
32	a	1498	UR3	C1'-N1-C2	2.04	120.39	117.04
1	A	2504	PSU	O4'-C1'-C2'	2.04	107.98	105.15
1	A	2457	PSU	C5-C6-N1	-2.04	119.31	122.14
32	a	1518	MA6	C10-N6-C9	-2.04	109.64	116.18
32	a	1498	UR3	C3'-C2'-C1'	2.04	105.31	101.46
32	a	1519	MA6	C4-N9-C8	2.04	107.88	105.74
32	a	967	5MC	O4'-C1'-N1	2.03	112.96	108.36
1	A	2552	OMU	O2-C2-N3	-2.03	117.75	121.49
32	a	1518	MA6	C3'-C2'-C1'	2.02	105.28	101.46

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	746	PSU	O4'-C4'-C5'-O5'
32	a	1402	4OC	O4'-C4'-C5'-O5'
32	a	1518	MA6	C5-C6-N6-C9
53	v	252	MEQ	C-CA-CB-CG
1	A	1939	5MU	O4'-C4'-C5'-O5'
1	A	2445	2MG	C3'-C4'-C5'-O5'
1	A	2457	PSU	O4'-C4'-C5'-O5'
32	a	1518	MA6	O4'-C4'-C5'-O5'
32	a	1519	MA6	O4'-C4'-C5'-O5'
1	A	1835	2MG	C3'-C4'-C5'-O5'
1	A	1939	5MU	C3'-C4'-C5'-O5'
1	A	2445	2MG	O4'-C4'-C5'-O5'
32	a	966	2MG	O4'-C4'-C5'-O5'
32	a	966	2MG	C3'-C4'-C5'-O5'
1	A	746	PSU	C3'-C4'-C5'-O5'
32	a	1402	4OC	C3'-C4'-C5'-O5'
1	A	1835	2MG	O4'-C4'-C5'-O5'
32	a	1207	2MG	C3'-C4'-C5'-O5'
1	A	2457	PSU	C3'-C4'-C5'-O5'
32	a	1207	2MG	O4'-C4'-C5'-O5'
32	a	1518	MA6	C3'-C4'-C5'-O5'
32	a	1519	MA6	C3'-C4'-C5'-O5'
32	a	1207	2MG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
32	a	1519	MA6	C5-C6-N6-C9
32	a	1518	MA6	N1-C6-N6-C9
1	A	746	PSU	O4'-C1'-C5-C4
32	a	1519	MA6	C4'-C5'-O5'-P

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	2504	PSU	14	0
1	A	1939	5MU	1	0
32	a	966	2MG	2	0
32	a	967	5MC	1	0
1	A	1962	5MC	1	0
32	a	1518	MA6	2	0
1	A	2605	PSU	1	0
1	A	1835	2MG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 125 ligands modelled in this entry, 125 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

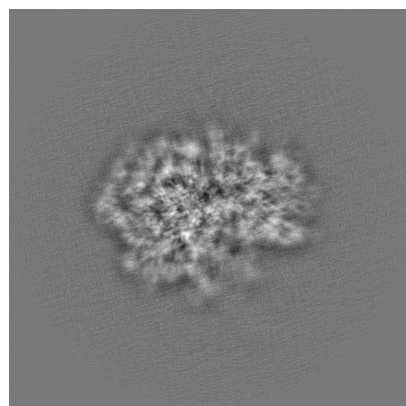
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8505. These allow visual inspection of the internal detail of the map and identification of artifacts.

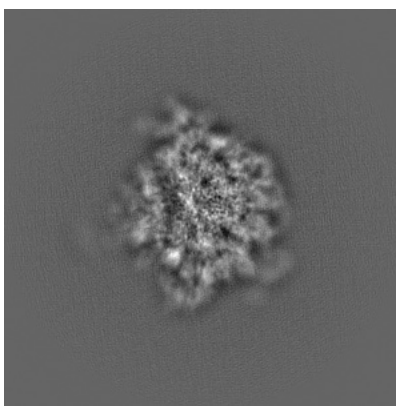
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

