Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 10:37 AM JST

PDB ID	:	44II / pdb_000044ii
EMDB ID	:	EMD-82632
Title	:	Structural basis of ribosomal RNA modification of A- and P-tRNA bound 70S
Deposited on	:	2026-07-30
Resolution	:	2.84 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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)	:	2.50

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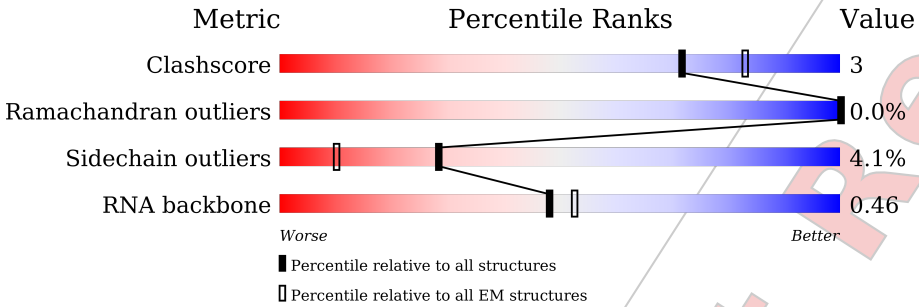
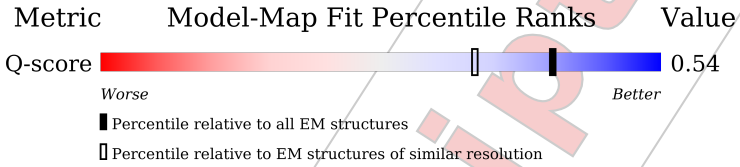
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.84 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	11884 (2.34 - 3.34)

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 <=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	0	2904	75% 19% • 5%
2	1	120	77% 22% •

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Mol	Chain	Length	Quality of chain
3	2	1542	65% 30%
4	3	10	70% 30%
5	4	77	6% 62% 32% 5%
6	5	76	5% 70% 22% 8%
7	A	273	87% 12%
8	B	209	94% 5%
9	C	201	94% 6%
10	D	179	80% 16%
11	E	177	88% 9%
12	F	149	64% 87% 11%
13	G	142	93% 7%
14	H	123	87% 13%
15	I	144	88% 11%
16	J	136	86% 14%
17	K	127	82% 11% 7%
18	L	117	92% 6%
19	M	115	89% 10%
20	N	118	94% 5%
21	O	103	90% 10%
22	P	110	91% 6%
23	Q	100	88% 5% 7%
24	R	104	5% 93%
25	S	94	89% 9%
26	T	85	82% 6% 12%
27	U	78	82% 15%

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Mol	Chain	Length	Quality of chain
28	V	63	84% 11% 5%
29	W	59	90% 7%
30	X	70	10% 71% 13% 14%
31	a	57	82% 14%
32	b	55	75% 18% 7%
33	c	46	89% 9%
34	d	65	97%
35	e	38	89% 11%
36	f	241	11% 70% 20% 7%
37	g	233	70% 18% 12%
38	h	206	19% 87% 11%
39	i	167	80% 11% 7%
40	j	131	66% 13% 19%
41	k	179	21% 66% 16% 16%
42	l	130	85% 14%
43	m	130	5% 67% 28%
44	n	103	20% 75% 19%
45	o	129	81% 10% 9%
46	p	124	5% 84% 15%
47	q	118	75% 21%
48	r	101	6% 82% 15%
49	s	89	82% 16%
50	t	82	16% 84% 15%
51	u	84	79% 17% 5%
52	v	75	80% 8% 12%

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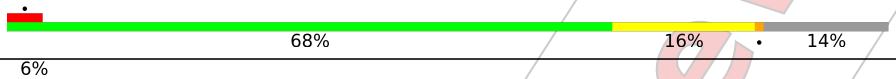
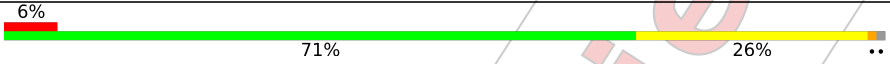
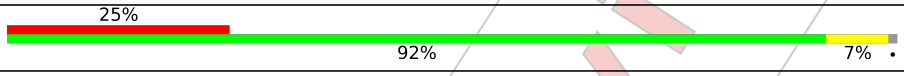
Mol	Chain	Length	Quality of chain
53	w	92	
54	x	87	
55	y	71	

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2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 142656 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
			Total	C	N	O	P		
1	0	2758	59219	26417	10911	19134	2757	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1	120	2566	1144	468	835	119	0	0

- Molecule 3 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	2	1534	32917	14681	6041	10661	1534	0	0

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	3	10	215	97	41	67	10	0	0

- Molecule 5 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
5	4	77	1642	734	297	534	76	1	0	0

- Molecule 6 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
6	5	76	1625	729	283	537	75	1	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	208	Total	C	N	O	S	0	0
			1559	976	287	292	4		

- Molecule 9 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	173	Total	C	N	O	S	0	0
			1295	814	237	242	2		

- Molecule 12 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 13 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 14 is a protein called Large ribosomal subunit protein uL14.

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 15 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 16 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 17 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 18 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 19 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 22 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 23 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	75	Total	C	N	O	S	0	0
			572	355	116	100	1		

- Molecule 27 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

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Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	60	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 29 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	57	Total	C	N	O	S	0	0
			439	276	86	75	2		

- Molecule 30 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 31 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 32 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	b	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 33 is a protein called Large ribosomal subunit protein bL34.

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

- Molecule 34 is a protein called Large ribosomal subunit protein bL35.

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

- Molecule 35 is a protein called Large ribosomal subunit protein bL36A.

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

- Molecule 36 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 37 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 38 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 39 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 40 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 41 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 42 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 43 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 44 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 45 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 46 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 47 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 48 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 49 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 50 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 51 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 52 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 53 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 54 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 55 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

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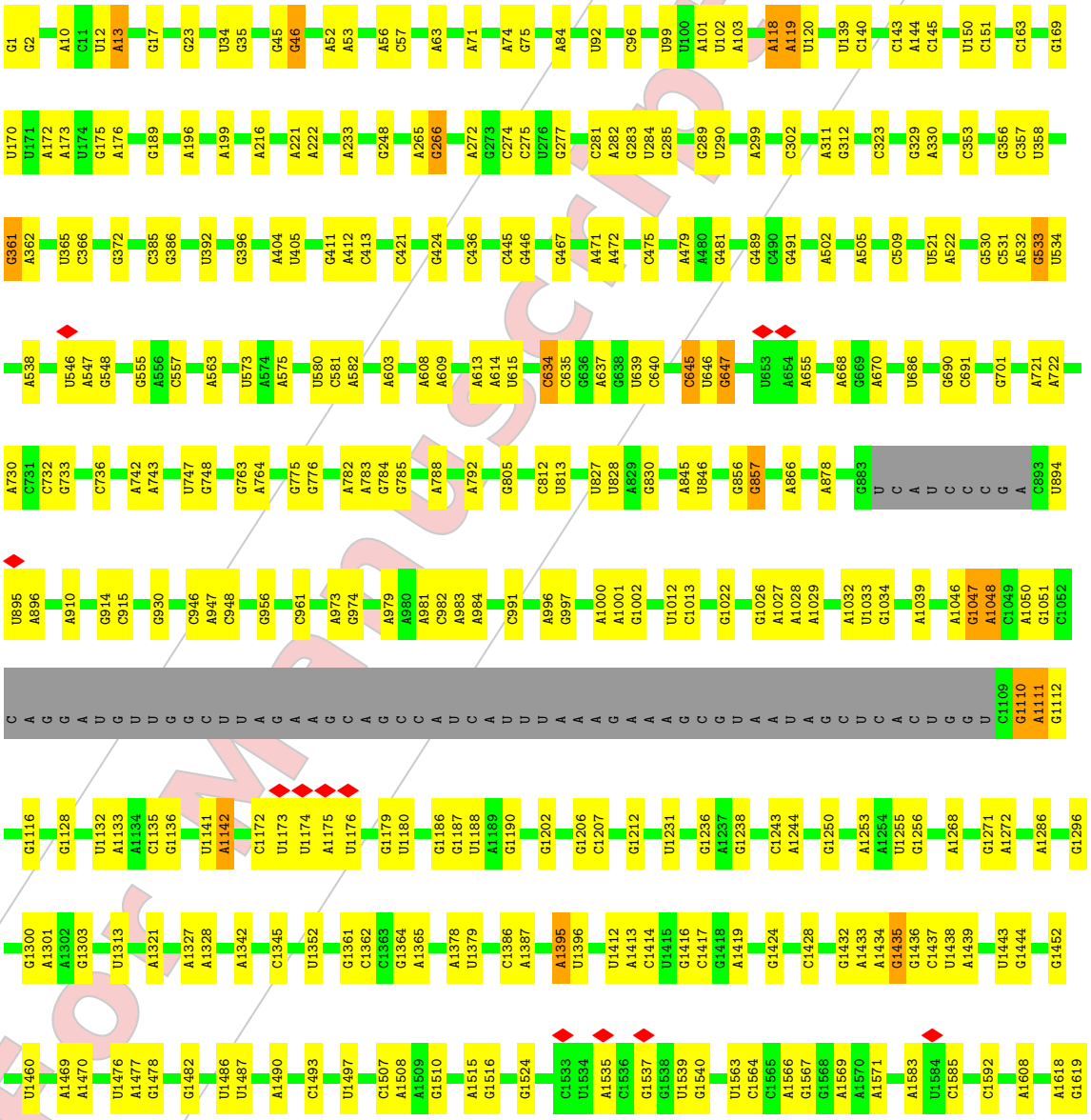
3 Residue-property plots (i)

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

Chain 0: 



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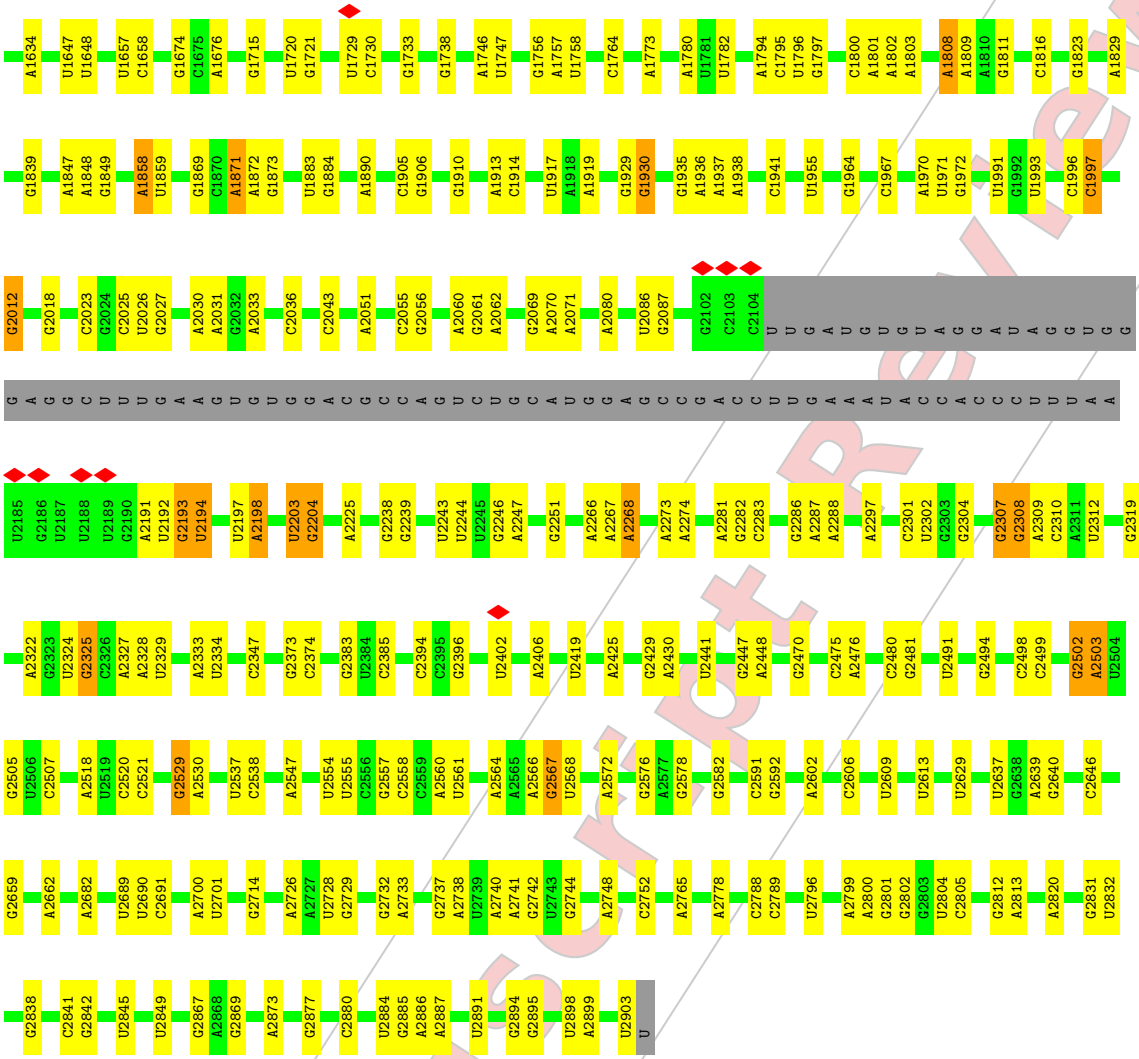


• Molecule 2: 5S rRNA

Chain 1:

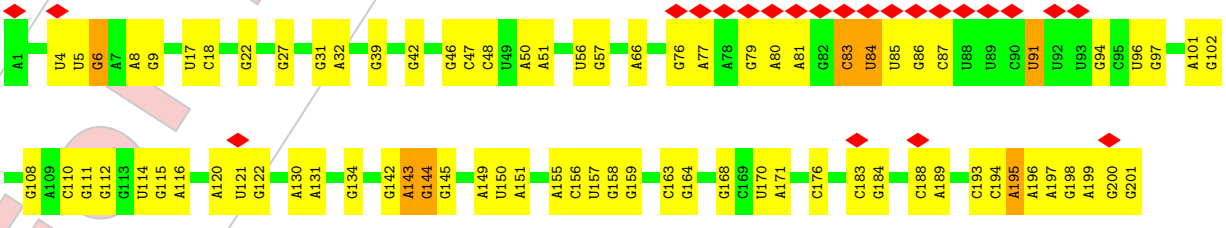




• Molecule 3: 16S rRNA

Chain 2:





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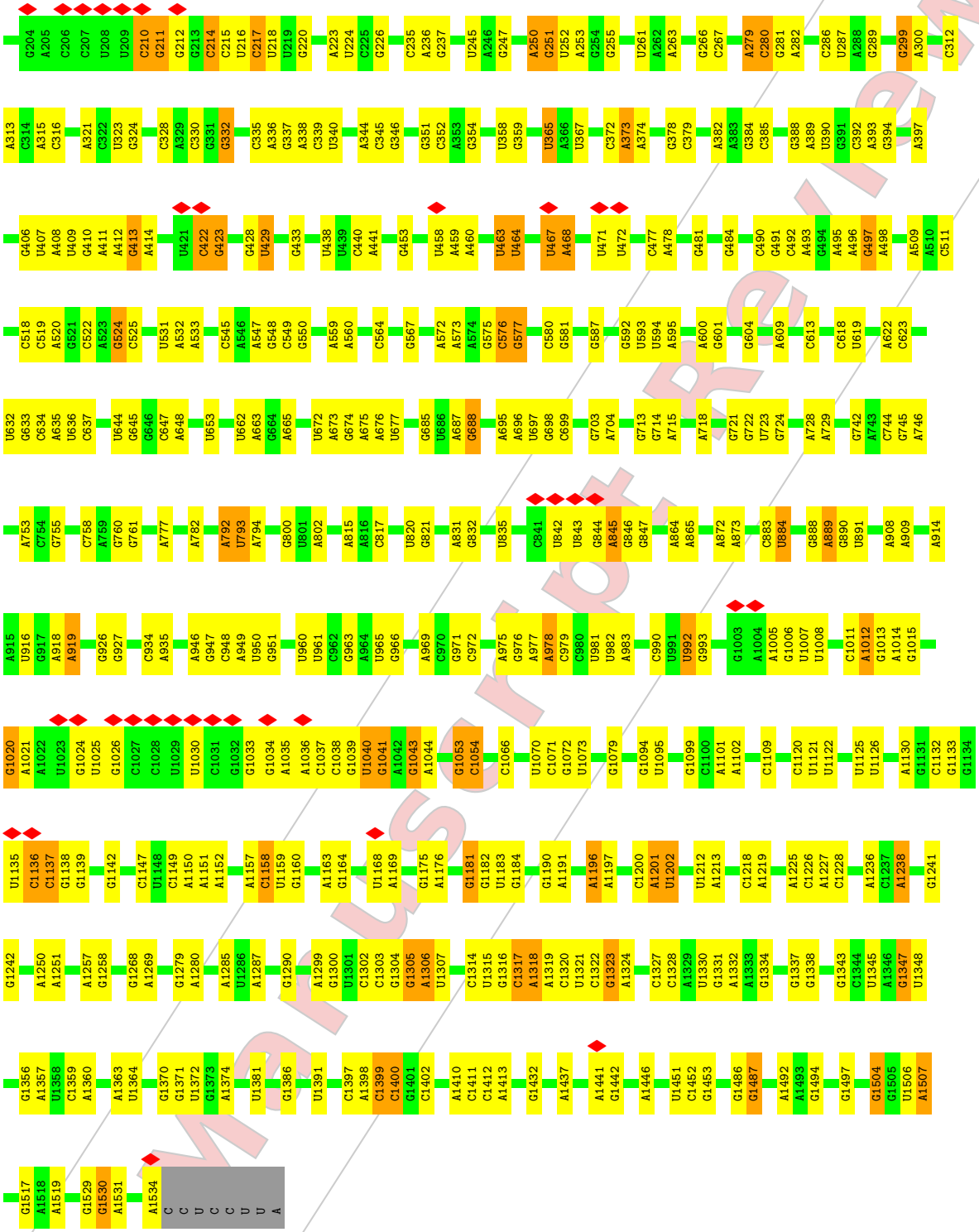

• Molecule 4: mRNA

Chain 3:





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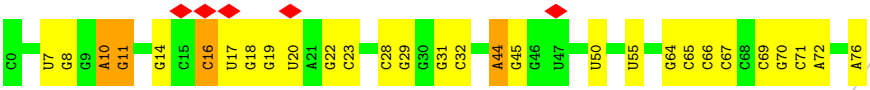
• Molecule 5: P-site tRNA