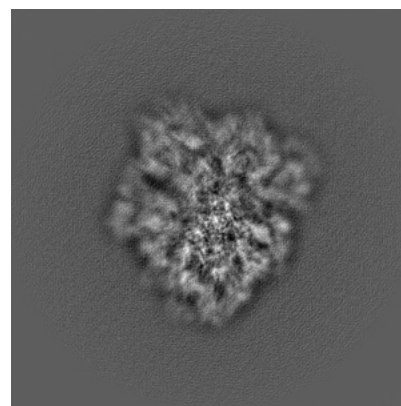
6.1.1 Primary map



X

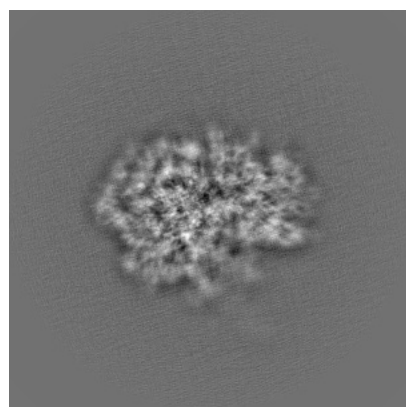


Y

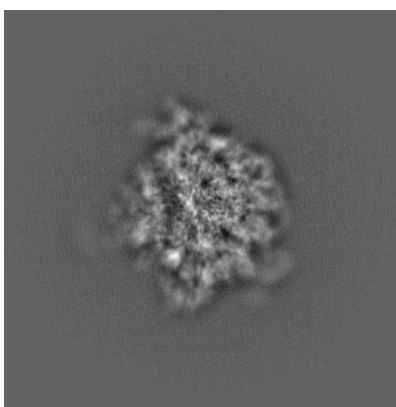


Z

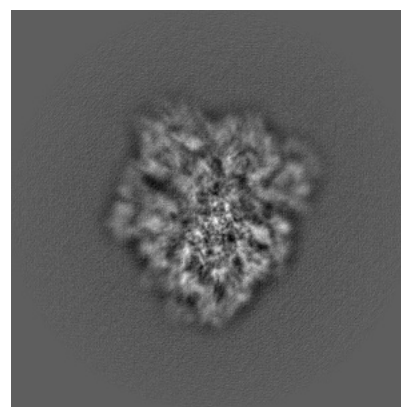
6.1.2 Raw map



X



Y

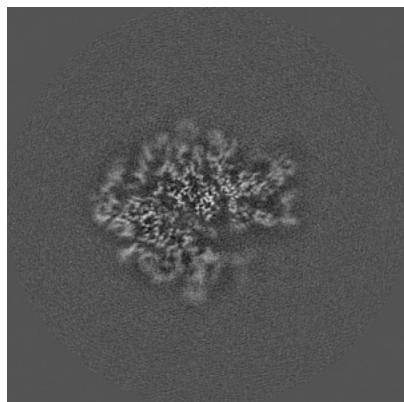


Z

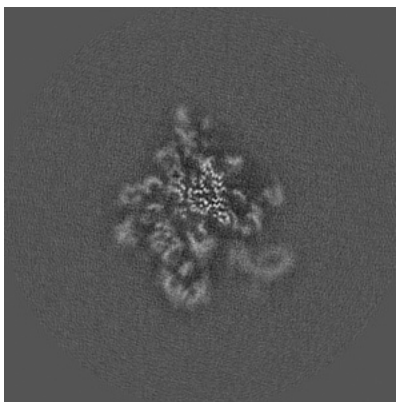
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

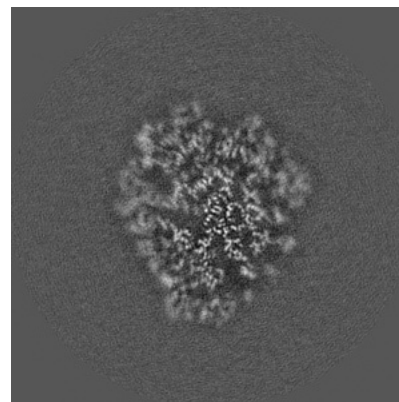
6.2.1 Primary map



X Index: 192

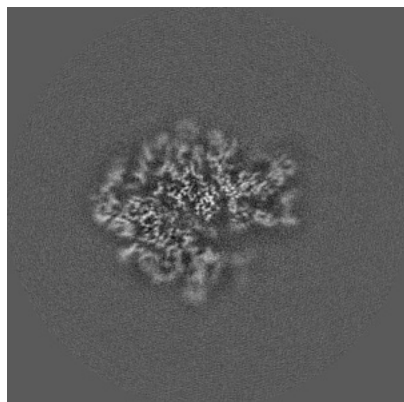


Y Index: 192

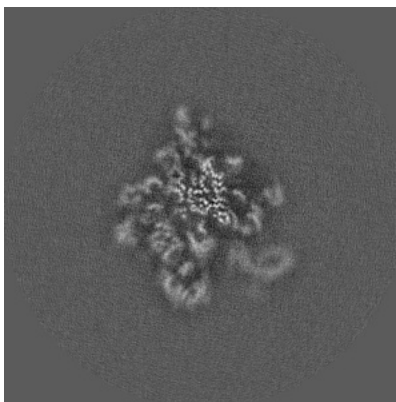


Z Index: 192

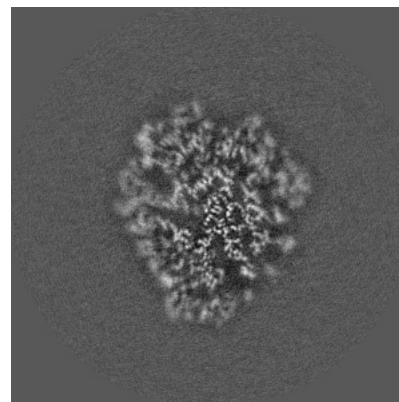
6.2.2 Raw map



X Index: 192



Y Index: 192

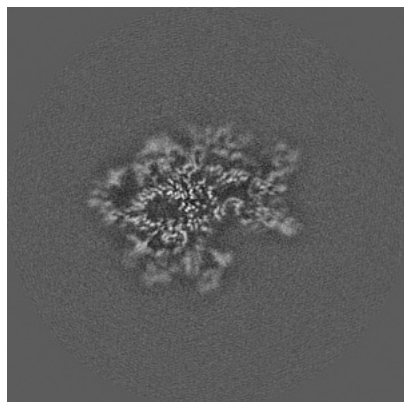


Z Index: 192

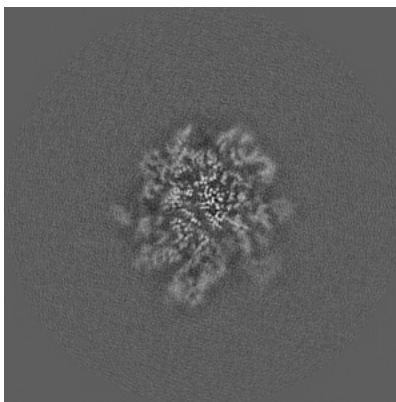
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