Chain 4:

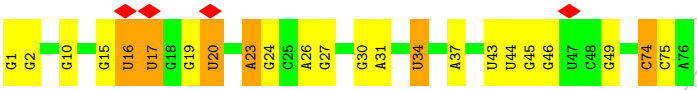




• Molecule 6: A-site tRNA

Chain 5:

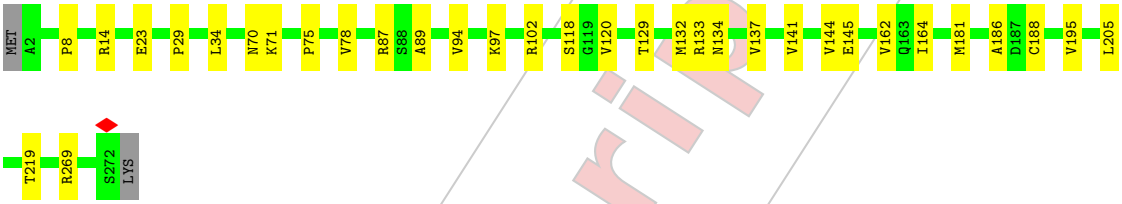




• Molecule 7: Large ribosomal subunit protein uL2

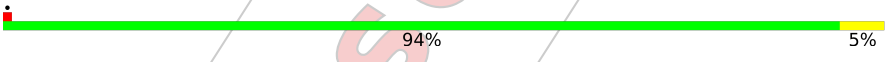
Chain A:

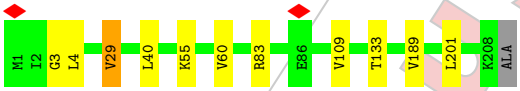




• Molecule 8: Large ribosomal subunit protein uL3

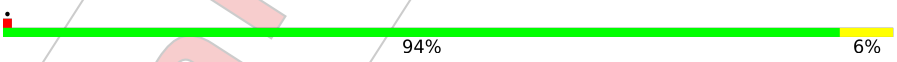
Chain B:





• Molecule 9: Large ribosomal subunit protein uL4

Chain C:

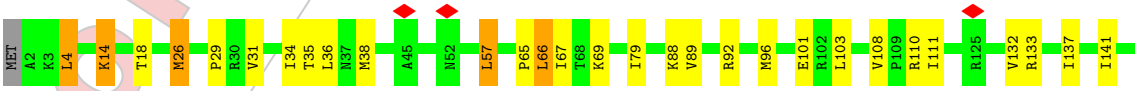




• Molecule 10: Large ribosomal subunit protein uL5

Chain D:





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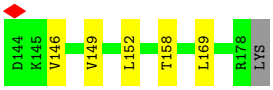
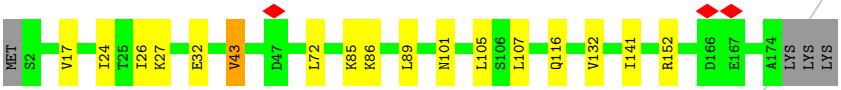


• Molecule 11: Large ribosomal subunit protein uL6

Chain E:

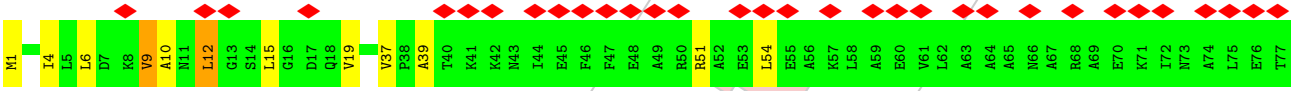




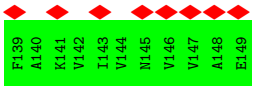
• Molecule 12: Large ribosomal subunit protein bL9

Chain F:



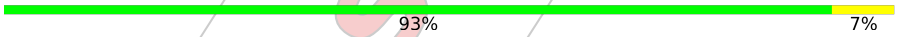


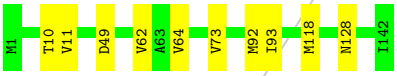




• Molecule 13: Large ribosomal subunit protein uL13

Chain G:

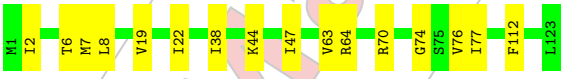




• Molecule 14: Large ribosomal subunit protein uL14

Chain H:

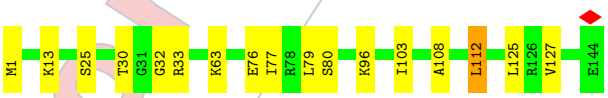




• Molecule 15: Large ribosomal subunit protein uL15

Chain I:





• Molecule 16: Large ribosomal subunit protein uL16

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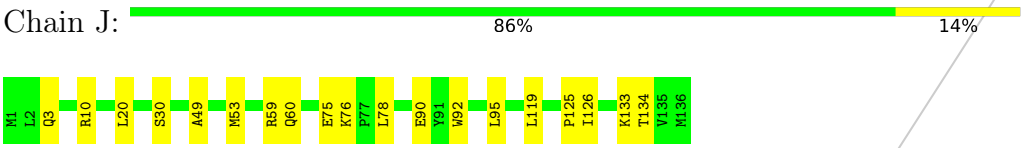
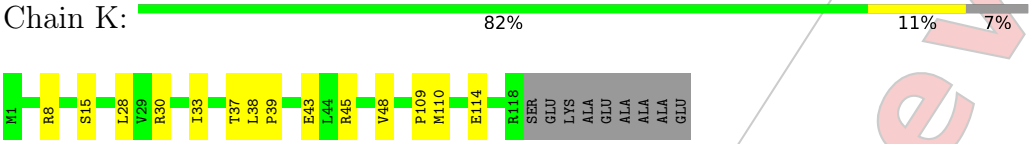
Chain J:



• Molecule 17: Large ribosomal subunit protein bL17

Chain K:



• Molecule 18: Large ribosomal subunit protein uL18

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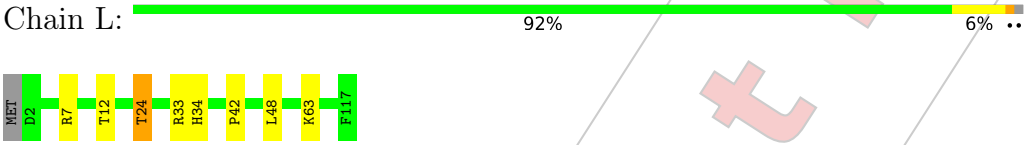
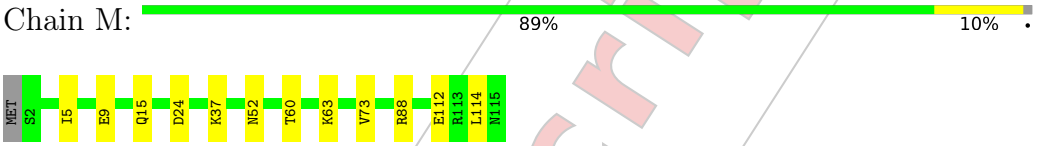


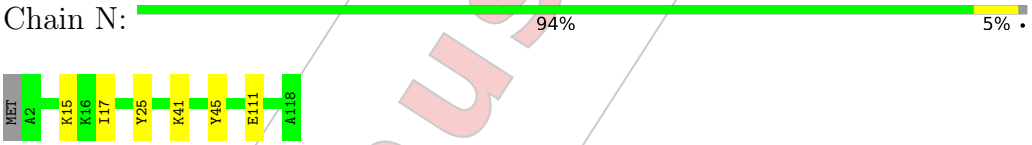
• Molecule 19: Large ribosomal subunit protein bL19

Chain M:



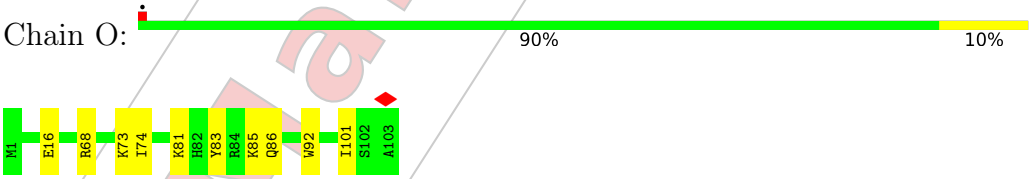
• Molecule 20: 50S ribosomal protein L20

Chain N:



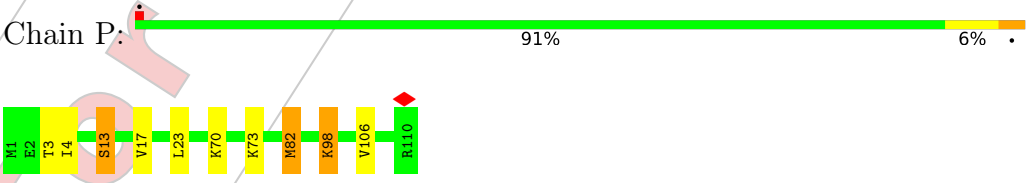
• Molecule 21: Large ribosomal subunit protein bL21

Chain O:



• Molecule 22: Large ribosomal subunit protein uL22

Chain P:



• Molecule 23: Large ribosomal subunit protein uL23

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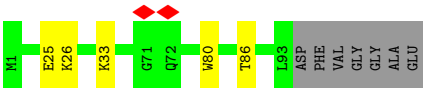
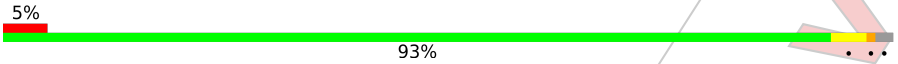
Chain Q:

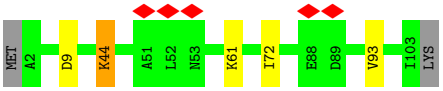




• Molecule 24: Large ribosomal subunit protein uL24

Chain R:

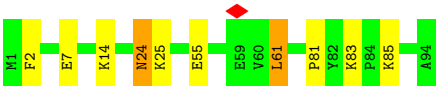




• Molecule 25: 50S ribosomal protein L25

Chain S:

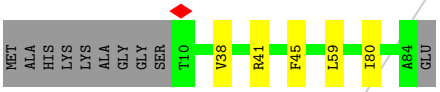




• Molecule 26: Large ribosomal subunit protein bL27

Chain T:





• Molecule 27: Large ribosomal subunit protein bL28

Chain U:

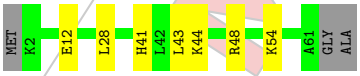




• Molecule 28: 50S ribosomal protein L29

Chain V:

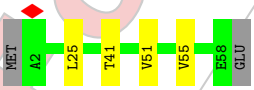




• Molecule 29: Large ribosomal subunit protein uL30

Chain W:





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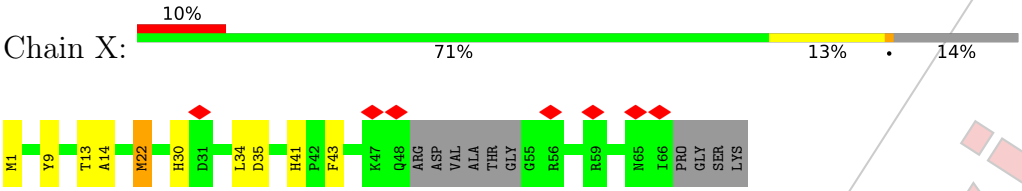
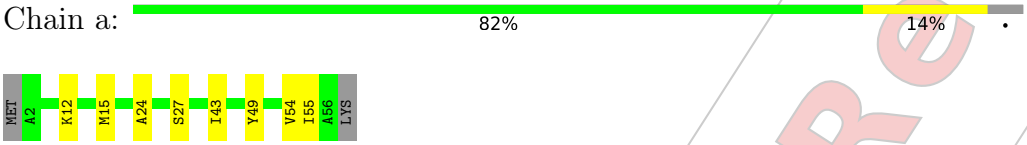
• Molecule 30: Large ribosomal subunit protein bL31

Chain X:



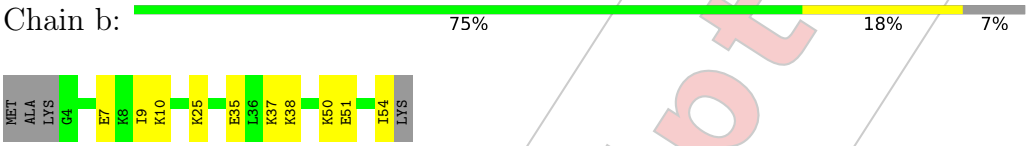
• Molecule 31: Large ribosomal subunit protein bL32

Chain a:



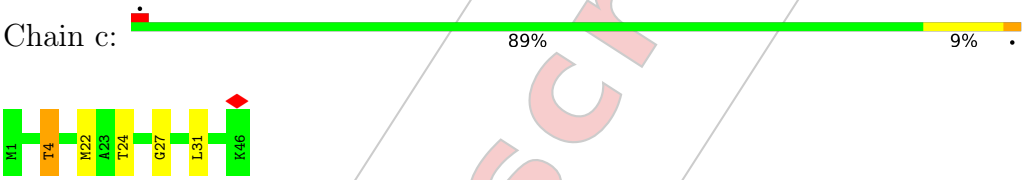
• Molecule 32: Large ribosomal subunit protein bL33

Chain b:



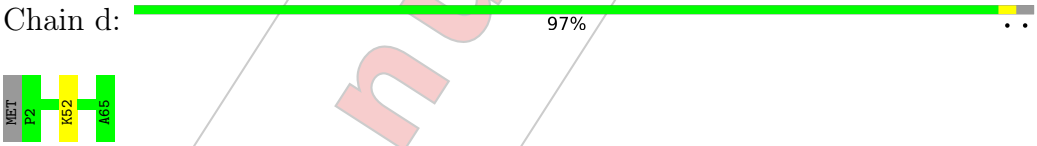
• Molecule 33: Large ribosomal subunit protein bL34

Chain c:



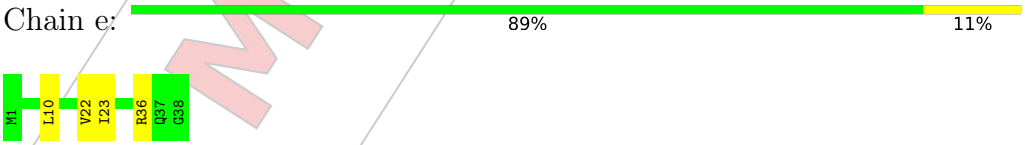
• Molecule 34: Large ribosomal subunit protein bL35

Chain d:



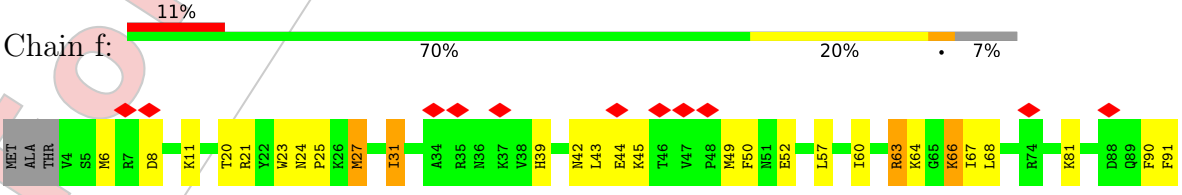
• Molecule 35: Large ribosomal subunit protein bL36A

Chain e:



• Molecule 36: Small ribosomal subunit protein uS2

Chain f:



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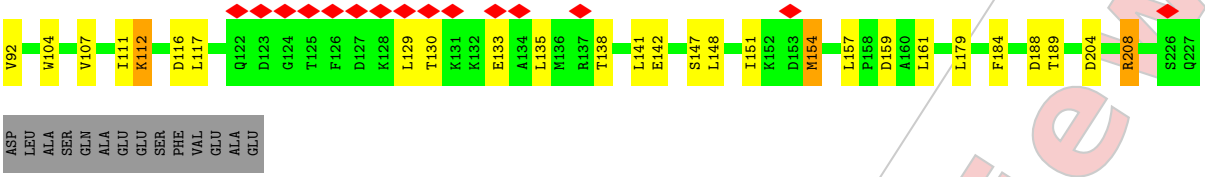
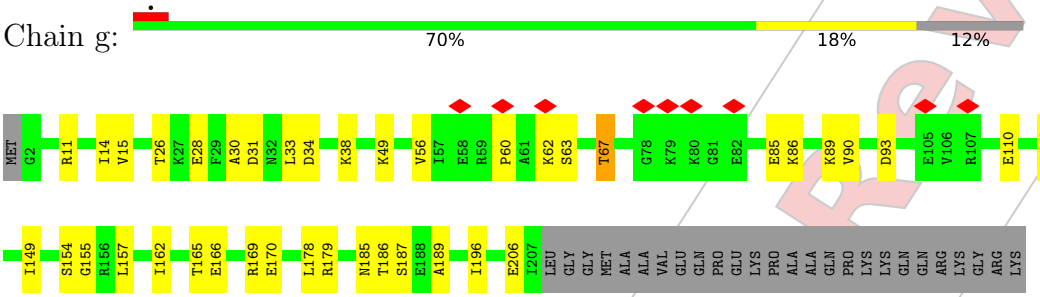
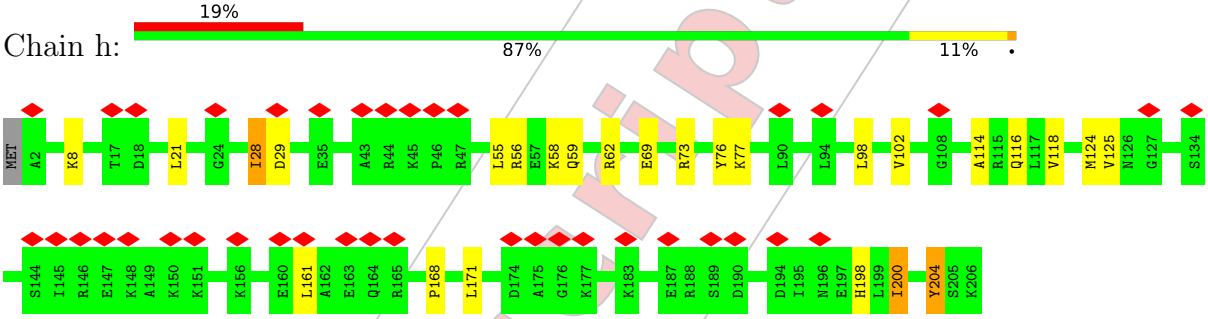