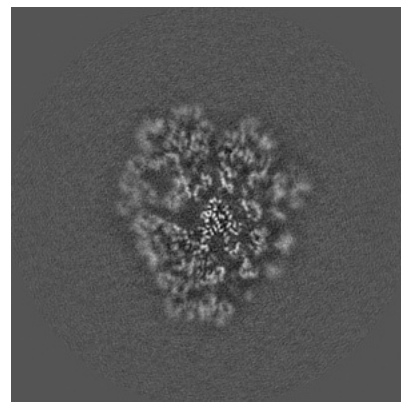
6.3.1 Primary map



X Index: 201

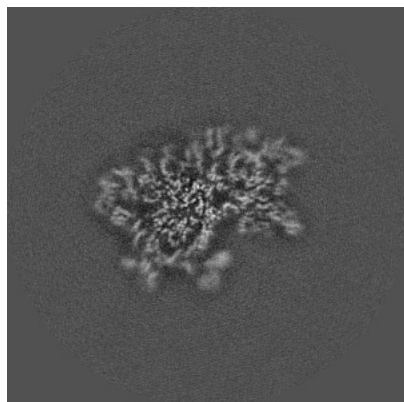


Y Index: 170

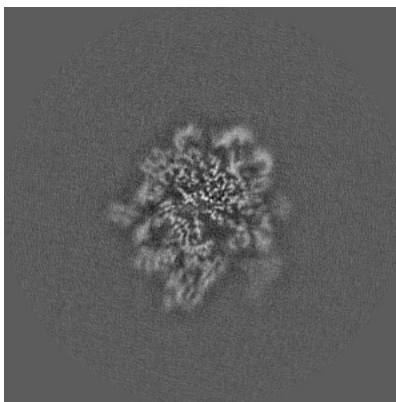


Z Index: 195

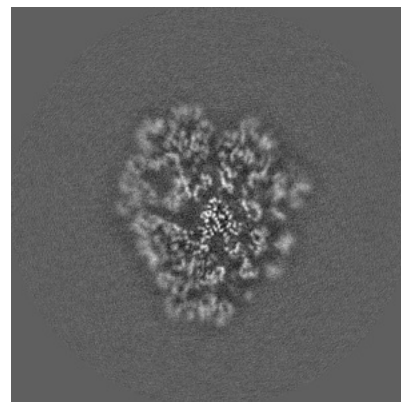
6.3.2 Raw map



X Index: 207



Y Index: 174

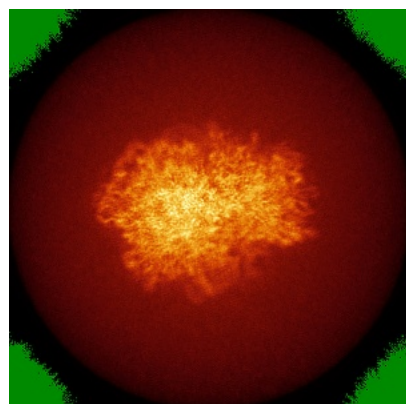


Z Index: 195

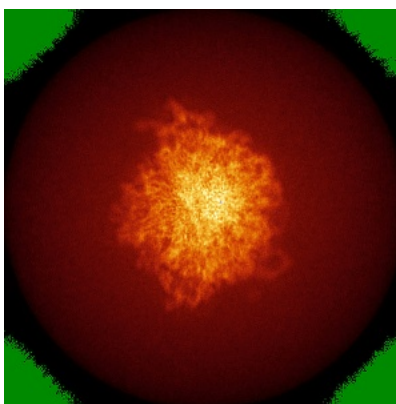
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

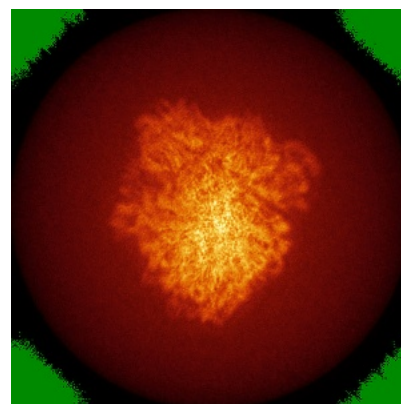
6.4.1 Primary map



X

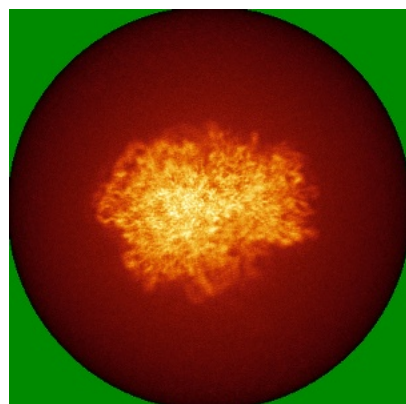


Y

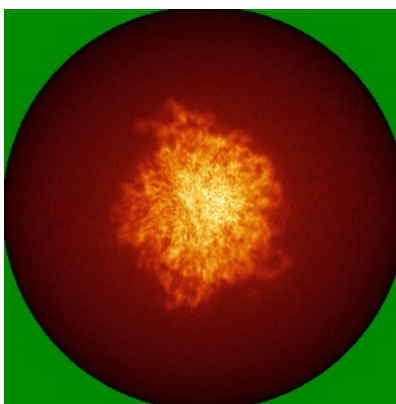


Z

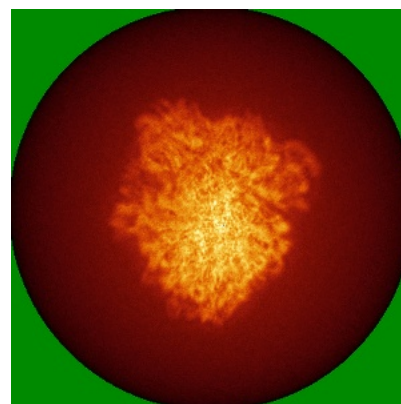
6.4.2 Raw map



X



Y

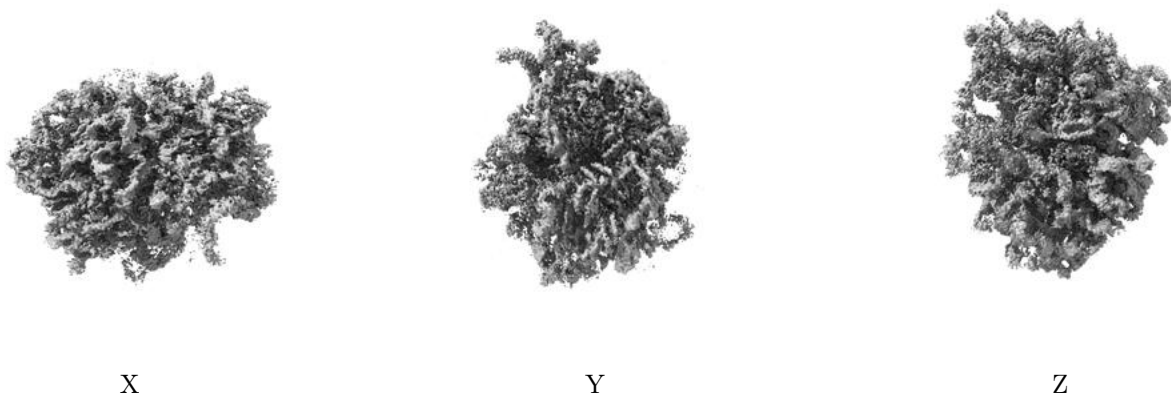


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

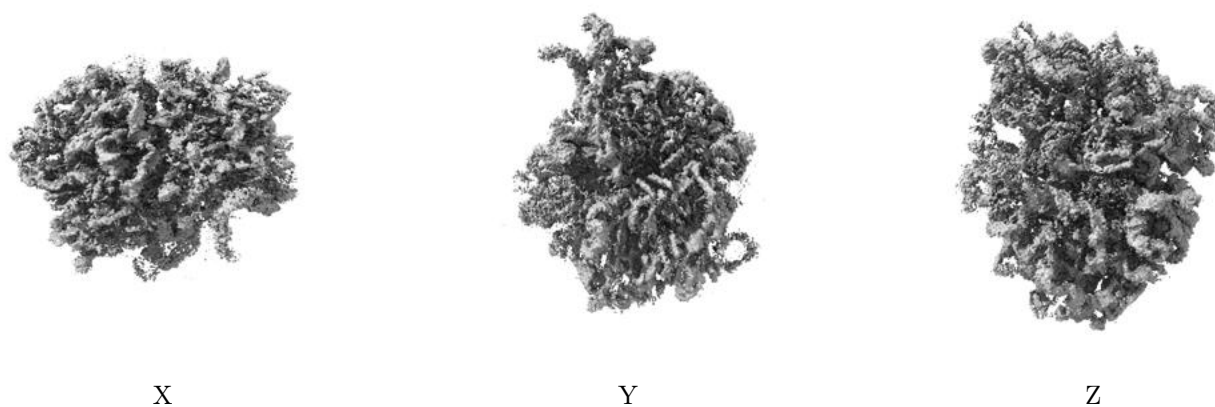
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

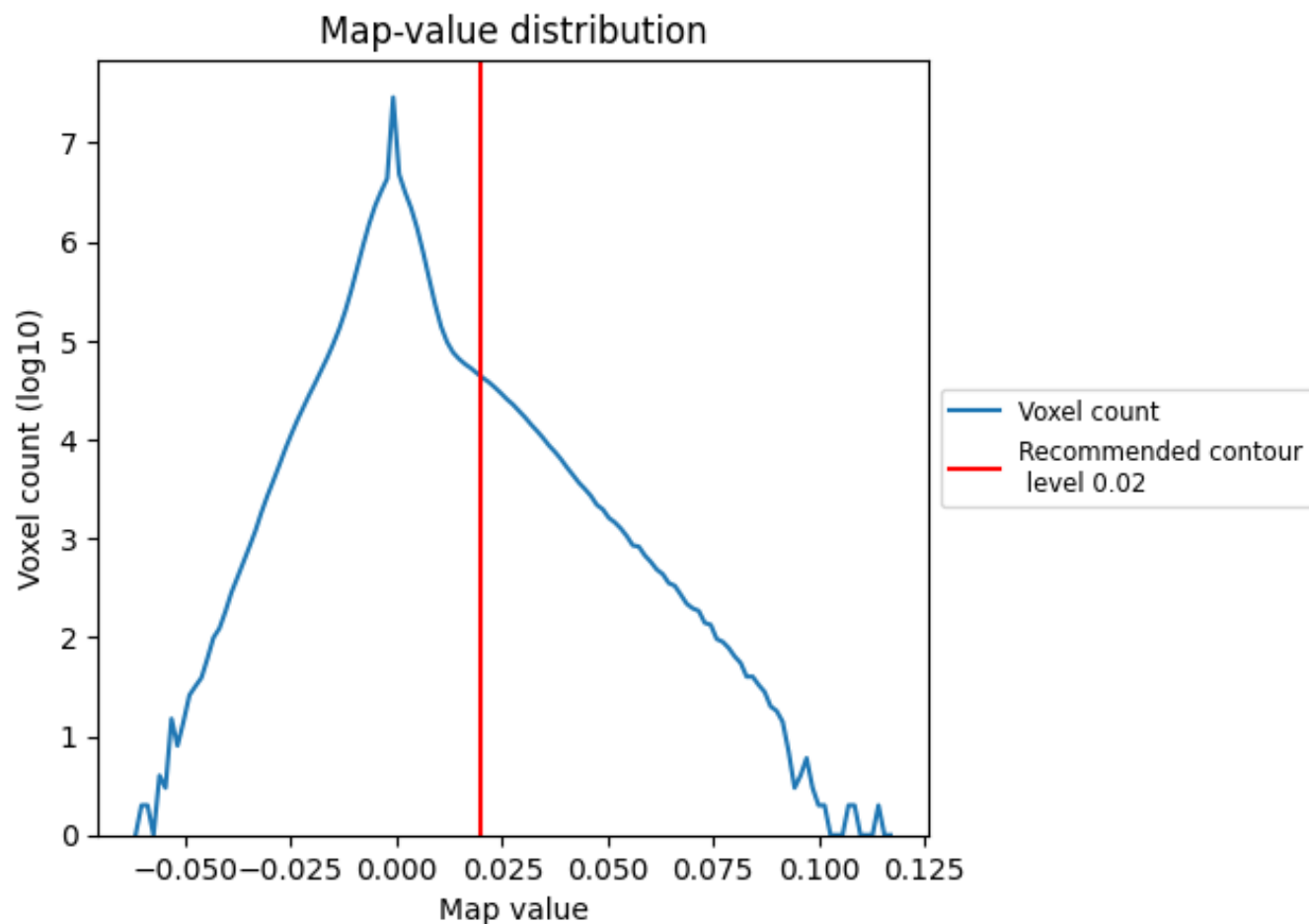
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