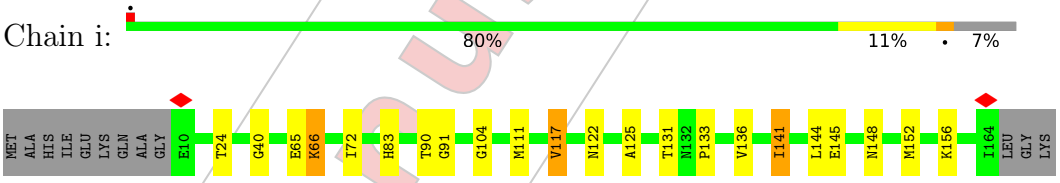
• Molecule 37: Small ribosomal subunit protein uS3



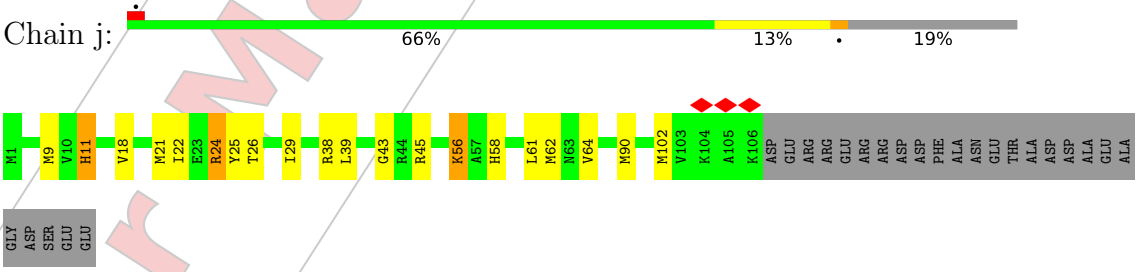
• Molecule 38: Small ribosomal subunit protein uS4



• Molecule 39: Small ribosomal subunit protein uS5



• Molecule 40: Small ribosomal subunit protein bS6



• Molecule 41: Small ribosomal subunit protein uS7



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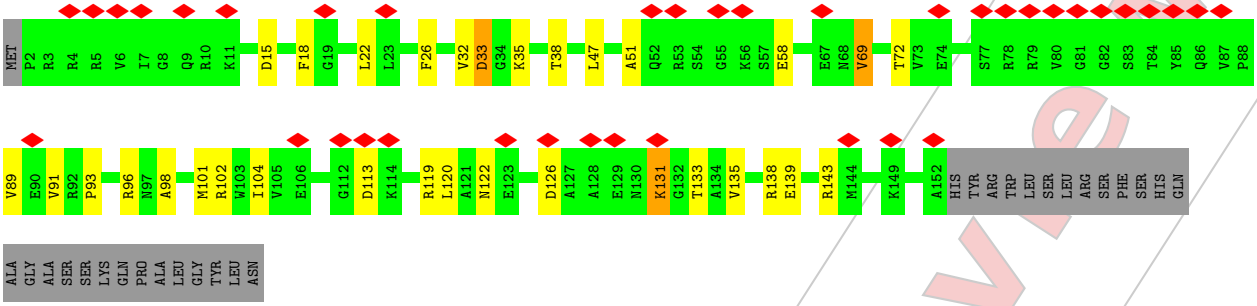
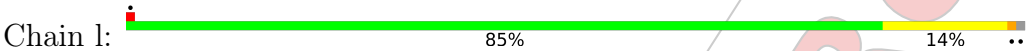
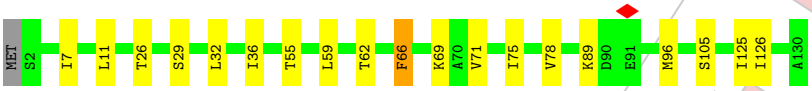


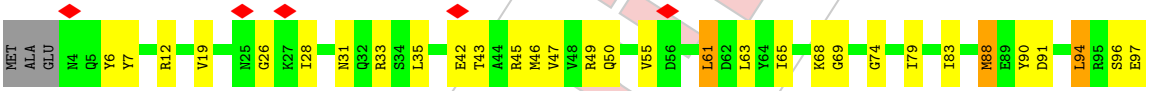
• Molecule 42: Small ribosomal subunit protein uS8



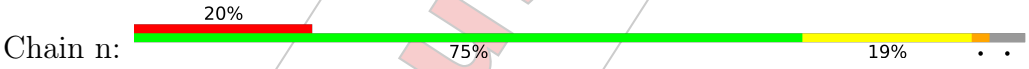


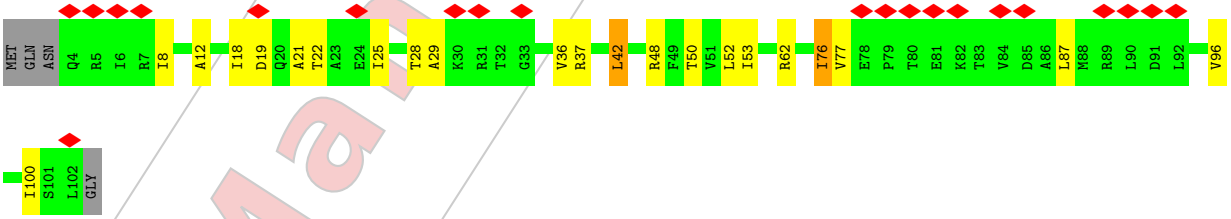
• Molecule 43: Small ribosomal subunit protein uS9



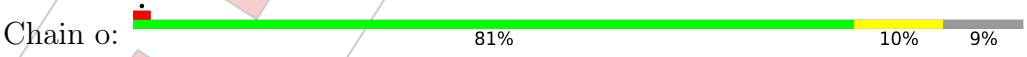


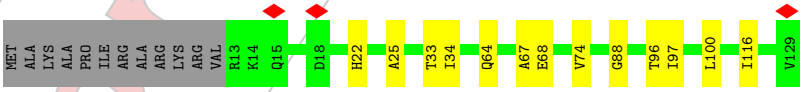
• Molecule 44: Small ribosomal subunit protein uS10



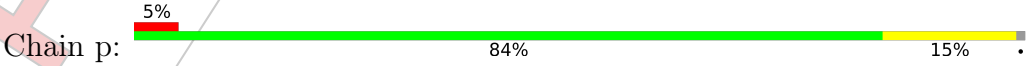


• Molecule 45: Small ribosomal subunit protein uS11





• Molecule 46: Small ribosomal subunit protein uS12



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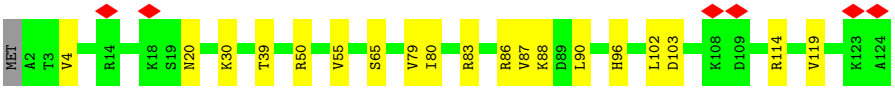
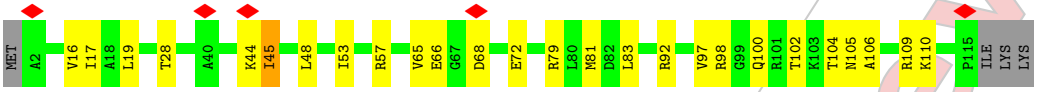
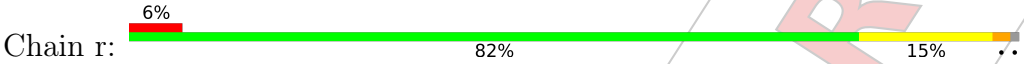


• Molecule 47: Small ribosomal subunit protein uS13



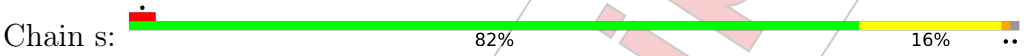


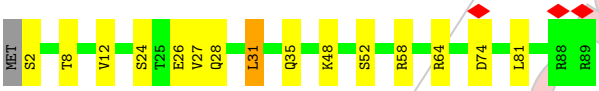
• Molecule 48: Small ribosomal subunit protein uS14



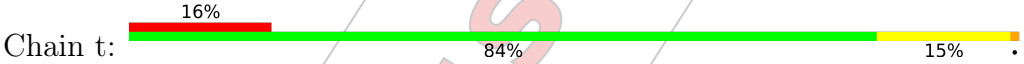


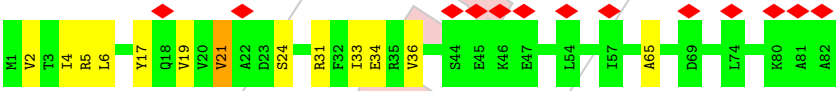
• Molecule 49: Small ribosomal subunit protein uS15



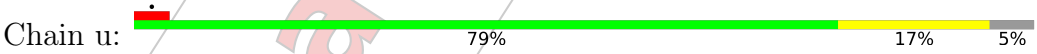


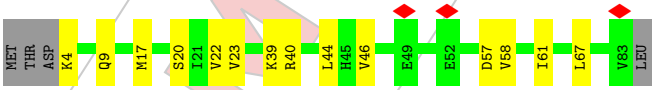
• Molecule 50: Small ribosomal subunit protein bS16



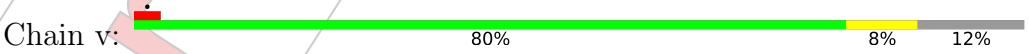


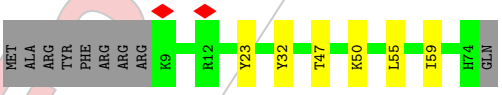
• Molecule 51: Small ribosomal subunit protein uS17





• Molecule 52: Small ribosomal subunit protein bS18





• Molecule 53: Small ribosomal subunit protein uS19

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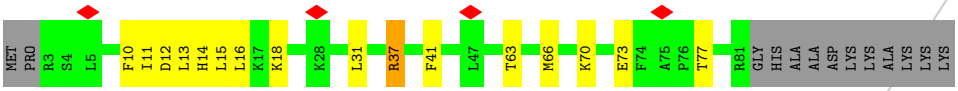
Chain w:

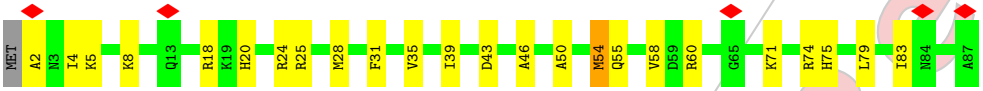




• Molecule 54: Small ribosomal subunit protein bS20

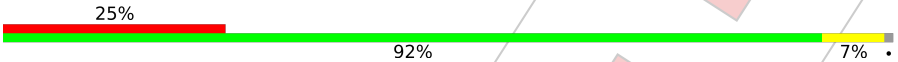
Chain x:

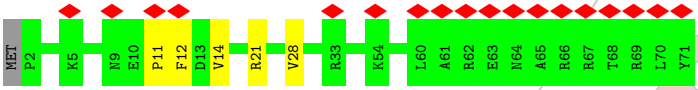




• Molecule 55: Small ribosomal subunit protein bS21

Chain y:





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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6805	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.442	Depositor
Minimum map value	-0.199	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	465.6, 465.6, 465.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	Depositor

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5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, U8U, T6A, H2U, OMC, 4SU

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	0	0.33	0/66326	0.35	0/103471
2	1	0.29	0/2869	0.30	0/4474
3	2	0.28	0/36859	0.36	0/57501
4	3	0.25	0/241	0.25	0/373
5	4	0.25	0/1766	0.30	0/2753
6	5	0.26	0/1663	0.29	0/2588
7	A	0.29	0/2121	0.40	0/2852
8	B	0.29	0/1580	0.36	0/2127
9	C	0.25	0/1571	0.35	0/2113
10	D	0.22	0/1434	0.45	0/1926
11	E	0.21	0/1315	0.36	0/1783
12	F	0.12	0/1122	0.36	1/1515 (0.1%)
13	G	0.30	0/1152	0.38	0/1551
14	H	0.27	0/956	0.41	0/1279
15	I	0.25	0/1062	0.37	0/1413
16	J	0.30	0/1093	0.42	0/1460
17	K	0.27	0/958	0.39	0/1281
18	L	0.24	0/902	0.39	0/1209
19	M	0.28	0/929	0.36	0/1242
20	N	0.31	0/960	0.37	0/1278
21	O	0.26	0/829	0.43	0/1107
22	P	0.25	0/864	0.41	0/1156
23	Q	0.23	0/744	0.35	0/994
24	R	0.25	0/787	0.33	0/1051
25	S	0.25	0/766	0.38	0/1025
26	T	0.31	0/579	0.39	0/767
27	U	0.27	0/635	0.42	0/848
28	V	0.22	0/492	0.32	0/655
29	W	0.23	0/443	0.32	0/593
30	X	0.13	0/488	0.31	0/649
31	a	0.26	0/440	0.34	0/588
32	b	0.24	0/424	0.35	0/565

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Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	c	0.32	0/380	0.37	0/498
34	d	0.30	0/513	0.40	0/676
35	e	0.31	0/303	0.35	0/397
36	f	0.19	0/1784	0.43	0/2403
37	g	0.24	0/1651	0.41	0/2225
38	h	0.16	0/1665	0.39	0/2227
39	i	0.23	0/1157	0.38	0/1557
40	j	0.20	0/881	0.41	0/1189
41	k	0.16	0/1195	0.38	0/1602
42	l	0.26	0/989	0.41	0/1326
43	m	0.23	0/1034	0.44	0/1375
44	n	0.19	0/805	0.47	0/1089
45	o	0.21	0/893	0.39	0/1205
46	p	0.17	0/969	0.38	0/1300
47	q	0.22	0/892	0.47	2/1193 (0.2%)
48	r	0.23	0/817	0.33	0/1088
49	s	0.25	0/722	0.39	0/964
50	t	0.17	0/659	0.40	0/884
51	u	0.22	0/657	0.42	0/881
52	v	0.23	0/553	0.33	0/742
53	w	0.19	0/652	0.37	0/877
54	x	0.21	0/676	0.48	0/895
55	y	0.14	0/598	0.26	0/792
All	All	0.29	0/154815	0.36	3/231572 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	121	VAL	N-CA-C	-5.88	107.02	112.43
47	q	44	LYS	CA-C-N	5.16	131.26	121.97
47	q	44	LYS	C-N-CA	5.16	131.26	121.97

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

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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	0	59219	0	29790	168	0
2	1	2566	0	1302	14	0
3	2	32917	0	16564	218	0
4	3	215	0	108	1	0
5	4	1642	0	841	12	0
6	5	1625	0	836	9	0
7	A	2082	0	2154	14	0
8	B	1559	0	1611	7	0
9	C	1552	0	1619	4	0
10	D	1410	0	1444	24	0
11	E	1295	0	1332	9	0
12	F	1111	0	1148	10	0
13	G	1129	0	1162	3	0
14	H	947	0	1023	7	0
15	I	1053	0	1129	7	0
16	J	1074	0	1157	7	0
17	K	945	0	989	7	0
18	L	892	0	923	3	0
19	M	917	0	962	6	0
20	N	947	0	1019	3	0
21	O	816	0	839	7	0
22	P	857	0	922	8	0
23	Q	738	0	807	2	0
24	R	779	0	831	1	0
25	S	753	0	780	6	0
26	T	572	0	593	3	0
27	U	625	0	652	8	0
28	V	491	0	523	4	0
29	W	439	0	482	2	0
30	X	480	0	482	5	0
31	a	434	0	445	4	0
32	b	417	0	451	4	0
33	c	377	0	418	3	0
34	d	504	0	572	0	0
35	e	302	0	343	2	0
36	f	1753	0	1780	33	0
37	g	1624	0	1696	26	0
38	h	1643	0	1707	14	0
39	i	1144	0	1185	12	0
40	j	862	0	864	12	0
41	k	1181	0	1238	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	l	979	0	1031	11	0
43	m	1022	0	1070	25	0
44	n	795	0	836	13	0
45	o	877	0	887	7	0
46	p	955	0	1016	7	0
47	q	883	0	941	17	0
48	r	805	0	844	17	0
49	s	714	0	734	8	0
50	t	649	0	666	7	0
51	u	648	0	691	8	0
52	v	544	0	565	4	0
53	w	637	0	665	12	0
54	x	670	0	719	17	0
55	y	590	0	629	3	0
All	All	142656	0	96017	798	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 3.

All (798) 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)
3:2:151:A:H62	3:2:170:U:H3	1.17	0.91
5:4:50:U:H3	5:4:64:G:H1	1.20	0.88
25:S:24:ASN:O	25:S:24:ASN:ND2	2.07	0.87
3:2:409:U:H3	3:2:433:G:H1	1.22	0.83
10:D:38:MET:HE3	10:D:57:LEU:HG	1.59	0.82
50:t:5:ARG:HH22	50:t:24:SER:HA	1.45	0.82
10:D:4:LEU:HD13	10:D:101:GLU:HB2	1.61	0.82
3:2:1356:G:H2'	3:2:1357:A:H8	1.47	0.80
41:k:47:LEU:HB3	41:k:58:GLU:HG2	1.67	0.76
50:t:19:VAL:HG13	50:t:36:VAL:HG23	1.67	0.76
46:p:87:VAL:HG11	46:p:90:LEU:HD12	1.68	0.76
10:D:29:PRO:HG2	10:D:169:LEU:HD13	1.66	0.76
35:e:22:VAL:HG11	35:e:36:ARG:HH21	1.55	0.72
36:f:8:ASP:HA	36:f:11:LYS:HG2	1.72	0.71
46:p:86:ARG:HH21	46:p:88:LYS:HD2	1.57	0.70
14:H:70:ARG:HH21	14:H:74:GLY:HA2	1.53	0.70
9:C:108:ILE:HA	15:I:1:MET:HE1	1.74	0.70
31:a:54:VAL:HG23	31:a:55:ILE:HG12	1.74	0.70
6:5:30:G:H2'	6:5:31:A:H8	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:46:LEU:HD12	53:w:13:LEU:HD13	1.72	0.69
17:K:33:ILE:HG13	17:K:114:GLU:HB3	1.73	0.69
3:2:1218:C:H2'	3:2:1219:A:C8	2.28	0.69
1:0:2324:U:H3'	1:0:2325:G:H5"	1.74	0.69
1:0:856:G:H2'	1:0:857:G:C8	2.27	0.68
3:2:176:C:H5"	54:x:24:ARG:HH12	1.56	0.68
10:D:31:VAL:HA	10:D:158:THR:HG22	1.75	0.68
3:2:1013:G:H21	3:2:1219:A:H1'	1.58	0.68
22:P:4:ILE:HG13	22:P:106:VAL:HG22	1.75	0.67
1:0:1047:G:H21	1:0:1111:A:N6	1.91	0.67
3:2:337:G:H2'	3:2:338:A:C8	2.28	0.67
25:S:24:ASN:HD22	25:S:24:ASN:C	2.00	0.67
43:m:35:LEU:HD22	43:m:49:ARG:HH22	1.59	0.66
54:x:71:LYS:HD3	54:x:74:ARG:NH1	2.11	0.66
3:2:1356:G:H2'	3:2:1357:A:C8	2.32	0.65
37:g:26:THR:HG23	48:r:76:LYS:HE3	1.78	0.65
1:0:981:A:H8	1:0:2027:G:H21	1.42	0.65
15:I:30:THR:HG22	15:I:33:ARG:H	1.61	0.65
3:2:946:A:H2'	3:2:947:G:H8	1.62	0.65
7:A:132:MET:HE2	7:A:164:ILE:HD11	1.77	0.65
25:S:2:PHE:HB2	25:S:61:LEU:HD12	1.78	0.65
1:0:2796:U:H3	1:0:2799:A:H61	1.44	0.65
49:s:8:THR:HG23	49:s:31:LEU:HD21	1.78	0.65
8:B:4:LEU:HD23	8:B:29:VAL:HG11	1.77	0.65
1:0:1802:A:H2'	1:0:1803:A:C8	2.31	0.64
3:2:946:A:H2'	3:2:947:G:C8	2.33	0.64
5:4:69:C:H2'	5:4:70:G:H8	1.62	0.64
49:s:8:THR:O	49:s:12:VAL:HG23	1.98	0.64
1:0:1469:A:H2'	1:0:1470:A:C8	2.33	0.64
54:x:71:LYS:HD3	54:x:74:ARG:HH11	1.63	0.64
30:X:41:HIS:HD2	30:X:43:PHE:HB3	1.63	0.64
38:h:56:ARG:HE	38:h:56:ARG:HA	1.63	0.64
3:2:407:U:H2'	3:2:408:A:H8	1.63	0.63
11:E:86:LYS:HE3	11:E:132:VAL:HG13	1.79	0.63
8:B:55:LYS:HD3	8:B:60:VAL:HG22	1.79	0.63
3:2:490:C:H2'	3:2:491:G:H8	1.64	0.63
1:0:2637:U:H5"	8:B:83:ARG:HH12	1.62	0.62
43:m:19:VAL:HG22	43:m:65:ILE:HG12	1.81	0.62
41:k:26:PHE:HZ	41:k:120:LEU:HD21	1.65	0.62
1:0:2812:G:H2'	1:0:2813:A:C8	2.35	0.62
3:2:407:U:H2'	3:2:408:A:C8	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:459:A:H2'	3:2:460:A:H8	1.64	0.62
47:q:81:MET:HE3	47:q:92:ARG:HG2	1.82	0.62
7:A:144:VAL:HG21	7:A:162:VAL:HG11	1.81	0.62
3:2:5:U:H4'	3:2:6:G:C2	2.35	0.62
44:n:12:ALA:HB2	44:n:96:VAL:HG22	1.83	0.61
27:U:43:GLU:OE1	27:U:45:ARG:HB2	2.00	0.61
54:x:25:ARG:HG3	54:x:25:ARG:HH11	1.65	0.61
3:2:1218:C:H2'	3:2:1219:A:H8	1.64	0.61
11:E:101:ASN:HD21	11:E:116:GLN:HE22	1.48	0.61
3:2:1040:U:H2'	3:2:1041:G:C8	2.35	0.61
7:A:141:VAL:HG23	7:A:162:VAL:HG13	1.83	0.61
3:2:1323:G:H2'	3:2:1324:A:C8	2.35	0.61
21:O:16:GLU:HG2	21:O:101:ILE:HD12	1.83	0.61
54:x:35:VAL:HG22	54:x:50:ALA:HB1	1.81	0.61
3:2:673:A:H2'	3:2:674:G:C8	2.37	0.60
37:g:56:VAL:HB	37:g:67:THR:HG23	1.83	0.60
3:2:216:U:H2'	3:2:217:C:C6	2.36	0.60
3:2:1345:U:H5"	43:m:122:ARG:HH21	1.66	0.60
3:2:1014:A:H2'	3:2:1015:G:C8	2.36	0.60
3:2:688:G:H1	3:2:699:C:H5	1.50	0.60
47:q:16:VAL:HG13	47:q:17:ILE:HG23	1.83	0.60
3:2:888:G:H3'	3:2:889:A:H5"	1.84	0.60
27:U:59:ILE:HG12	27:U:67:VAL:HG21	1.82	0.60
41:k:135:VAL:O	41:k:139:GLU:HG3	2.02	0.60
45:o:116:ILE:HD11	55:y:28:VAL:HG13	1.83	0.60
39:i:156:LYS:HG2	42:l:71:VAL:HG22	1.83	0.60
3:2:337:G:H2'	3:2:338:A:H8	1.67	0.59
42:l:11:LEU:HD22	42:l:75:ILE:HD11	1.83	0.59
42:l:78:VAL:HG11	42:l:125:ILE:HD11	1.82	0.59
47:q:97:VAL:HG23	47:q:98:ARG:HG3	1.85	0.59
1:0:475:C:O2	1:0:479:A:N6	2.35	0.59
28:V:28:LEU:HD23	28:V:43:LEU:HD23	1.83	0.59
3:2:714:G:H2'	3:2:715:A:C8	2.37	0.59
51:u:9:GLN:HE22	51:u:58:VAL:HG12	1.68	0.59
12:F:4:ILE:HG23	12:F:39:ALA:HB2	1.85	0.58
41:k:69:VAL:HG21	41:k:104:ILE:HD11	1.86	0.58
43:m:61:LEU:HD13	43:m:63:LEU:HD11	1.85	0.58
55:y:11:PRO:HB2	55:y:14:VAL:HG23	1.85	0.58
1:0:2394:C:H5"	15:I:63:LYS:HE2	1.86	0.58
41:k:98:ALA:O	41:k:102:ARG:HG3	2.04	0.58
3:2:79:G:H1	3:2:91:U:H1'	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:i:40:GLY:HA3	39:i:117:VAL:HG13	1.86	0.58
3:2:1303:C:H5	3:2:1334:G:H22	1.52	0.58
1:0:1808:A:H3'	1:0:1809:A:C8	2.39	0.58
50:t:5:ARG:NH2	50:t:24:SER:HA	2.17	0.58
43:m:88:MET:HA	43:m:88:MET:HE2	1.87	0.57
1:0:118:A:H5'	1:0:119:A:H8	1.69	0.57
3:2:458:U:H2'	3:2:459:A:H8	1.69	0.57
3:2:358:U:H2'	3:2:359:G:H8	1.68	0.57
1:0:1050:A:H2'	1:0:1051:G:C8	2.40	0.57
15:I:79:LEU:HD11	15:I:112:LEU:HD22	1.86	0.57
11:E:24:ILE:HD11	11:E:43:VAL:HG11	1.86	0.57
37:g:14:ILE:HG22	37:g:15:VAL:HG13	1.87	0.57
47:q:45:ILE:HA	47:q:48:LEU:HG	1.85	0.57
3:2:1347:G:H5"	43:m:109:ARG:HB2	1.86	0.56
54:x:5:LYS:HA	54:x:8:LYS:HG2	1.86	0.56
25:S:24:ASN:ND2	25:S:24:ASN:C	2.62	0.56
6:5:30:G:H2'	6:5:31:A:C8	2.38	0.56
3:2:17:U:H2'	3:2:18:C:C6	2.41	0.56
1:0:2193:G:H2'	1:0:2194:U:C6	2.41	0.56
27:U:66:THR:O	27:U:70:GLU:HG2	2.06	0.56
43:m:91:ASP:HB3	43:m:94:LEU:HD11	1.88	0.56
1:0:2521:C:O2'	1:0:2564:A:H8	1.89	0.56
22:P:82:MET:HE2	22:P:98:LYS:HD3	1.88	0.56
39:i:72:ILE:HD12	39:i:145:GLU:HG2	1.88	0.55
3:2:949:A:H2	47:q:105:ASN:HD21	1.53	0.55
1:0:2070:A:H2'	1:0:2071:A:C8	2.40	0.55
7:A:75:PRO:HG2	7:A:97:LYS:CE	2.36	0.55
54:x:54:MET:HE2	54:x:58:VAL:HG11	1.88	0.55
54:x:31:PHE:O	54:x:35:VAL:HG23	2.07	0.55
6:5:23:A:H2'	6:5:24:G:H8	1.72	0.55
43:m:12:ARG:HG2	43:m:74:GLY:HA2	1.89	0.55
46:p:55:VAL:HG11	46:p:80:ILE:HD11	1.89	0.55
47:q:79:ARG:HG2	47:q:79:ARG:HH11	1.71	0.55
1:0:742:A:H2'	1:0:743:A:C8	2.42	0.55
16:J:49:ALA:O	16:J:53:MET:HG2	2.06	0.55
36:f:151:ILE:HA	36:f:154:MET:SD	2.47	0.55
40:j:29:ILE:HD12	40:j:64:VAL:HG11	1.89	0.55
3:2:1504:G:OP1	3:2:1507:A:H4'	2.07	0.54
36:f:66:LYS:HB3	36:f:90:PHE:HE2	1.72	0.54
43:m:19:VAL:HG11	43:m:83:ILE:HD13	1.89	0.54
3:2:409:U:O4	3:2:433:G:O6	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:u:46:VAL:HG21	51:u:61:ILE:HG21	1.90	0.54
1:0:1847:A:O2'	1:0:1848:A:H8	1.90	0.54
14:H:7:MET:HE1	14:H:44:LYS:HG3	1.90	0.54
37:g:117:ALA:HB1	37:g:187:SER:HB3	1.89	0.54
3:2:979:C:O2	48:r:59:ARG:HD2	2.08	0.54
3:2:96:U:H2'	3:2:97:G:H8	1.72	0.54
3:2:1314:C:H2'	3:2:1315:U:H6	1.72	0.54
10:D:14:LYS:O	10:D:18:THR:HG23	2.08	0.54
45:o:64:GLN:O	45:o:68:GLU:HG3	2.07	0.54
54:x:43:ASP:HB3	54:x:46:ALA:HB3	1.89	0.54
10:D:79:ILE:HD12	10:D:79:ILE:O	2.07	0.54
36:f:188:ASP:HB2	36:f:204:ASP:OD2	2.08	0.54
1:0:2307:G:H4'	1:0:2308:G:O5'	2.06	0.53
2:1:55:U:H1'	10:D:26:MET:HE2	1.89	0.53
3:2:250:A:H4'	3:2:251:G:O5'	2.08	0.53
3:2:384:G:H2'	3:2:385:C:C6	2.43	0.53
3:2:1318:A:O2'	53:w:37:ARG:HG3	2.08	0.53
3:2:42:G:H21	3:2:622:A:H8	1.56	0.53
3:2:477:C:H2'	3:2:478:A:C8	2.44	0.53
11:E:107:LEU:HD12	11:E:152:ARG:HH11	1.71	0.53
12:F:110:VAL:HG11	12:F:132:PHE:HE2	1.74	0.53
3:2:1008:U:H1'	3:2:1020:G:H22	1.73	0.53
1:0:521:U:H2'	1:0:522:A:C8	2.44	0.53
1:0:2267:A:H5"	1:0:2268:A:H5'	1.91	0.53
3:2:195:A:H2'	3:2:196:A:C8	2.44	0.53
12:F:110:VAL:HG11	12:F:132:PHE:CE2	2.44	0.53
1:0:1:G:H2'	1:0:2:G:H8	1.74	0.53
40:j:9:MET:HA	40:j:58:HIS:O	2.08	0.53
44:n:37:ARG:HH22	44:n:77:VAL:HG22	1.74	0.53
3:2:144:G:H2'	3:2:145:G:C8	2.44	0.53
51:u:23:VAL:HG22	51:u:44:LEU:HB2	1.90	0.53
1:0:2737:G:H2'	1:0:2738:A:C8	2.44	0.53
6:5:74:C:H2'	6:5:75:C:O4'	2.09	0.53
41:k:113:ASP:HB2	41:k:119:ARG:HG2	1.89	0.53
3:2:199:A:H2'	3:2:200:G:H8	1.74	0.53
3:2:545:C:H5'	38:h:69:GLU:OE2	2.09	0.53
3:2:1149:C:H2'	3:2:1150:A:C8	2.43	0.53
5:4:69:C:H2'	5:4:70:G:C8	2.43	0.53
37:g:121:THR:HG23	37:g:189:ALA:HB2	1.91	0.53
1:0:1434:A:HO2'	1:0:1435:G:H8	1.54	0.53
3:2:335:C:H2'	3:2:336:A:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:145:GLU:HB2	7:A:188:CYS:HB3	1.90	0.53
18:L:24:THR:HG22	18:L:42:PRO:HD3	1.91	0.53
43:m:26:GLY:HA2	43:m:61:LEU:O	2.09	0.53
3:2:1317:C:N4	48:r:53:ARG:HE	2.07	0.52
5:4:71:C:H2'	5:4:72:A:C8	2.43	0.52
3:2:492:C:H2'	3:2:493:A:C8	2.44	0.52
26:T:45:PHE:HB3	26:T:80:ILE:HD13	1.92	0.52
47:q:53:ILE:HG22	47:q:57:ARG:HH21	1.75	0.52
47:q:106:ALA:O	47:q:110:LYS:HB2	2.09	0.52
3:2:883:C:O2'	3:2:884:U:H5'	2.10	0.52
12:F:97:ARG:HD3	12:F:112:LYS:HZ1	1.75	0.52
37:g:169:ARG:HG2	37:g:170:GLU:N	2.25	0.52
43:m:88:MET:HE3	43:m:98:LEU:HD12	1.90	0.52
1:0:742:A:H2'	1:0:743:A:H8	1.75	0.52
53:w:11:ILE:HG12	53:w:16:LEU:HB2	1.92	0.52
1:0:12:U:H2'	1:0:13:A:H5'	1.90	0.52
3:2:1318:A:H5'	53:w:10:PHE:CE1	2.44	0.52
36:f:117:LEU:HB3	36:f:141:LEU:HD12	1.92	0.52
38:h:76:TYR:CE2	38:h:204:TYR:HB3	2.44	0.52
3:2:695:A:H2'	3:2:696:A:C8	2.45	0.52
3:2:393:A:C2	3:2:394:G:C8	2.98	0.52
53:w:14:HIS:H	53:w:14:HIS:CD2	2.27	0.52
1:0:1:G:H2'	1:0:2:G:C8	2.45	0.52
3:2:1323:G:H2'	3:2:1324:A:H8	1.74	0.52
43:m:45:ARG:O	43:m:49:ARG:HG2	2.09	0.52
7:A:71:LYS:HD2	7:A:102:ARG:HH21	1.75	0.52
16:J:75:GLU:HB2	16:J:90:GLU:HG3	1.91	0.51
44:n:29:ALA:HB1	44:n:36:VAL:HG11	1.92	0.51
47:q:68:ASP:O	47:q:72:GLU:HG2	2.10	0.51
50:t:6:LEU:HD12	50:t:17:TYR:HB3	1.90	0.51
1:0:2557:G:H2'	1:0:2558:C:C6	2.45	0.51
39:i:111:MET:HE1	39:i:125:ALA:HB1	1.92	0.51
49:s:2:SER:HA	49:s:35:GLN:HE22	1.74	0.51
53:w:18:LYS:HG2	53:w:31:LEU:HD21	1.92	0.51
3:2:696:A:H2'	3:2:697:U:H6	1.75	0.51
3:2:1040:U:H2'	3:2:1041:G:H8	1.75	0.51
3:2:299:G:H2'	3:2:300:A:C8	2.45	0.51
3:2:458:U:H2'	3:2:459:A:C8	2.45	0.51
3:2:1236:A:H4'	3:2:1304:G:H4'	1.91	0.51
5:4:28:C:H2'	5:4:29:G:H8	1.75	0.51
2:1:54:G:H21	10:D:26:MET:HE1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:200:G:H2'	3:2:201:G:H8	1.76	0.51
31:a:43:ILE:HG22	31:a:49:TYR:HB2	1.93	0.51
38:h:114:ALA:O	38:h:118:VAL:HG12	2.10	0.51
41:k:126:ASP:HB3	41:k:131:LYS:O	2.10	0.51
3:2:490:C:H2'	3:2:491:G:C8	2.44	0.51
33:c:24:THR:HG23	33:c:27:GLY:H	1.75	0.51
3:2:1054:C:H6	3:2:1196:A:HO2'	1.56	0.51
3:2:142:G:H2'	3:2:143:A:C8	2.46	0.51
1:0:144:A:H2'	1:0:145:C:C6	2.46	0.51
3:2:820:U:H5	3:2:873:A:N7	2.08	0.51
45:o:34:ILE:HD12	45:o:74:VAL:HG21	1.93	0.51
36:f:57:LEU:HG	36:f:184:PHE:HE2	1.74	0.51
1:0:668:A:H2'	1:0:670:A:H62	1.76	0.50
1:0:1563:U:H2'	1:0:1564:C:C6	2.46	0.50
37:g:85:GLU:O	37:g:89:LYS:HG3	2.11	0.50
37:g:179:ARG:O	37:g:179:ARG:HG3	2.11	0.50
42:l:32:LEU:O	42:l:36:ILE:HG12	2.11	0.50
1:0:2804:U:H2'	1:0:2805:C:C6	2.46	0.50
3:2:662:U:H2'	3:2:663:A:C8	2.46	0.50
3:2:1530:G:H2'	3:2:1531:A:H8	1.75	0.50
9:C:111:GLU:HG3	9:C:115:GLN:OE1	2.11	0.50
11:E:17:VAL:HG22	11:E:26:ILE:HD12	1.91	0.50
40:j:90:MET:HE1	52:v:23:TYR:CE1	2.46	0.50
43:m:6:TYR:HE2	43:m:90:TYR:HD1	1.59	0.50
1:0:1187:G:H5'	21:O:83:TYR:CE2	2.45	0.50
3:2:215:C:H2'	3:2:216:U:C6	2.46	0.50
33:c:22:MET:HE3	33:c:31:LEU:HD22	1.93	0.50
3:2:215:C:H2'	3:2:216:U:H6	1.76	0.50
23:Q:33:LYS:HE2	23:Q:80:TRP:CZ3	2.46	0.50
36:f:130:THR:HB	36:f:133:GLU:HB2	1.94	0.50
46:p:79:VAL:O	46:p:103:ASP:HB3	2.11	0.50
1:0:2788:C:H2'	1:0:2789:C:C6	2.47	0.50
32:b:35:GLU:HG2	32:b:50:LYS:HG3	1.92	0.50
1:0:1720:U:H2'	1:0:1721:G:O4'	2.12	0.50
37:g:33:LEU:HD21	48:r:93:ILE:HG13	1.94	0.50
44:n:53:ILE:HB	48:r:85:ARG:NH1	2.26	0.50
54:x:2:ALA:HB3	54:x:8:LYS:HZ3	1.77	0.50
3:2:155:A:H2'	3:2:156:C:H6	1.77	0.50
3:2:918:A:H2'	3:2:919:A:C8	2.47	0.50
3:2:1486:G:H2'	3:2:1487:G:O4'	2.11	0.50
26:T:38:VAL:HG12	26:T:59:LEU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:533:G:H2'	1:0:534:U:C6	2.47	0.50
1:0:2502:G:H5'	1:0:2503:A:H5'	1.94	0.50
1:0:2567:G:H2'	1:0:2568:U:C6	2.47	0.50
1:0:2637:U:H5"	8:B:83:ARG:NH1	2.27	0.50
37:g:110:GLU:OE2	37:g:144:LEU:HD13	2.11	0.50
44:n:36:VAL:HG12	44:n:76:ILE:HG23	1.94	0.50
44:n:52:LEU:HD23	44:n:62:ARG:HG2	1.94	0.50
3:2:96:U:H2'	3:2:97:G:C8	2.47	0.49
3:2:647:C:H2'	3:2:648:A:C8	2.47	0.49
10:D:103:LEU:HG	10:D:108:VAL:HG23	1.94	0.49
48:r:89:MET:HE2	48:r:89:MET:HA	1.94	0.49
1:0:1047:G:N2	1:0:1111:A:N6	2.58	0.49
3:2:1399:C:H4'	3:2:1400:C:O5'	2.13	0.49
1:0:1433:A:O2'	1:0:1434:A:H5'	2.12	0.49
36:f:68:LEU:HB3	36:f:161:LEU:HD23	1.92	0.49
3:2:279:A:H5"	3:2:280:C:H3'	1.95	0.49
21:O:73:LYS:C	21:O:74:ILE:HD12	2.37	0.49
13:G:128:ASN:O	13:G:128:ASN:ND2	2.40	0.49
50:t:2:VAL:HB	50:t:65:ALA:HA	1.95	0.49
50:t:33:ILE:HG22	50:t:34:GLU:HG3	1.95	0.49
18:L:33:ARG:HB3	18:L:34:HIS:CD2	2.48	0.49
36:f:104:TRP:HA	36:f:107:VAL:HG22	1.94	0.49
3:2:674:G:H2'	3:2:675:A:H8	1.78	0.49
37:g:179:ARG:HG3	37:g:206:GLU:HB3	1.94	0.49
1:0:2246:G:H2'	1:0:2247:A:C8	2.48	0.49
3:2:235:C:H2'	3:2:236:A:C8	2.48	0.49
1:0:956:G:H5"	16:J:76:LYS:HD2	1.94	0.49
1:0:2030:A:C2	1:0:2499:C:H5"	2.48	0.49
3:2:744:C:H2'	3:2:745:G:H8	1.78	0.49
38:h:76:TYR:CZ	38:h:204:TYR:HB3	2.48	0.49
2:1:54:G:N2	10:D:26:MET:HE1	2.27	0.48
3:2:698:G:H2'	3:2:699:C:O2	2.13	0.48
44:n:21:ALA:O	44:n:25:ILE:HG22	2.13	0.48
1:0:2051:A:H8	1:0:2051:A:OP2	1.95	0.48
53:w:37:ARG:O	53:w:37:ARG:HG2	2.13	0.48
43:m:97:GLU:HA	43:m:100:LYS:HE3	1.95	0.48
3:2:210:C:H4'	3:2:211:G:O5'	2.14	0.48
3:2:519:C:H2'	3:2:520:A:C8	2.48	0.48
36:f:31:ILE:HD11	36:f:39:HIS:CG	2.47	0.48
1:0:1746:A:H2'	1:0:1747:U:C6	2.49	0.48
41:k:138:ARG:HH21	41:k:139:GLU:HG2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1039:A:N1	1:0:1116:G:O6	2.46	0.48
3:2:199:A:H2'	3:2:200:G:C8	2.48	0.48
3:2:637:C:H5"	51:u:4:LYS:HD3	1.95	0.48
10:D:110:ARG:HB3	10:D:137:ILE:HG23	1.94	0.48
1:0:1386:C:H2'	1:0:1387:A:C8	2.48	0.48
1:0:1996:C:H4'	1:0:1997:C:OP1	2.14	0.48
1:0:2328:A:H2'	1:0:2329:U:C6	2.49	0.48
3:2:459:A:H2'	3:2:460:A:C8	2.46	0.48
36:f:147:SER:HB3	36:f:148:LEU:HD22	1.94	0.48
3:2:46:G:HO2'	3:2:365:U:H6	1.62	0.48
3:2:422:C:H4'	3:2:423:G:O5'	2.13	0.48
3:2:1135:U:H2'	3:2:1136:C:H2'	1.96	0.48
22:P:70:LYS:NZ	22:P:70:LYS:HB2	2.28	0.48
40:j:11:HIS:ND1	40:j:11:HIS:C	2.72	0.48
43:m:47:VAL:O	43:m:50:GLN:HG3	2.14	0.48
1:0:634:C:H2'	1:0:635:C:C6	2.49	0.48
7:A:133:ARG:HG3	7:A:186:ALA:HB1	1.96	0.48
36:f:60:ILE:HG21	36:f:67:ILE:HD11	1.96	0.48
45:o:22:HIS:HB2	45:o:33:THR:HG23	1.96	0.48
3:2:150:U:H2'	3:2:151:A:H8	1.79	0.47
1:0:608:A:H2'	1:0:609:A:C8	2.48	0.47
1:0:1858:A:H2'	1:0:1859:U:O4'	2.14	0.47
3:2:676:A:H2'	3:2:677:U:C6	2.49	0.47
9:C:132:LYS:HE3	9:C:132:LYS:HB3	1.55	0.47
1:0:2281:A:O2'	1:0:2282:G:H5'	2.13	0.47
3:2:143:A:H2	3:2:220:G:H1	1.61	0.47
7:A:181:MET:HG3	7:A:269:ARG:HH21	1.80	0.47
1:0:1361:G:H2'	1:0:1362:C:C6	2.49	0.47
3:2:193:C:H2'	3:2:194:C:H6	1.79	0.47
3:2:236:A:H2'	3:2:237:G:C8	2.49	0.47
3:2:1412:C:H2'	3:2:1413:A:C8	2.49	0.47
1:0:17:G:H4'	20:N:25:TYR:HE1	1.79	0.47
1:0:143:C:H2'	1:0:144:A:H8	1.80	0.47
1:0:788:A:N3	33:c:4:THR:HG23	2.29	0.47
3:2:744:C:H2'	3:2:745:G:C8	2.48	0.47
54:x:4:ILE:O	54:x:8:LYS:HE3	2.14	0.47
3:2:411:A:C4	3:2:413:G:H1'	2.49	0.47
3:2:831:A:H5'	36:f:21:ARG:HH11	1.80	0.47
3:2:1327:C:H2'	3:2:1328:C:C6	2.50	0.47
17:K:45:ARG:HA	17:K:48:VAL:HG12	1.94	0.47
1:0:1869:G:H2'	1:0:1871:A:OP2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2246:G:H2'	1:0:2247:A:H8	1.79	0.47
1:0:2740:A:H2'	1:0:2741:A:C8	2.50	0.47
3:2:149:A:H2'	3:2:150:U:C6	2.49	0.47
3:2:339:C:H2'	3:2:340:U:C6	2.50	0.47
3:2:1238:A:N7	3:2:1303:C:H1'	2.30	0.47
26:T:41:ARG:HA	26:T:41:ARG:HD3	1.68	0.47
36:f:157:LEU:HD21	36:f:179:LEU:HD13	1.97	0.47
40:j:22:ILE:O	40:j:26:THR:HG22	2.15	0.47
1:0:1486:U:H2'	1:0:1487:U:C6	2.49	0.47
1:0:2576:G:H5'	1:0:2578:G:N7	2.29	0.47
39:i:83:HIS:CE1	42:l:96:MET:HE3	2.50	0.47
41:k:91:VAL:HB	41:k:96:ARG:HD3	1.96	0.47
1:0:283:G:H2'	1:0:284:U:C6	2.49	0.47
3:2:792:A:H4'	3:2:793:U:O5'	2.15	0.47
7:A:118:SER:HB2	7:A:129:THR:HB	1.96	0.47
53:w:11:ILE:HB	53:w:41:PHE:HE1	1.80	0.47
1:0:365:U:H2'	1:0:366:C:C6	2.50	0.47
1:0:2243:U:H2'	1:0:2244:U:C6	2.50	0.47
1:0:356:G:H2'	1:0:357:C:C6	2.50	0.46
1:0:2799:A:O2'	1:0:2800:A:H5"	2.16	0.46
3:2:410:G:H2'	3:2:429:U:C4	2.50	0.46
3:2:1136:C:H4'	3:2:1137:C:OP2	2.15	0.46
3:2:1268:G:H2'	3:2:1269:A:C8	2.50	0.46
16:J:3:GLN:HE21	16:J:92:TRP:NE1	2.13	0.46
1:0:56:A:H2'	1:0:57:C:O4'	2.15	0.46
3:2:46:G:O2'	3:2:365:U:H6	1.98	0.46
3:2:576:C:H3'	3:2:577:G:H5"	1.96	0.46
40:j:24:ARG:H	40:j:24:ARG:HG3	1.54	0.46
3:2:332:G:O3'	54:x:2:ALA:HB2	2.16	0.46
3:2:600:A:H2'	3:2:601:G:H8	1.80	0.46
3:2:618:C:H5"	3:2:619:U:H5"	1.97	0.46
3:2:950:U:H2'	3:2:951:G:H8	1.81	0.46
37:g:154:SER:OG	37:g:165:THR:HG23	2.15	0.46
44:n:8:ILE:HG12	44:n:100:ILE:HG22	1.97	0.46
1:0:2301:C:H2'	1:0:2302:U:C6	2.50	0.46
3:2:463:U:H2'	3:2:464:U:C6	2.51	0.46
3:2:497:G:H2'	3:2:498:A:C8	2.51	0.46
3:2:1305:G:H1'	3:2:1332:A:N6	2.30	0.46
3:2:1316:G:N2	3:2:1318:A:H3'	2.31	0.46
49:s:26:GLU:HG3	49:s:81:LEU:HD22	1.96	0.46
1:0:580:U:H2'	1:0:581:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1539:U:H2'	1:0:1540:G:H8	1.81	0.46
1:0:2086:U:H2'	1:0:2087:G:C8	2.51	0.46
3:2:286:C:H2'	3:2:287:U:C6	2.50	0.46
6:5:1:G:H2'	6:5:2:G:H8	1.81	0.46
1:0:639:U:H2'	1:0:640:C:H6	1.81	0.46
1:0:2560:A:H2'	1:0:2561:U:C6	2.50	0.46
1:0:2841:C:H2'	1:0:2842:G:C8	2.51	0.46
3:2:845:A:H2'	3:2:846:G:O4'	2.16	0.46