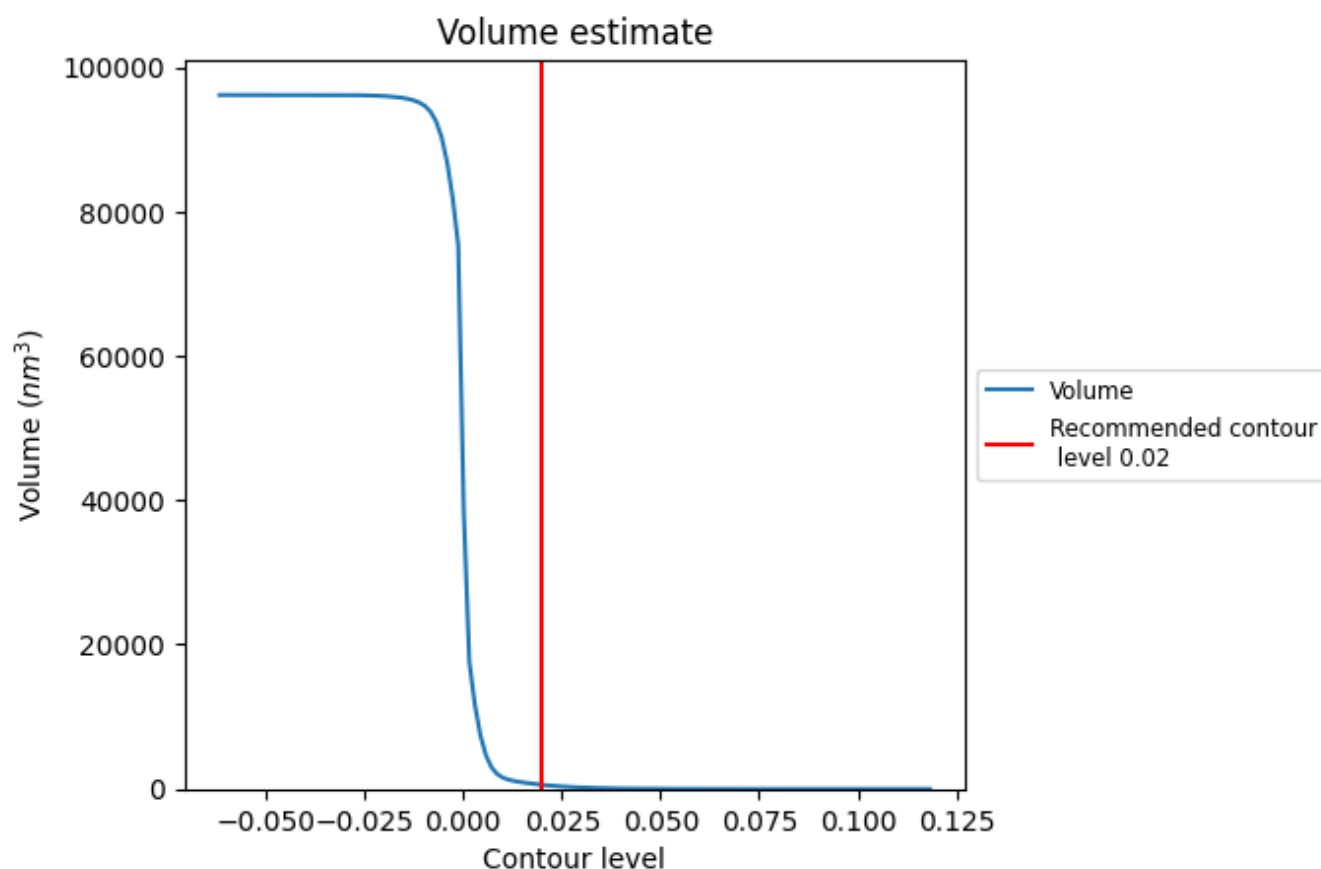
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