3:2:1315:U:O2	3:2:1360:A:H2	1.98	0.46
3:2:1343:G:H1'	43:m:123:ARG:HH12	1.80	0.46
8:B:4:LEU:HD23	8:B:29:VAL:CG1	2.45	0.46
39:i:72:ILE:HD13	39:i:141:ILE:HG23	1.98	0.46
1:0:645:C:H2'	1:0:647:G:N7	2.31	0.46
1:0:2898:U:H2'	1:0:2899:A:H8	1.81	0.46
3:2:1201:A:H1'	3:2:1202:U:OP2	2.16	0.46
38:h:168:PRO:HG2	38:h:171:LEU:HD22	1.98	0.46
43:m:118:LEU:HG	43:m:124:ARG:HG2	1.97	0.46
49:s:58:ARG:HH11	49:s:58:ARG:HG3	1.81	0.46
52:v:32:TYR:CG	52:v:55:LEU:HD21	2.50	0.46
1:0:2373:G:H2'	1:0:2374:C:H6	1.80	0.46
2:1:57:A:N6	10:D:26:MET:HE3	2.30	0.46
3:2:236:A:H2'	3:2:237:G:H8	1.81	0.46
11:E:27:LYS:HG3	11:E:32:GLU:HB2	1.98	0.46
54:x:74:ARG:HG3	54:x:75:HIS:N	2.30	0.46
1:0:45:G:H5'	1:0:46:G:OP1	2.16	0.46
3:2:580:C:H2'	3:2:581:G:O4'	2.16	0.46
3:2:1158:C:H5	3:2:1181:G:H22	1.64	0.46
10:D:65:PRO:HA	10:D:89:VAL:HG22	1.98	0.46
10:D:132:VAL:HB	10:D:152:LEU:HD23	1.98	0.46
14:H:2:ILE:HD12	14:H:6:THR:HG21	1.97	0.46
1:0:2529:G:H5"	1:0:2530:A:H5"	1.98	0.46
36:f:81:LYS:HD2	36:f:91:PHE:CE2	2.51	0.46
41:k:51:ALA:HB2	41:k:58:GLU:HG3	1.97	0.46
45:o:67:ALA:HB2	45:o:96:THR:HG23	1.97	0.46
1:0:1443:U:H2'	1:0:1444:G:H8	1.82	0.45
3:2:846:G:H2'	3:2:847:G:C8	2.51	0.45
3:2:948:C:H5'	3:2:1306:A:O2'	2.16	0.45
3:2:1038:C:H2'	3:2:1039:G:H8	1.81	0.45
5:4:16:C:H5"	5:4:17:U:H5'	1.96	0.45
36:f:151:ILE:HD12	36:f:154:MET:HE1	1.98	0.45
47:q:65:VAL:HG13	47:q:66:GLU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2662:A:O5'	1:0:2662:A:H8	1.97	0.45
3:2:950:U:H2'	3:2:951:G:C8	2.50	0.45
1:0:721:A:H2'	1:0:722:A:C8	2.51	0.45
1:0:1905:C:H3'	1:0:1930:G:C8	2.51	0.45
30:X:1:MET:HB2	30:X:1:MET:HE3	1.71	0.45
48:r:9:ARG:O	48:r:13:ARG:HG3	2.16	0.45
3:2:157:U:H2'	3:2:158:G:H8	1.80	0.45
3:2:713:G:H2'	3:2:714:G:C8	2.51	0.45
16:J:20:LEU:HD13	25:S:81:PRO:HG2	1.98	0.45
38:h:28:ILE:HD12	38:h:29:ASP:N	2.31	0.45
1:0:1794:A:H2'	1:0:1795:C:C6	2.51	0.45
1:0:2639:A:H2'	1:0:2640:G:O4'	2.16	0.45
3:2:200:G:H2'	3:2:201:G:C8	2.52	0.45
3:2:217:C:H2'	3:2:218:U:C6	2.51	0.45
3:2:1327:C:H2'	3:2:1328:C:H6	1.81	0.45
3:2:1328:C:OP1	47:q:28:THR:HG21	2.16	0.45
19:M:24:ASP:HB2	19:M:88:ARG:O	2.16	0.45
19:M:60:THR:OG1	19:M:73:VAL:HG22	2.16	0.45
43:m:79:ILE:O	43:m:83:ILE:HG12	2.17	0.45
1:0:1000:A:H2'	1:0:1001:A:C8	2.52	0.45
3:2:373:A:C2	3:2:374:A:C8	3.04	0.45
36:f:50:PHE:C	36:f:52:GLU:H	2.25	0.45
36:f:129:LEU:HD13	36:f:130:THR:HG23	1.98	0.45
49:s:24:SER:O	49:s:28:GLN:HG3	2.17	0.45
51:u:39:LYS:C	51:u:40:ARG:HD2	2.42	0.45
3:2:110:C:H2'	3:2:111:G:O4'	2.17	0.45
3:2:235:C:H2'	3:2:236:A:H8	1.80	0.45
3:2:358:U:H2'	3:2:359:G:C8	2.49	0.45
36:f:184:PHE:CD1	36:f:184:PHE:N	2.84	0.45
1:0:2266:A:H4'	1:0:2267:A:N3	2.32	0.45
3:2:1250:A:H2'	3:2:1251:A:C8	2.52	0.45
11:E:24:ILE:HG21	11:E:72:LEU:HD11	1.97	0.45
27:U:18:ARG:HA	27:U:23:ASN:O	2.17	0.45
32:b:10:LYS:HD2	32:b:54:ILE:HG13	1.99	0.45
3:2:389:A:C6	3:2:390:U:H1'	2.52	0.45
37:g:11:ARG:NH1	37:g:178:LEU:HA	2.32	0.45
40:j:39:LEU:HD23	40:j:62:MET:HB3	1.99	0.45
45:o:97:ILE:HG22	55:y:12:PHE:HZ	1.81	0.45
3:2:155:A:H2'	3:2:156:C:C6	2.51	0.45
5:4:71:C:H2'	5:4:72:A:H8	1.80	0.45
6:5:44:U:H2'	6:5:45:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1386:C:H2'	1:0:1387:A:H8	1.82	0.44
1:0:2554:U:H2'	1:0:2555:U:O2	2.16	0.44
3:2:864:A:H2'	3:2:865:A:C8	2.51	0.44
53:w:12:ASP:OD1	53:w:15:LEU:HB3	2.17	0.44
1:0:930:G:H1'	29:W:25:LEU:HD21	1.98	0.44
1:0:1657:U:H2'	1:0:1658:C:H6	1.82	0.44
1:0:2273:A:H2'	1:0:2274:A:C8	2.51	0.44
2:1:34:A:H5"	2:1:35:C:OP1	2.17	0.44
3:2:1241:G:H2'	3:2:1242:G:H8	1.83	0.44
12:F:6:LEU:HD11	12:F:37:VAL:HG23	1.98	0.44
12:F:9:VAL:HG12	12:F:10:ALA:H	1.82	0.44
36:f:135:LEU:O	36:f:138:THR:HG22	2.17	0.44
39:i:133:PRO:HA	39:i:136:VAL:HG12	2.00	0.44
1:0:150:U:H2'	1:0:151:C:C6	2.53	0.44
3:2:286:C:H2'	3:2:287:U:H6	1.83	0.44
3:2:1327:C:C2	3:2:1328:C:C5	3.06	0.44
46:p:83:ARG:HE	46:p:96:HIS:HB3	1.82	0.44
1:0:445:C:H2'	1:0:446:G:O4'	2.17	0.44
1:0:1432:G:H2'	1:0:1433:A:C8	2.53	0.44
1:0:2012:G:OP1	22:P:98:LYS:HE3	2.17	0.44
3:2:1011:C:H2'	3:2:1012:A:O4'	2.18	0.44
54:x:39:ILE:HD11	54:x:83:ILE:HG13	2.00	0.44
3:2:214:C:C2	3:2:215:C:C5	3.05	0.44
3:2:1053:G:N7	3:2:1200:C:H5"	2.33	0.44
5:4:10:A:H2'	5:4:11:G:C8	2.53	0.44
18:L:63:LYS:HB2	18:L:63:LYS:HE2	1.77	0.44
40:j:21:MET:HG2	40:j:25:TYR:CE2	2.53	0.44
3:2:1163:A:H2'	3:2:1164:G:H8	1.82	0.44
3:2:1330:U:H2'	3:2:1331:G:O4'	2.17	0.44
3:2:1371:G:C6	3:2:1372:U:C4	3.06	0.44
3:2:1410:A:H2'	3:2:1411:C:C6	2.52	0.44
22:P:13:SER:O	22:P:17:VAL:HG23	2.18	0.44
36:f:6:MET:HE2	36:f:6:MET:HB2	1.79	0.44
36:f:208:ARG:H	36:f:208:ARG:HG2	1.64	0.44
43:m:28:ILE:HD11	43:m:65:ILE:HD12	1.98	0.44
1:0:580:U:H2'	1:0:581:C:H6	1.82	0.44
1:0:639:U:H2'	1:0:640:C:C6	2.53	0.44
3:2:471:U:H2'	3:2:472:U:C6	2.53	0.44
10:D:108:VAL:O	10:D:111:ILE:HD12	2.18	0.44
11:E:105:LEU:HB3	11:E:107:LEU:HD23	2.00	0.44
24:R:44:LYS:HD2	24:R:61:LYS:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:35:ASP:CG	47:q:57:ARG:HH12	2.25	0.44
38:h:55:LEU:O	38:h:59:GLN:HG2	2.18	0.44
3:2:1175:G:H2'	3:2:1176:A:H8	1.82	0.44
6:5:23:A:H2'	6:5:24:G:C8	2.51	0.44
28:V:12:GLU:H	28:V:12:GLU:CD	2.26	0.44
48:r:59:ARG:HE	48:r:59:ARG:HB3	1.60	0.44
49:s:64:ARG:HE	49:s:64:ARG:HA	1.82	0.44
51:u:17:MET:SD	51:u:20:SER:HB2	2.57	0.44
1:0:1476:U:H2'	1:0:1477:A:H8	1.83	0.44
3:2:1345:U:H5"	43:m:122:ARG:NH2	2.31	0.44
19:M:5:ILE:O	19:M:9:GLU:HG3	2.18	0.44
37:g:28:GLU:HA	37:g:31:ASP:OD2	2.18	0.44
1:0:1032:A:H1'	35:e:23:ILE:HD13	2.00	0.43
1:0:2537:U:H2'	1:0:2538:C:C6	2.53	0.43
2:1:60:C:H2'	2:1:61:G:H8	1.82	0.43
2:1:118:C:H2'	2:1:119:A:H8	1.83	0.43
3:2:636:U:H2'	3:2:637:C:C6	2.52	0.43
48:r:9:ARG:HB3	48:r:13:ARG:NH1	2.32	0.43
48:r:85:ARG:O	48:r:89:MET:HG2	2.18	0.43
1:0:1796:U:H2'	1:0:1797:G:H8	1.82	0.43
1:0:2191:A:H2'	1:0:2192:U:C6	2.53	0.43
11:E:85:LYS:HG3	11:E:141:ILE:HG12	1.98	0.43
30:X:14:ALA:HB1	30:X:34:LEU:HD23	1.99	0.43
38:h:56:ARG:HH21	38:h:59:GLN:HG3	1.82	0.43
1:0:471:A:H2'	1:0:472:A:O4'	2.18	0.43
1:0:2373:G:H2'	1:0:2374:C:C6	2.53	0.43
3:2:908:A:H2'	3:2:909:A:C8	2.53	0.43
3:2:1121:U:H2'	3:2:1122:U:C6	2.53	0.43
5:4:65:C:H2'	5:4:66:C:C6	2.54	0.43
17:K:109:PRO:O	17:K:110:MET:HE2	2.17	0.43
32:b:38:LYS:HE2	32:b:38:LYS:HB3	1.93	0.43
50:t:4:ILE:HG13	50:t:21:VAL:HB	2.01	0.43
1:0:169:G:H2'	1:0:170:U:C6	2.54	0.43
1:0:973:A:H5"	21:O:81:LYS:HD2	1.99	0.43
1:0:1141:U:H4'	1:0:1142:A:O4'	2.17	0.43
8:B:3:GLY:O	8:B:4:LEU:HD12	2.18	0.43
38:h:8:LYS:HG3	38:h:21:LEU:HD13	1.99	0.43
2:1:66:A:H2	2:1:68:C:H41	1.66	0.43
3:2:1307:U:O3'	47:q:109:ARG:HD2	2.17	0.43
12:F:130:VAL:HG23	12:F:132:PHE:HE1	1.83	0.43
14:H:76:VAL:C	14:H:77:ILE:HD12	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:25:LYS:HE2	32:b:51:GLU:OE1	2.18	0.43
41:k:93:PRO:HA	41:k:96:ARG:HG3	1.99	0.43
48:r:51:LEU:H	48:r:51:LEU:HD12	1.82	0.43
1:0:1028:A:H2'	1:0:1029:A:C8	2.52	0.43
2:1:1:U:H2'	2:1:2:G:H8	1.84	0.43
3:2:1132:C:H2'	3:2:1133:G:C8	2.54	0.43
21:O:73:LYS:HB3	21:O:73:LYS:HE2	1.75	0.43
36:f:42:ASN:O	36:f:43:LEU:HB2	2.19	0.43
1:0:2327:A:H2'	1:0:2328:A:C8	2.54	0.43
7:A:75:PRO:HG2	7:A:97:LYS:HE2	2.01	0.43
19:M:112:GLU:HG2	19:M:114:LEU:HG	1.99	0.43
23:Q:25:GLU:OE1	23:Q:26:LYS:HG2	2.19	0.43
53:w:12:ASP:HB2	53:w:14:HIS:CD2	2.54	0.43
1:0:289:G:H2'	1:0:290:U:C6	2.54	0.43
1:0:1361:G:H2'	1:0:1362:C:H6	1.83	0.43
1:0:1486:U:H2'	1:0:1487:U:H6	1.83	0.43
1:0:2025:C:H2'	1:0:2026:U:C6	2.54	0.43
3:2:1163:A:H2'	3:2:1164:G:C8	2.54	0.43
1:0:1327:A:H2'	1:0:1328:A:O4'	2.19	0.43
1:0:1434:A:O2'	1:0:1435:G:H8	2.02	0.43
2:1:118:C:H2'	2:1:119:A:C8	2.54	0.43
3:2:193:C:H2'	3:2:194:C:C6	2.54	0.43
3:2:728:A:H2'	3:2:729:A:C8	2.54	0.43
21:O:68:ARG:HD3	21:O:92:TRP:CE2	2.54	0.43
22:P:73:LYS:HB2	22:P:73:LYS:HE2	1.70	0.43
36:f:161:LEU:HD23	36:f:161:LEU:HA	1.85	0.43
1:0:2480:C:H2'	1:0:2481:G:O4'	2.19	0.43
1:0:2804:U:H2'	1:0:2805:C:H6	1.83	0.43
3:2:676:A:H2'	3:2:677:U:H6	1.84	0.43
3:2:745:G:H2'	3:2:746:A:C8	2.54	0.43
37:g:60:PRO:HD2	37:g:63:SER:C	2.44	0.43
40:j:45:ARG:O	40:j:56:LYS:HA	2.19	0.43
45:o:25:ALA:O	45:o:88:GLY:HA3	2.18	0.43
17:K:8:ARG:HD2	17:K:43:GLU:HG2	2.01	0.42
36:f:27:MET:HE2	36:f:189:THR:HA	2.00	0.42
36:f:27:MET:HE3	36:f:27:MET:HB3	1.77	0.42
37:g:30:ALA:HB1	48:r:65:ARG:HH12	1.83	0.42
54:x:24:ARG:O	54:x:28:MET:HG2	2.19	0.42
1:0:2203:U:H5"	1:0:2204:G:OP1	2.19	0.42
1:0:2728:U:O2'	1:0:2729:G:H8	2.02	0.42
2:1:45:A:O4'	10:D:92:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:672:U:H2'	3:2:673:A:H8	1.83	0.42
3:2:1072:G:H2'	3:2:1073:U:C6	2.54	0.42
5:4:10:A:H2'	5:4:11:G:H8	1.84	0.42
7:A:8:PRO:HB3	7:A:14:ARG:HG3	2.01	0.42
8:B:109:VAL:CG1	8:B:201:LEU:HD22	2.49	0.42
10:D:35:THR:C	10:D:36:LEU:HD23	2.44	0.42
40:j:45:ARG:HH22	40:j:102:MET:HE2	1.84	0.42
3:2:782:A:H62	3:2:800:G:H21	1.68	0.42
10:D:88:LYS:HE2	10:D:88:LYS:HB3	1.82	0.42
17:K:28:LEU:HD23	17:K:48:VAL:HG21	2.01	0.42
38:h:98:LEU:O	38:h:102:VAL:HG23	2.19	0.42
42:l:29:SER:HB2	42:l:59:LEU:HB2	1.99	0.42
1:0:581:C:H2'	1:0:582:A:C8	2.55	0.42
1:0:947:A:H2'	1:0:948:C:C6	2.54	0.42
1:0:984:A:N3	1:0:984:A:H2'	2.34	0.42
1:0:2845:U:H5"	19:M:52:ASN:O	2.20	0.42
3:2:261:U:H2'	3:2:263:A:OP2	2.20	0.42
10:D:133:ARG:O	10:D:133:ARG:HG2	2.19	0.42
47:q:83:LEU:HD11	53:w:66:MET:HG3	2.01	0.42
2:1:60:C:H2'	2:1:61:G:C8	2.54	0.42
3:2:323:U:H2'	3:2:324:G:O4'	2.19	0.42
3:2:835:U:OP1	52:v:50:LYS:HG3	2.20	0.42
46:p:114:ARG:HB3	46:p:119:VAL:HB	2.00	0.42
37:g:11:ARG:HG2	37:g:11:ARG:HH11	1.85	0.42
1:0:45:G:H5'	1:0:46:G:H5'	2.02	0.42
1:0:172:A:H2'	1:0:173:A:C8	2.54	0.42
3:2:1359:C:H6	3:2:1359:C:O5'	2.02	0.42
37:g:30:ALA:HB1	48:r:65:ARG:HH22	1.84	0.42
39:i:148:ASN:HA	39:i:152:MET:HE3	2.02	0.42
40:j:43:GLY:HA2	40:j:58:HIS:CE1	2.55	0.42
42:l:69:LYS:HE2	42:l:69:LYS:HB2	1.83	0.42
3:2:56:U:H2'	3:2:57:G:C8	2.54	0.42
3:2:576:C:H3'	3:2:577:G:C5'	2.50	0.42
10:D:67:ILE:HG22	10:D:69:LYS:NZ	2.34	0.42
14:H:38:ILE:HD11	14:H:112:PHE:HZ	1.85	0.42
36:f:20:THR:HG22	36:f:39:HIS:CE1	2.55	0.42
41:k:22:LEU:HD12	41:k:22:LEU:HA	1.89	0.42
44:n:48:ARG:NH1	48:r:101:TRP:CD2	2.87	0.42
1:0:1395:A:O2'	1:0:1396:U:H5"	2.18	0.42
1:0:2700:A:H2'	1:0:2701:U:C6	2.55	0.42
1:0:2728:U:HO2'	1:0:2729:G:H8	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:592:G:H2'	3:2:593:U:C6	2.54	0.42
3:2:600:A:H2'	3:2:601:G:C8	2.55	0.42
3:2:745:G:H2'	3:2:746:A:H8	1.84	0.42
3:2:889:A:H8	3:2:889:A:OP1	2.03	0.42
22:P:73:LYS:NZ	22:P:106:VAL:HG21	2.35	0.42
31:a:12:LYS:HA	31:a:15:MET:HG3	2.02	0.42
44:n:87:LEU:HD12	44:n:87:LEU:HA	1.88	0.42
49:s:27:VAL:O	49:s:31:LEU:HD12	2.19	0.42
53:w:70:LYS:O	53:w:73:GLU:HG3	2.20	0.42
1:0:979:A:H2'	1:0:982:C:H42	1.84	0.42
1:0:1243:C:H2'	1:0:1244:A:O4'	2.19	0.42
6:5:27:G:H1	6:5:43:U:H3	1.68	0.42
25:S:83:LYS:HD2	25:S:85:LYS:HZ2	1.85	0.42
37:g:86:LYS:O	37:g:90:VAL:HG23	2.20	0.42
1:0:361:G:H8	1:0:361:G:OP2	2.03	0.41
3:2:594:U:H2'	3:2:595:A:O4'	2.20	0.41
3:2:644:U:C2	3:2:645:G:C8	3.08	0.41
3:2:846:G:H2'	3:2:847:G:H8	1.83	0.41
3:2:1147:C:H4'	43:m:7:TYR:CZ	2.55	0.41
28:V:44:LYS:O	28:V:48:ARG:HG2	2.20	0.41
47:q:79:ARG:HG2	47:q:79:ARG:NH1	2.33	0.41
1:0:189:G:OP1	27:U:26:LYS:HD2	2.20	0.41
1:0:634:C:H2'	1:0:635:C:H6	1.85	0.41
1:0:2301:C:H2'	1:0:2302:U:H6	1.85	0.41
1:0:2801:G:H2'	1:0:2802:G:H8	1.86	0.41
3:2:214:C:H2'	3:2:215:C:C6	2.56	0.41
3:2:378:G:H2'	3:2:379:C:C6	2.55	0.41
3:2:1149:C:H2'	3:2:1150:A:H8	1.83	0.41
15:I:96:LYS:HD3	15:I:103:ILE:HA	2.01	0.41
36:f:66:LYS:H	36:f:159:ASP:HB2	1.85	0.41
42:l:7:ILE:O	42:l:11:LEU:HG	2.20	0.41
42:l:105:SER:HB2	42:l:126:ILE:HD11	2.01	0.41
1:0:265:A:H4'	1:0:266:G:OP1	2.20	0.41
1:0:1048:A:H62	1:0:1110:G:H21	1.69	0.41
3:2:978:A:C4	3:2:1319:A:C2	3.09	0.41
4:3:21:A:H2	6:5:34:U8U:HN3	1.68	0.41
47:q:65:VAL:HG13	47:q:66:GLU:H	1.85	0.41
1:0:12:U:C2'	1:0:13:A:H5'	2.50	0.41
1:0:1412:U:H2'	1:0:1413:A:C8	2.56	0.41
3:2:634:C:C2	3:2:635:A:C8	3.08	0.41
3:2:1226:C:H2'	47:q:102:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:49:ASP:OD2	13:G:118:MET:HG3	2.20	0.41
17:K:30:ARG:NH1	17:K:30:ARG:HB2	2.35	0.41
36:f:45:LYS:HG2	36:f:50:PHE:HB2	2.02	0.41
39:i:156:LYS:HD2	42:l:71:VAL:HA	2.01	0.41
1:0:1047:G:N2	1:0:1111:A:C5	2.88	0.41
1:0:1179:G:H2'	1:0:1180:U:C6	2.56	0.41
1:0:1469:A:H2'	1:0:1470:A:H8	1.83	0.41
3:2:467:U:H4'	3:2:468:A:OP2	2.20	0.41
10:D:67:ILE:HG22	10:D:69:LYS:HZ1	1.86	0.41
21:O:85:LYS:HG2	21:O:86:GLN:N	2.36	0.41
30:X:14:ALA:HB3	30:X:22:MET:HG2	2.03	0.41
36:f:24:ASN:HA	36:f:25:PRO:HD3	1.90	0.41
51:u:9:GLN:NE2	51:u:58:VAL:HG12	2.32	0.41
1:0:175:G:H2'	1:0:176:A:C8	2.55	0.41
1:0:1438:U:H2'	1:0:1439:A:H8	1.84	0.41
1:0:1507:C:H2'	1:0:1508:A:O4'	2.21	0.41
2:1:106:G:H2'	2:1:107:G:O4'	2.20	0.41
3:2:17:U:H2'	3:2:18:C:H6	1.84	0.41
3:2:114:U:H2'	3:2:115:G:C8	2.56	0.41
3:2:149:A:C5	3:2:150:U:C4	3.09	0.41
3:2:312:C:H2'	3:2:313:A:C8	2.55	0.41
5:4:66:C:H2'	5:4:67:C:C6	2.56	0.41
44:n:19:ASP:O	44:n:22:THR:HG22	2.21	0.41
1:0:1802:A:H2'	1:0:1803:A:H8	1.79	0.41
1:0:1883:U:H2'	1:0:1884:G:O4'	2.20	0.41
1:0:2591:C:H2'	1:0:2592:G:C8	2.55	0.41
3:2:83:C:H4'	3:2:84:U:OP1	2.20	0.41
3:2:1126:U:H5	44:n:42:LEU:HD21	1.86	0.41
5:4:44:A:H2'	5:4:45:G:O4'	2.21	0.41
14:H:8:LEU:HB2	14:H:19:VAL:HG23	2.02	0.41
37:g:162:ILE:HD13	37:g:162:ILE:HA	1.88	0.41
38:h:58:LYS:HA	38:h:200:ILE:HD11	2.02	0.41
46:p:30:LYS:HD2	46:p:30:LYS:HA	1.93	0.41
1:0:1413:A:H2'	1:0:1414:C:H6	1.86	0.41
3:2:392:C:C2	3:2:393:A:C8	3.08	0.41
3:2:524:G:H2'	3:2:525:C:C6	2.56	0.41
3:2:1014:A:H1'	3:2:1218:C:O2'	2.21	0.41
3:2:1070:U:H2'	3:2:1071:C:H6	1.86	0.41
3:2:1314:C:H2'	3:2:1315:U:C6	2.52	0.41
10:D:141:ILE:HD11	10:D:146:VAL:HG22	2.01	0.41
12:F:51:ARG:HG2	12:F:54:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:157:LEU:HD13	37:g:166:GLU:OE1	2.21	0.41
39:i:104:GLY:O	39:i:122:ASN:HA	2.20	0.41
1:0:357:C:H2'	1:0:358:U:C6	2.55	0.41
1:0:973:A:H5'	1:0:1188:U:H1'	2.02	0.41
1:0:1435:G:H2'	1:0:1436:G:H8	1.86	0.41
1:0:2197:U:O2'	1:0:2198:A:H2'	2.21	0.41
2:1:1:U:H2'	2:1:2:G:C8	2.56	0.41
3:2:214:C:H2'	3:2:215:C:H6	1.85	0.41
3:2:674:G:H2'	3:2:675:A:C8	2.55	0.41
14:H:63:VAL:HG23	14:H:64:ARG:HG3	2.02	0.41
22:P:23:LEU:HD22	31:a:24:ALA:HB2	2.03	0.41
36:f:42:ASN:C	36:f:44:GLU:H	2.29	0.41
36:f:63:ARG:O	36:f:64:LYS:HG2	2.20	0.41
44:n:37:ARG:NH2	44:n:77:VAL:HG22	2.35	0.41
54:x:28:MET:HE3	54:x:28:MET:HB2	1.91	0.41
54:x:79:LEU:HD23	54:x:79:LEU:HA	1.78	0.41
1:0:1190:G:H5"	15:I:32:GLY:HA2	2.01	0.41
3:2:223:A:H2'	3:2:224:U:C6	2.56	0.41
3:2:549:C:H2'	3:2:550:G:O4'	2.21	0.41
3:2:685:G:O5'	3:2:685:G:H8	2.04	0.41
3:2:844:G:H21	3:2:844:G:P	2.44	0.41
3:2:1219:A:H5"	48:r:53:ARG:NH1	2.36	0.41
7:A:29:PRO:HG2	7:A:34:LEU:HD21	2.02	0.41
12:F:1:MET:HE2	27:U:60:ASP:OD1	2.21	0.41
20:N:41:LYS:HE2	20:N:45:TYR:OH	2.19	0.41
39:i:90:THR:HG22	39:i:91:GLY:N	2.35	0.41
51:u:17:MET:HB2	51:u:20:SER:O	2.19	0.41
3:2:159:G:H1	3:2:163:C:N4	2.19	0.40
16:J:133:LYS:HG3	16:J:134:THR:N	2.35	0.40
19:M:114:LEU:HD23	19:M:114:LEU:HA	1.91	0.40
36:f:111:ILE:HG13	36:f:112:LYS:N	2.36	0.40
37:g:62:LYS:HD3	37:g:62:LYS:HA	1.89	0.40
37:g:155:GLY:O	37:g:196:ILE:HG12	2.20	0.40
38:h:73:ARG:HG2	38:h:77:LYS:NZ	2.37	0.40
43:m:42:GLU:HA	43:m:45:ARG:HD2	2.02	0.40
1:0:118:A:H5'	1:0:119:A:C8	2.53	0.40
1:0:732:C:H2'	1:0:733:G:O4'	2.21	0.40
1:0:1047:G:N2	1:0:1111:A:C6	2.88	0.40
1:0:1413:A:H2'	1:0:1414:C:C6	2.55	0.40
1:0:1437:C:H2'	1:0:1438:U:C6	2.56	0.40
3:2:636:U:H2'	3:2:637:C:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:908:A:H2'	3:2:909:A:H8	1.86	0.40
7:A:87:ARG:HG3	7:A:89:ALA:H	1.87	0.40
27:U:22:LEU:HD12	27:U:22:LEU:HA	1.79	0.40
29:W:51:VAL:O	29:W:55:VAL:HG22	2.22	0.40
37:g:34:ASP:HB2	48:r:65:ARG:HH21	1.86	0.40
39:i:66:LYS:HB2	39:i:66:LYS:HE3	1.61	0.40
40:j:38:ARG:NH2	40:j:61:LEU:HD21	2.37	0.40
41:k:35:LYS:HB3	41:k:38:THR:HB	2.02	0.40
43:m:31:ASN:O	43:m:33:ARG:HG3	2.21	0.40
52:v:55:LEU:O	52:v:59:ILE:HG13	2.21	0.40
1:0:2243:U:H2'	1:0:2244:U:H6	1.87	0.40
3:2:440:C:C2	3:2:441:A:C8	3.09	0.40
3:2:453:G:H8	3:2:453:G:OP2	2.04	0.40
3:2:1314:C:C2	3:2:1315:U:C5	3.09	0.40
7:A:78:VAL:HG22	7:A:94:VAL:HG12	2.03	0.40
10:D:34:ILE:HD12	10:D:96:MET:HG3	2.03	0.40
37:g:56:VAL:HB	37:g:67:THR:CG2	2.49	0.40
37:g:114:LYS:HB2	37:g:185:ASN:ND2	2.36	0.40
41:k:33:ASP:O	41:k:33:ASP:OD1	2.40	0.40
42:l:66:PHE:HD1	42:l:66:PHE:HA	1.69	0.40
43:m:43:THR:O	43:m:46:MET:HG3	2.22	0.40
43:m:68:LYS:HD2	43:m:69:GLY:N	2.36	0.40
1:0:96:C:H4'	28:V:41:HIS:CE1	2.56	0.40
1:0:274:C:H2'	1:0:275:C:C6	2.57	0.40
1:0:2841:C:H2'	1:0:2842:G:H8	1.86	0.40
3:2:101:A:C4	3:2:102:G:C8	3.10	0.40
3:2:110:C:C2	3:2:111:G:C8	3.09	0.40
3:2:992:U:O4	3:2:1043:G:H2'	2.22	0.40
3:2:1120:C:H2'	3:2:1121:U:H6	1.87	0.40
9:C:102:ARG:O	9:C:106:LYS:HG3	2.21	0.40
10:D:66:LEU:HD21	10:D:88:LYS:HE3	2.02	0.40
12:F:12:LEU:HB2	12:F:19:VAL:HG21	2.03	0.40
13:G:92:MET:HE3	13:G:92:MET:HB3	1.79	0.40
15:I:108:ALA:HB3	15:I:125:LEU:HD22	2.03	0.40
16:J:125:PRO:C	16:J:126:ILE:HG12	2.46	0.40
17:K:38:LEU:HB3	17:K:39:PRO:HD3	2.04	0.40
27:U:45:ARG:HH12	27:U:47:VAL:HG22	1.86	0.40
1:0:52:A:H2'	1:0:53:A:C8	2.57	0.40
20:N:15:LYS:HE2	20:N:15:LYS:HB3	1.86	0.40
38:h:161:LEU:HD23	38:h:161:LEU:HA	1.97	0.40
41:k:15:ASP:HB2	41:k:18:PHE:O	2.21	0.40

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There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	
7	A	269/273 (98%)	257 (96%)	12 (4%)	0	100	100
8	B	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
9	C	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
10	D	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
11	E	171/177 (97%)	163 (95%)	8 (5%)	0	100	100
12	F	147/149 (99%)	141 (96%)	6 (4%)	0	100	100
13	G	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
14	H	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
15	I	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
16	J	134/136 (98%)	122 (91%)	12 (9%)	0	100	100
17	K	116/127 (91%)	108 (93%)	8 (7%)	0	100	100
18	L	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
19	M	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
20	N	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
21	O	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
22	P	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
23	Q	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
24	R	100/104 (96%)	95 (95%)	5 (5%)	0	100	100
25	S	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
26	T	73/85 (86%)	73 (100%)	0	0	100	100
27	U	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
28	V	58/63 (92%)	57 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	W	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
30	X	56/70 (80%)	51 (91%)	5 (9%)	0	100	100
31	a	53/57 (93%)	51 (96%)	2 (4%)	0	100	100
32	b	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
33	c	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
34	d	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
35	e	36/38 (95%)	36 (100%)	0	0	100	100
36	f	222/241 (92%)	205 (92%)	17 (8%)	0	100	100
37	g	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
38	h	203/206 (98%)	202 (100%)	1 (0%)	0	100	100
39	i	153/167 (92%)	147 (96%)	6 (4%)	0	100	100
40	j	104/131 (79%)	101 (97%)	2 (2%)	1 (1%)	12	24
41	k	149/179 (83%)	144 (97%)	5 (3%)	0	100	100
42	l	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
43	m	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
44	n	97/103 (94%)	92 (95%)	5 (5%)	0	100	100
45	o	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
46	p	121/124 (98%)	118 (98%)	3 (2%)	0	100	100
47	q	112/118 (95%)	100 (89%)	11 (10%)	1 (1%)	14	27
48	r	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
49	s	86/89 (97%)	86 (100%)	0	0	100	100
50	t	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
51	u	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
52	v	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
53	w	77/92 (84%)	73 (95%)	4 (5%)	0	100	100
54	x	84/87 (97%)	84 (100%)	0	0	100	100
55	y	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
All	All	5581/5909 (94%)	5352 (96%)	227 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
47	q	45	ILE