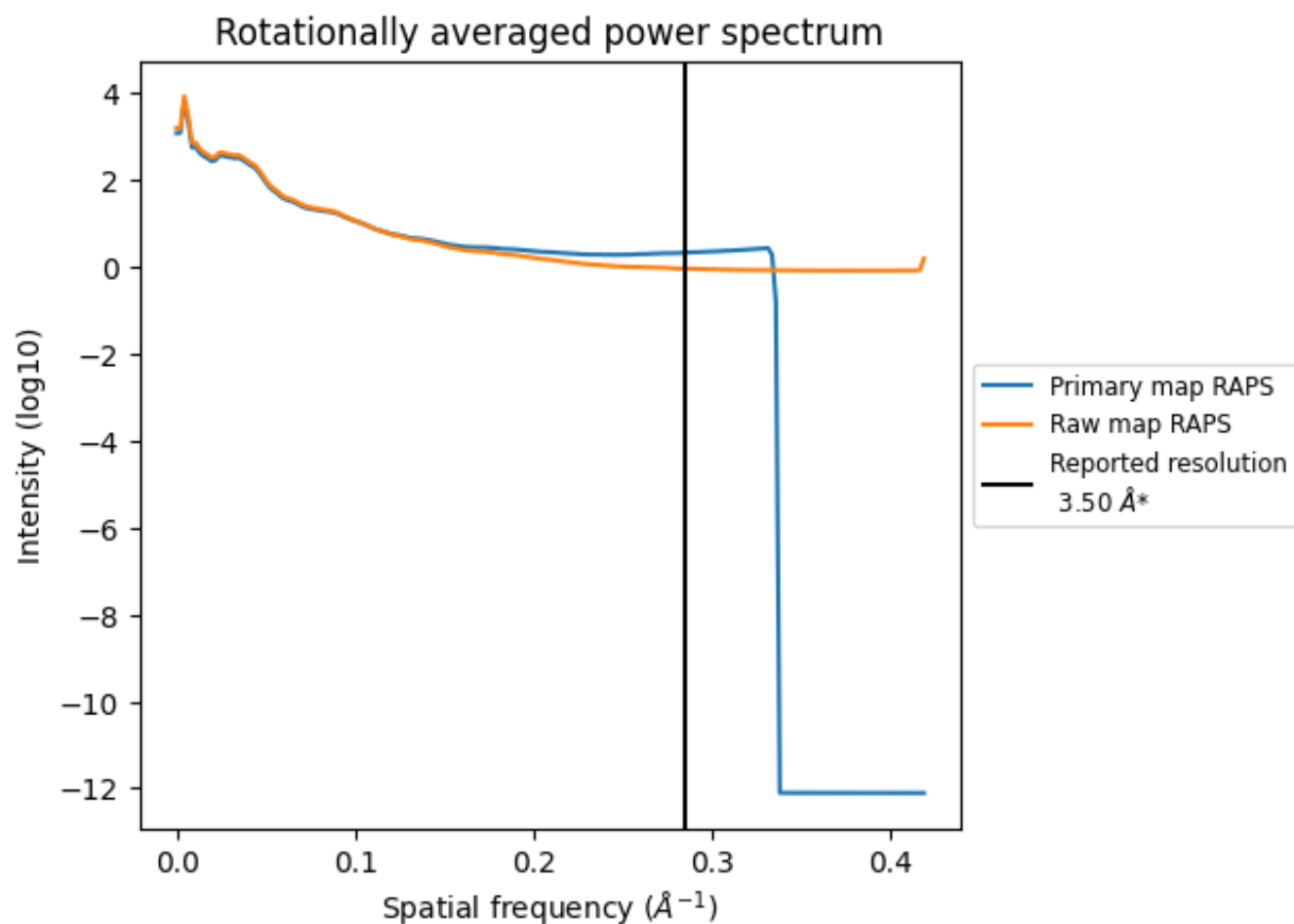
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 571 nm³; this corresponds to an approximate mass of 516 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

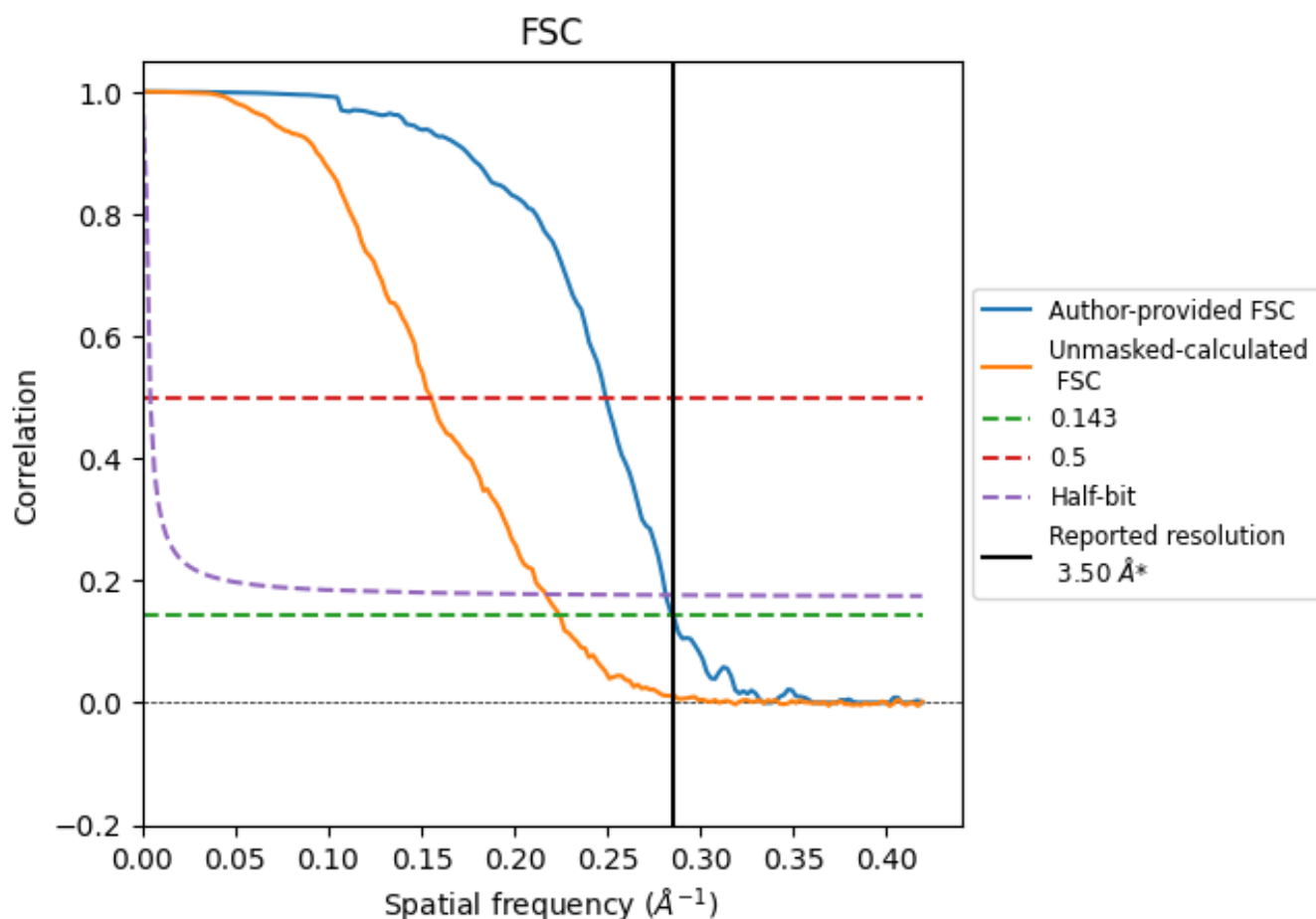


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.286 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