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Mol	Chain	Res	Type
40	j	56	LYS

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	
7	A	216/218 (99%)	208 (96%)	8 (4%)	30	55
8	B	164/164 (100%)	160 (98%)	4 (2%)	43	67
9	C	165/165 (100%)	159 (96%)	6 (4%)	31	56
10	D	148/150 (99%)	142 (96%)	6 (4%)	27	52
11	E	134/138 (97%)	132 (98%)	2 (2%)	57	77
12	F	114/114 (100%)	110 (96%)	4 (4%)	32	57
13	G	116/116 (100%)	110 (95%)	6 (5%)	21	43
14	H	104/104 (100%)	102 (98%)	2 (2%)	50	73
15	I	103/103 (100%)	96 (93%)	7 (7%)	14	31
16	J	109/109 (100%)	102 (94%)	7 (6%)	16	33
17	K	98/103 (95%)	96 (98%)	2 (2%)	48	72
18	L	86/87 (99%)	82 (95%)	4 (5%)	23	47
19	M	99/100 (99%)	96 (97%)	3 (3%)	36	60
20	N	89/90 (99%)	87 (98%)	2 (2%)	45	69
21	O	84/84 (100%)	84 (100%)	0	100	100
22	P	93/93 (100%)	89 (96%)	4 (4%)	26	50
23	Q	80/84 (95%)	79 (99%)	1 (1%)	61	79
24	R	83/85 (98%)	79 (95%)	4 (5%)	23	46
25	S	78/78 (100%)	72 (92%)	6 (8%)	12	26
26	T	57/63 (90%)	57 (100%)	0	100	100
27	U	67/68 (98%)	65 (97%)	2 (3%)	36	60
28	V	54/55 (98%)	53 (98%)	1 (2%)	50	73
29	W	47/49 (96%)	46 (98%)	1 (2%)	47	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	X	55/62 (89%)	51 (93%)	4 (7%)	13	28
31	a	46/48 (96%)	45 (98%)	1 (2%)	45	69
32	b	46/49 (94%)	43 (94%)	3 (6%)	15	32
33	c	38/38 (100%)	37 (97%)	1 (3%)	40	65
34	d	51/52 (98%)	50 (98%)	1 (2%)	48	72
35	e	34/34 (100%)	33 (97%)	1 (3%)	37	61
36	f	186/199 (94%)	174 (94%)	12 (6%)	15	32
37	g	170/190 (90%)	164 (96%)	6 (4%)	32	57
38	h	172/173 (99%)	164 (95%)	8 (5%)	23	47
39	i	118/126 (94%)	111 (94%)	7 (6%)	18	37
40	j	92/112 (82%)	89 (97%)	3 (3%)	33	58
41	k	124/147 (84%)	114 (92%)	10 (8%)	11	24
42	l	104/105 (99%)	99 (95%)	5 (5%)	23	46
43	m	105/107 (98%)	97 (92%)	8 (8%)	12	26
44	n	87/90 (97%)	82 (94%)	5 (6%)	18	39
45	o	90/99 (91%)	89 (99%)	1 (1%)	65	81
46	p	103/104 (99%)	97 (94%)	6 (6%)	18	38
47	q	92/96 (96%)	89 (97%)	3 (3%)	33	58
48	r	83/84 (99%)	76 (92%)	7 (8%)	10	22
49	s	76/77 (99%)	72 (95%)	4 (5%)	20	42
50	t	65/65 (100%)	63 (97%)	2 (3%)	35	59
51	u	74/78 (95%)	71 (96%)	3 (4%)	27	52
52	v	57/65 (88%)	56 (98%)	1 (2%)	51	74
53	w	70/79 (89%)	67 (96%)	3 (4%)	26	50
54	x	65/66 (98%)	60 (92%)	5 (8%)	12	26
55	y	60/61 (98%)	59 (98%)	1 (2%)	53	75
All	All	4651/4826 (96%)	4458 (96%)	193 (4%)	28	52

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	A	23	GLU
7	A	70	ASN

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Mol	Chain	Res	Type
7	A	120	VAL
7	A	134	ASN
7	A	137	VAL
7	A	195	VAL
7	A	205	LEU
7	A	219	THR
8	B	29	VAL
8	B	40	LEU
8	B	133	THR
8	B	189	VAL
9	C	65	THR
9	C	69	ARG
9	C	91	ASP
9	C	105	LEU
9	C	122	GLU
9	C	163	ASN
10	D	4	LEU
10	D	14	LYS
10	D	26	MET
10	D	57	LEU
10	D	66	LEU
10	D	149	VAL
11	E	43	VAL
11	E	89	LEU
12	F	9	VAL
12	F	12	LEU
12	F	15	LEU
12	F	90	LEU
13	G	10	THR
13	G	11	VAL
13	G	62	VAL
13	G	64	VAL
13	G	73	VAL
13	G	93	ILE
14	H	22	ILE
14	H	47	ILE
15	I	13	LYS
15	I	25	SER
15	I	76	GLU
15	I	77	ILE
15	I	80	SER
15	I	112	LEU

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Mol	Chain	Res	Type
15	I	127	VAL
16	J	10	ARG
16	J	30	SER
16	J	59	ARG
16	J	60	GLN
16	J	78	LEU
16	J	95	LEU
16	J	119	LEU
17	K	15	SER
17	K	37	THR
18	L	7	ARG
18	L	12	THR
18	L	24	THR
18	L	48	LEU
19	M	15	GLN
19	M	37	LYS
19	M	63	LYS
20	N	17	ILE
20	N	111	GLU
22	P	3	THR
22	P	13	SER
22	P	82	MET
22	P	98	LYS
23	Q	86	THR
24	R	9	ASP
24	R	44	LYS
24	R	72	ILE
24	R	93	VAL
25	S	7	GLU
25	S	14	LYS
25	S	24	ASN
25	S	25	LYS
25	S	55	GLU
25	S	61	LEU
27	U	22	LEU
27	U	25	THR
28	V	54	LYS
29	W	41	THR
30	X	9	TYR
30	X	13	THR
30	X	22	MET
30	X	30	HIS

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Mol	Chain	Res	Type
31	a	27	SER
32	b	7	GLU
32	b	9	ILE
32	b	37	LYS
33	c	4	THR
34	d	52	LYS
35	e	10	LEU
36	f	23	TRP
36	f	27	MET
36	f	31	ILE
36	f	49	MET
36	f	63	ARG
36	f	66	LYS
36	f	92	VAL
36	f	112	LYS
36	f	116	ASP
36	f	142	GLU
36	f	154	MET
36	f	208	ARG
37	g	38	LYS
37	g	49	LYS
37	g	67	THR
37	g	93	ASP
37	g	149	ILE
37	g	186	THR
38	h	28	ILE
38	h	62	ARG
38	h	116	GLN
38	h	124	MET
38	h	125	VAL
38	h	198	HIS
38	h	200	ILE
38	h	204	TYR
39	i	24	THR
39	i	65	GLU
39	i	66	LYS
39	i	117	VAL
39	i	131	THR
39	i	141	ILE
39	i	144	LEU
40	j	11	HIS
40	j	18	VAL

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Mol	Chain	Res	Type
40	j	24	ARG
41	k	32	VAL
41	k	33	ASP
41	k	69	VAL
41	k	72	THR
41	k	89	VAL
41	k	101	MET
41	k	122	ASN
41	k	131	LYS
41	k	133	THR
41	k	143	ARG
42	l	26	THR
42	l	55	THR
42	l	62	THR
42	l	66	PHE
42	l	89	LYS
43	m	55	VAL
43	m	61	LEU
43	m	88	MET
43	m	94	LEU
43	m	96	SER
43	m	105	THR
43	m	109	ARG
43	m	119	ARG
44	n	18	ILE
44	n	28	THR
44	n	42	LEU
44	n	50	THR
44	n	76	ILE
45	o	100	LEU
46	p	4	VAL
46	p	20	ASN
46	p	39	THR
46	p	50	ARG
46	p	65	SER
46	p	102	LEU
47	q	19	LEU
47	q	100	GLN
47	q	104	THR
48	r	5	SER
48	r	47	LYS
48	r	49	GLN

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Mol	Chain	Res	Type
48	r	59	ARG
48	r	93	ILE
48	r	97	LYS
48	r	100	SER
49	s	31	LEU
49	s	48	LYS
49	s	52	SER
49	s	74	ASP
50	t	21	VAL
50	t	31	ARG
51	u	22	VAL
51	u	57	ASP
51	u	67	LEU
52	v	47	THR
53	w	37	ARG
53	w	63	THR
53	w	77	THR
54	x	18	ARG
54	x	20	HIS
54	x	54	MET
54	x	55	GLN
54	x	60	ARG
55	y	21	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
7	A	25	HIS
7	A	58	HIS
7	A	70	ASN
7	A	260	ASN
8	B	49	GLN
8	B	150	GLN
9	C	94	GLN
11	E	101	ASN
13	G	47	HIS
14	H	88	ASN
16	J	3	GLN
18	L	38	GLN
19	M	10	GLN
19	M	56	HIS
20	N	44	GLN

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Mol	Chain	Res	Type
22	P	9	HIS
23	Q	91	GLN
25	S	80	HIS
27	U	36	HIS
30	X	6	HIS
35	e	13	ASN
37	g	3	GLN
38	h	36	GLN
38	h	71	GLN
38	h	116	GLN
38	h	126	ASN
38	h	140	ASN
42	l	4	GLN
42	l	21	ASN
43	m	32	GLN
43	m	50	GLN
43	m	81	HIS
44	n	58	ASN
45	o	15	GLN
47	q	91	HIS
47	q	105	ASN
50	t	9	HIS
51	u	50	ASN
53	w	43	ASN
54	x	21	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2754/2904 (94%)	374 (13%)	5 (0%)
2	1	119/120 (99%)	14 (11%)	0
3	2	1533/1542 (99%)	283 (18%)	40 (2%)
4	3	9/10 (90%)	2 (22%)	0
5	4	76/77 (98%)	13 (17%)	1 (1%)
6	5	75/76 (98%)	10 (13%)	1 (1%)
All	All	4566/4729 (96%)	696 (15%)	47 (1%)

All (696) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	10	A

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Mol	Chain	Res	Type
1	0	13	A
1	0	23	G
1	0	34	U
1	0	35	G
1	0	46	G
1	0	63	A
1	0	71	A
1	0	74	A
1	0	75	G
1	0	84	A
1	0	92	U
1	0	99	U
1	0	101	A
1	0	102	U
1	0	103	A
1	0	118	A
1	0	119	A
1	0	120	U
1	0	139	U
1	0	140	C
1	0	163	C
1	0	196	A
1	0	199	A
1	0	216	A
1	0	221	A
1	0	222	A
1	0	233	A
1	0	248	G
1	0	266	G
1	0	272	A
1	0	277	G
1	0	281	C
1	0	282	A
1	0	285	G
1	0	299	A
1	0	302	C
1	0	311	A
1	0	312	G
1	0	323	C
1	0	329	G
1	0	330	A
1	0	353	C