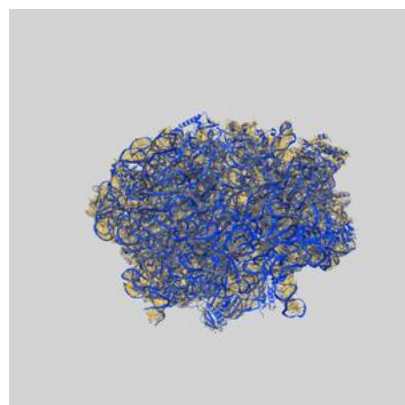
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	4.01	3.55
Unmasked-calculated*	4.46	6.44	4.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.46 differs from the reported value 3.5 by more than 10 %

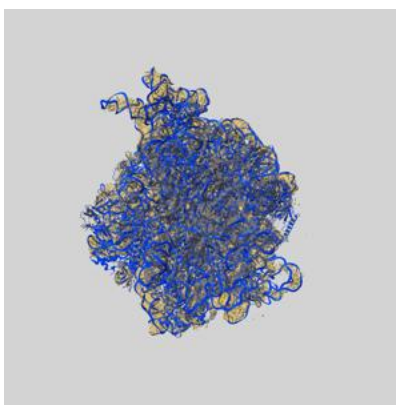
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8505 and PDB model 5U4I. Per-residue inclusion information can be found in section 3 on page 16.

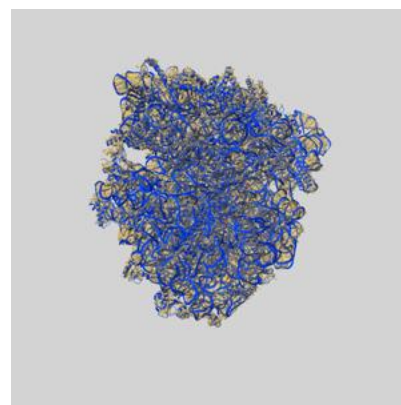
9.1 Map-model overlay [i](#)



X



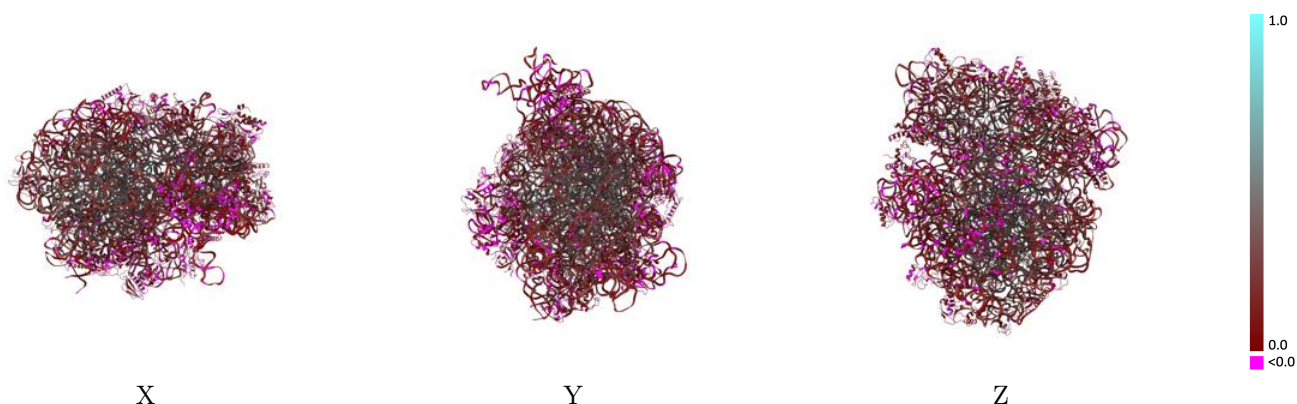
Y



Z

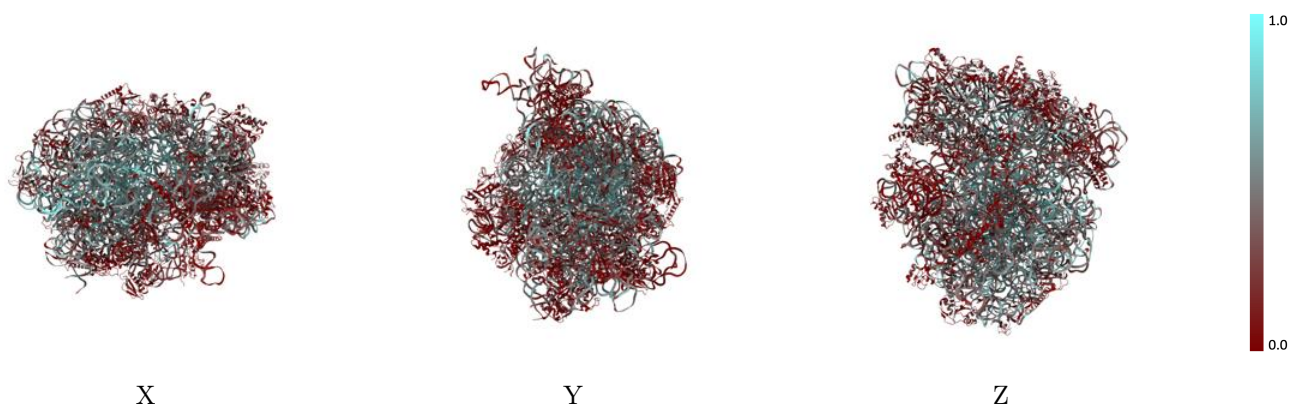
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



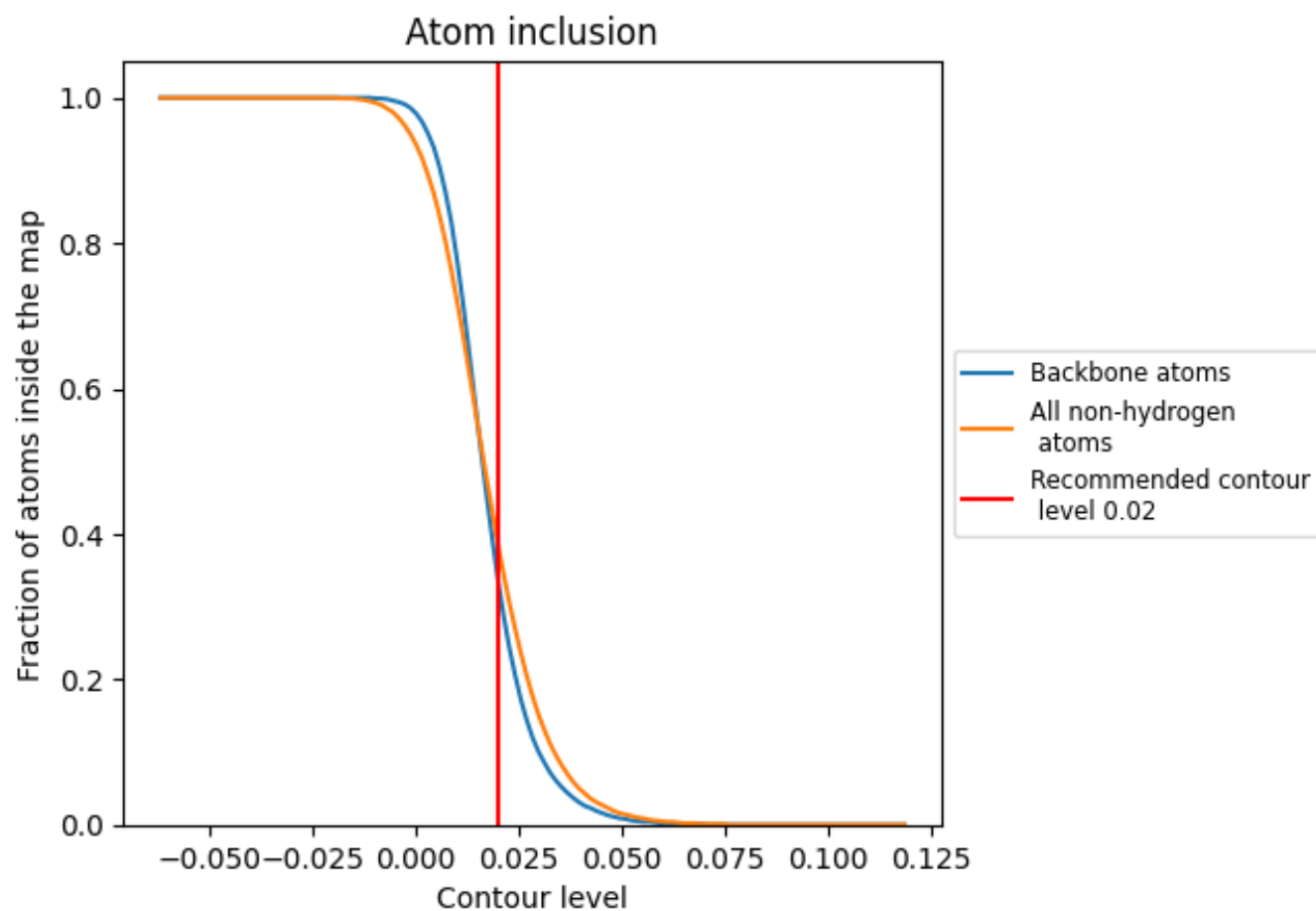
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 33% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3830	 0.2260
0	 0.1900	 0.1590
1	 0.2480	 0.2150
2	 0.0620	 0.0860
3	 0.3610	 0.3810
4	 0.0710	 0.2420
5	 0.0340	 0.1190
A	 0.5160	 0.2680
B	 0.3300	 0.1370
C	 0.2930	 0.2720
D	 0.1460	 0.1590
E	 0.2040	 0.1900
F	 0.1110	 0.1000
G	 0.0680	 0.0720
H	 0.0090	 0.0470
J	 0.0020	 0.0490
K	 0.0960	 0.1390
L	 0.2190	 0.2160
M	 0.1410	 0.1840
N	 0.2000	 0.1900
O	 0.1870	 0.2130
P	 0.0820	 0.0970
Q	 0.0930	 0.1020
R	 0.2160	 0.2310
S	 0.2150	 0.2020
T	 0.3700	 0.2930
U	 0.1870	 0.2110
V	 0.2090	 0.2040
W	 0.1060	 0.0790
X	 0.0860	 0.1640
Y	 0.1000	 0.1340
Z	 0.2270	 0.1710
a	 0.4510	 0.2410
b	 0.1410	 0.1220
c	 0.2430	 0.2010



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Chain	Atom inclusion	Q-score
d	 0.1000	 0.1590
e	 0.2730	 0.2490
f	 0.1720	 0.1020
g	 0.1770	 0.1410
h	 0.1700	 0.1550
i	 0.1200	 0.1520
j	 0.0990	 0.1540
k	 0.1510	 0.1510
l	 0.3090	 0.2900
m	 0.1470	 0.1640
n	 0.1430	 0.1670
o	 0.3030	 0.1620
p	 0.0450	 0.0090
q	 0.1230	 0.1480
r	 0.0700	 0.1120
s	 0.1140	 0.1500
t	 0.0340	 0.0500
u	 0.1940	 0.1490
v	 0.1830	 0.2170
w	 0.2820	 0.2930
x	 0.5740	 0.3170
y	 0.1070	 0.1170
z	 0.3280	 0.3360