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Mol	Chain	Res	Type
1	0	361	G
1	0	362	A
1	0	372	G
1	0	385	C
1	0	386	G
1	0	392	U
1	0	396	G
1	0	404	A
1	0	405	U
1	0	411	G
1	0	412	A
1	0	413	C
1	0	421	C
1	0	424	G
1	0	436	C
1	0	467	G
1	0	481	G
1	0	489	G
1	0	491	G
1	0	502	A
1	0	505	A
1	0	509	C
1	0	530	G
1	0	531	C
1	0	532	A
1	0	533	G
1	0	538	A
1	0	547	A
1	0	548	G
1	0	555	G
1	0	557	C
1	0	563	A
1	0	573	U
1	0	575	A
1	0	603	A
1	0	613	A
1	0	614	A
1	0	615	U
1	0	634	C
1	0	637	A
1	0	645	C
1	0	646	U

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Mol	Chain	Res	Type
1	0	647	G
1	0	655	A
1	0	686	U
1	0	690	G
1	0	691	C
1	0	701	G
1	0	730	A
1	0	736	C
1	0	747	U
1	0	748	G
1	0	763	G
1	0	764	A
1	0	775	G
1	0	776	G
1	0	782	A
1	0	783	A
1	0	784	G
1	0	785	G
1	0	792	A
1	0	805	G
1	0	812	C
1	0	813	U
1	0	827	U
1	0	828	U
1	0	830	G
1	0	845	A
1	0	846	U
1	0	857	G
1	0	866	A
1	0	878	A
1	0	894	U
1	0	895	U
1	0	896	A
1	0	910	A
1	0	914	G
1	0	915	C
1	0	946	C
1	0	961	C
1	0	974	G
1	0	983	A
1	0	991	C
1	0	996	A

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Mol	Chain	Res	Type
1	0	997	G
1	0	1002	G
1	0	1012	U
1	0	1013	C
1	0	1022	G
1	0	1026	G
1	0	1027	A
1	0	1033	U
1	0	1034	G
1	0	1046	A
1	0	1047	G
1	0	1048	A
1	0	1110	G
1	0	1111	A
1	0	1112	G
1	0	1128	G
1	0	1132	U
1	0	1133	A
1	0	1135	C
1	0	1136	G
1	0	1142	A
1	0	1172	C
1	0	1173	U
1	0	1174	U
1	0	1175	A
1	0	1176	U
1	0	1186	G
1	0	1202	G
1	0	1206	G
1	0	1207	C
1	0	1212	G
1	0	1231	U
1	0	1236	G
1	0	1238	G
1	0	1250	G
1	0	1253	A
1	0	1255	U
1	0	1256	G
1	0	1268	A
1	0	1271	G
1	0	1272	A
1	0	1286	A

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Mol	Chain	Res	Type
1	0	1296	G
1	0	1300	G
1	0	1301	A
1	0	1303	G
1	0	1313	U
1	0	1321	A
1	0	1342	A
1	0	1345	C
1	0	1352	U
1	0	1364	G
1	0	1365	A
1	0	1378	A
1	0	1379	U
1	0	1395	A
1	0	1416	G
1	0	1417	C
1	0	1419	A
1	0	1424	G
1	0	1428	C
1	0	1435	G
1	0	1452	G
1	0	1460	U
1	0	1478	G
1	0	1482	G
1	0	1490	A
1	0	1493	C
1	0	1497	U
1	0	1510	G
1	0	1515	A
1	0	1516	G
1	0	1524	G
1	0	1535	A
1	0	1537	G
1	0	1566	A
1	0	1567	G
1	0	1569	A
1	0	1571	A
1	0	1583	A
1	0	1585	C
1	0	1592	C
1	0	1608	A
1	0	1618	A

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Mol	Chain	Res	Type
1	0	1619	G
1	0	1634	A
1	0	1647	U
1	0	1648	U
1	0	1674	G
1	0	1676	A
1	0	1715	G
1	0	1729	U
1	0	1730	C
1	0	1733	G
1	0	1738	G
1	0	1756	G
1	0	1757	A
1	0	1758	U
1	0	1764	C
1	0	1773	A
1	0	1780	A
1	0	1782	U
1	0	1800	C
1	0	1801	A
1	0	1808	A
1	0	1811	G
1	0	1816	C
1	0	1823	G
1	0	1829	A
1	0	1839	G
1	0	1849	G
1	0	1858	A
1	0	1871	A
1	0	1872	A
1	0	1873	G
1	0	1890	A
1	0	1906	G
1	0	1910	G
1	0	1913	A
1	0	1914	C
1	0	1917	U
1	0	1919	A
1	0	1929	G
1	0	1930	G
1	0	1935	G
1	0	1936	A

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Mol	Chain	Res	Type
1	0	1937	A
1	0	1938	A
1	0	1941	C
1	0	1955	U
1	0	1964	G
1	0	1967	C
1	0	1970	A
1	0	1971	U
1	0	1972	G
1	0	1991	U
1	0	1993	U
1	0	1997	C
1	0	2012	G
1	0	2018	G
1	0	2023	C
1	0	2031	A
1	0	2033	A
1	0	2036	C
1	0	2043	C
1	0	2055	C
1	0	2056	G
1	0	2060	A
1	0	2061	G
1	0	2062	A
1	0	2069	G
1	0	2080	A
1	0	2194	U
1	0	2198	A
1	0	2203	U
1	0	2204	G
1	0	2225	A
1	0	2238	G
1	0	2239	G
1	0	2251	G
1	0	2268	A
1	0	2283	C
1	0	2286	G
1	0	2287	A
1	0	2288	A
1	0	2297	A
1	0	2304	G
1	0	2307	G

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Mol	Chain	Res	Type
1	0	2308	G
1	0	2309	A
1	0	2310	C
1	0	2312	U
1	0	2319	G
1	0	2322	A
1	0	2325	G
1	0	2333	A
1	0	2334	U
1	0	2347	C
1	0	2383	G
1	0	2385	C
1	0	2396	G
1	0	2402	U
1	0	2406	A
1	0	2419	U
1	0	2425	A
1	0	2429	G
1	0	2430	A
1	0	2441	U
1	0	2447	G
1	0	2448	A
1	0	2470	G
1	0	2475	C
1	0	2476	A
1	0	2491	U
1	0	2494	G
1	0	2498	C
1	0	2502	G
1	0	2503	A
1	0	2505	G
1	0	2507	C
1	0	2518	A
1	0	2520	C
1	0	2529	G
1	0	2547	A
1	0	2566	A
1	0	2567	G
1	0	2572	A
1	0	2582	G
1	0	2602	A
1	0	2606	C

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Mol	Chain	Res	Type
1	0	2609	U
1	0	2613	U
1	0	2629	U
1	0	2646	C
1	0	2659	G
1	0	2682	A
1	0	2689	U
1	0	2690	U
1	0	2691	C
1	0	2714	G
1	0	2726	A
1	0	2732	G
1	0	2733	A
1	0	2742	G
1	0	2744	G
1	0	2748	A
1	0	2752	C
1	0	2765	A
1	0	2778	A
1	0	2820	A
1	0	2831	G
1	0	2832	U
1	0	2838	G
1	0	2849	U
1	0	2867	G
1	0	2869	G
1	0	2873	A
1	0	2877	G
1	0	2880	C
1	0	2884	U
1	0	2885	G
1	0	2886	A
1	0	2887	A
1	0	2891	U
1	0	2894	G
1	0	2895	G
1	0	2903	U
2	1	13	G
2	1	24	G
2	1	35	C
2	1	41	G
2	1	44	G

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Mol	Chain	Res	Type
2	1	56	G
2	1	61	G
2	1	67	G
2	1	69	G
2	1	89	U
2	1	90	C
2	1	98	G
2	1	105	G
2	1	109	A
3	2	4	U
3	2	6	G
3	2	8	A
3	2	9	G
3	2	22	G
3	2	27	G
3	2	31	G
3	2	32	A
3	2	39	G
3	2	47	C
3	2	48	C
3	2	50	A
3	2	51	A
3	2	66	A
3	2	76	G
3	2	77	A
3	2	80	A
3	2	81	A
3	2	84	U
3	2	85	U
3	2	86	G
3	2	87	C
3	2	91	U
3	2	94	G
3	2	108	G
3	2	112	G
3	2	116	A
3	2	120	A
3	2	121	U
3	2	122	G
3	2	131	A
3	2	134	G
3	2	143	A

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Mol	Chain	Res	Type
3	2	144	G
3	2	164	G
3	2	168	G
3	2	171	A
3	2	183	C
3	2	184	G
3	2	189	A
3	2	195	A
3	2	197	A
3	2	198	G
3	2	210	C
3	2	211	G
3	2	212	G
3	2	214	C
3	2	217	C
3	2	226	G
3	2	245	U
3	2	247	G
3	2	251	G
3	2	252	U
3	2	253	A
3	2	255	G
3	2	266	G
3	2	267	C
3	2	279	A
3	2	280	C
3	2	282	A
3	2	289	G
3	2	299	G
3	2	316	C
3	2	321	A
3	2	328	C
3	2	330	C
3	2	332	G
3	2	344	A
3	2	346	G
3	2	351	G
3	2	352	C
3	2	354	G
3	2	365	U
3	2	367	U
3	2	372	C

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Mol	Chain	Res	Type
3	2	373	A
3	2	382	A
3	2	388	G
3	2	397	A
3	2	406	G
3	2	412	A
3	2	413	G
3	2	414	A
3	2	422	C
3	2	423	G
3	2	429	U
3	2	438	U
3	2	464	U
3	2	468	A
3	2	481	G
3	2	484	G
3	2	496	A
3	2	497	G
3	2	509	A
3	2	511	C
3	2	518	C
3	2	522	C
3	2	524	G
3	2	531	U
3	2	532	A
3	2	533	A
3	2	547	A
3	2	548	G
3	2	559	A
3	2	560	A
3	2	564	C
3	2	567	G
3	2	572	A
3	2	573	A
3	2	576	C
3	2	577	G
3	2	587	G
3	2	604	G
3	2	609	A
3	2	613	C
3	2	623	C
3	2	632	U

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Mol	Chain	Res	Type
3	2	633	G
3	2	653	U
3	2	665	A
3	2	687	A
3	2	688	G
3	2	703	G
3	2	704	A
3	2	718	A
3	2	721	G
3	2	722	G
3	2	723	U
3	2	724	G
3	2	742	G
3	2	753	A
3	2	755	G
3	2	758	C
3	2	760	G
3	2	761	G
3	2	777	A
3	2	792	A
3	2	793	U
3	2	794	A
3	2	802	A
3	2	815	A
3	2	817	C
3	2	821	G
3	2	832	G
3	2	842	U
3	2	843	U
3	2	845	A
3	2	872	A
3	2	884	U
3	2	889	A
3	2	890	G
3	2	891	U
3	2	914	A
3	2	916	U
3	2	919	A
3	2	926	G
3	2	927	G
3	2	934	C
3	2	935	A

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Mol	Chain	Res	Type
3	2	960	U
3	2	961	U
3	2	963	G
3	2	965	U
3	2	966	G
3	2	969	A
3	2	971	G
3	2	972	C
3	2	975	A
3	2	976	G
3	2	977	A
3	2	978	A
3	2	981	U
3	2	983	A
3	2	990	C
3	2	992	U
3	2	993	G
3	2	1005	A
3	2	1006	G
3	2	1007	U
3	2	1012	A
3	2	1020	G
3	2	1021	A
3	2	1024	G
3	2	1025	U
3	2	1026	G
3	2	1030	U
3	2	1033	G
3	2	1034	G
3	2	1035	A
3	2	1036	A
3	2	1037	C
3	2	1041	G
3	2	1043	G
3	2	1044	A
3	2	1053	G
3	2	1054	C
3	2	1066	C
3	2	1079	G
3	2	1094	G
3	2	1095	U
3	2	1099	G

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Mol	Chain	Res	Type
3	2	1101	A
3	2	1102	A
3	2	1109	C
3	2	1125	U
3	2	1130	A
3	2	1136	C
3	2	1137	C
3	2	1138	G
3	2	1139	G
3	2	1142	G
3	2	1151	A
3	2	1152	A
3	2	1158	C
3	2	1159	U
3	2	1160	G
3	2	1168	U
3	2	1169	A
3	2	1181	G
3	2	1183	U
3	2	1184	G
3	2	1191	A
3	2	1196	A
3	2	1197	A
3	2	1202	U
3	2	1212	U
3	2	1213	A
3	2	1225	A
3	2	1227	A
3	2	1228	C
3	2	1238	A
3	2	1257	A
3	2	1258	G
3	2	1279	G
3	2	1280	A
3	2	1285	A
3	2	1287	A
3	2	1290	G
3	2	1299	A
3	2	1300	G
3	2	1302	C
3	2	1306	A
3	2	1317	C

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Mol	Chain	Res	Type
3	2	1318	A
3	2	1320	C
3	2	1321	U
3	2	1322	C
3	2	1323	G
3	2	1337	G
3	2	1338	G
3	2	1347	G
3	2	1348	U
3	2	1363	A
3	2	1364	U
3	2	1370	G
3	2	1374	A
3	2	1381	U
3	2	1386	G
3	2	1391	U
3	2	1397	C
3	2	1398	A
3	2	1400	C
3	2	1402	C
3	2	1432	G
3	2	1437	A
3	2	1441	A
3	2	1442	G
3	2	1446	A
3	2	1451	U
3	2	1452	C
3	2	1453	G
3	2	1487	G
3	2	1492	A
3	2	1494	G
3	2	1497	G
3	2	1504	G
3	2	1506	U
3	2	1507	A
3	2	1517	G
3	2	1519	A
3	2	1529	G
3	2	1530	G
3	2	1534	A
4	3	16	A
4	3	19	A

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Mol	Chain	Res	Type
5	4	8	G
5	4	11	G
5	4	14	G
5	4	16	C
5	4	18	G
5	4	19	G
5	4	20	U
5	4	22	G
5	4	23	C
5	4	31	G
5	4	44	A
5	4	55	U
5	4	76	A
6	5	10	G
6	5	16	H2U
6	5	17	H2U
6	5	19	G
6	5	20	H2U
6	5	23	A
6	5	26	A
6	5	46	G
6	5	49	G
6	5	74	C

All (47) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	546	U
1	0	1026	G
1	0	1111	A
1	0	2193	G
1	0	2307	G
3	2	80	A
3	2	83	C
3	2	130	A
3	2	188	C
3	2	210	C
3	2	250	A
3	2	251	G
3	2	281	G
3	2	315	A
3	2	345	C

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Mol	Chain	Res	Type
3	2	413	G
3	2	422	C
3	2	428	G
3	2	463	U
3	2	467	U
3	2	495	A
3	2	559	A
3	2	575	G
3	2	703	G
3	2	792	A
3	2	890	G
3	2	960	U
3	2	982	U
3	2	992	U
3	2	1024	G
3	2	1040	U
3	2	1053	G
3	2	1136	C
3	2	1137	C
3	2	1151	A
3	2	1157	A
3	2	1182	G
3	2	1190	G
3	2	1201	A
3	2	1305	G
3	2	1320	C
3	2	1347	G
3	2	1399	C
3	2	1451	U
3	2	1452	C
5	4	10	A
6	5	15	G

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

9 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.

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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	$\#\|Z\|>2$
5	4SU	4	7	5	18,21,22	3.72	8 (44%)	26,30,33	2.32	5 (19%)
5	OMC	4	32	5	19,22,23	0.72	1 (5%)	26,31,34	0.82	1 (3%)
6	H2U	5	20	6	18,21,22	0.47	0	21,30,33	1.10	1 (4%)
5	5MU	4	54	5	19,22,23	0.51	0	28,32,35	0.58	0
6	U8U	5	34	4,6	19,24,25	2.40	6 (31%)	23,34,37	1.36	3 (13%)
6	T6A	5	37	6	31,34,35	1.90	8 (25%)	44,49,52	2.23	9 (20%)
6	H2U	5	16	6	18,21,22	0.45	0	21,30,33	1.00	1 (4%)
6	H2U	5	17	6	18,21,22	0.45	0	21,30,33	1.07	1 (4%)
6	5MU	5	54	6	19,22,23	0.53	0	28,32,35	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	4SU	4	7	5	-	0/7/25/26	0/2/2/2
5	OMC	4	32	5	-	1/9/27/28	0/2/2/2
6	H2U	5	20	6	-	4/7/38/39	0/2/2/2
5	5MU	4	54	5	-	0/7/25/26	0/2/2/2
6	U8U	5	34	4,6	-	0/9/28/29	0/2/2/2
6	T6A	5	37	6	-	6/23/41/42	0/3/3/3
6	H2U	5	16	6	-	2/7/38/39	0/2/2/2
6	H2U	5	17	6	-	4/7/38/39	0/2/2/2
6	5MU	5	54	6	-	0/7/25/26	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	7	4SU	C4-N3	7.89	1.46	1.37
5	4	7	4SU	C2-N3	7.15	1.50	1.38
5	4	7	4SU	C4-S4	-6.75	1.55	1.68
6	5	34	U8U	C2-N3	5.33	1.49	1.37
6	5	37	T6A	C10-N6	5.03	1.47	1.37
5	4	7	4SU	C6-C5	5.01	1.46	1.35
6	5	34	U8U	C2-S2	-4.87	1.60	1.67
6	5	34	U8U	C6-C5	4.50	1.47	1.34
6	5	37	T6A	C10-N11	4.39	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	7	4SU	C5-C4	4.21	1.48	1.42
6	5	37	T6A	C6-N6	4.05	1.47	1.39
5	4	7	4SU	C2-N1	3.94	1.44	1.38
5	4	7	4SU	C6-N1	3.90	1.47	1.38
5	4	7	4SU	O2-C2	-3.82	1.16	1.23
6	5	34	U8U	C6-N1	3.80	1.44	1.38
6	5	37	T6A	O10-C10	-3.47	1.16	1.23
6	5	34	U8U	C4-N3	3.32	1.45	1.38
6	5	34	U8U	O4-C4	-2.76	1.18	1.23
6	5	37	T6A	C5-N7	-2.73	1.33	1.39
6	5	37	T6A	C5-C6	-2.12	1.36	1.41
6	5	37	T6A	C5-C4	-2.05	1.35	1.39
5	4	32	OMC	C4-N3	-2.03	1.30	1.34
6	5	37	T6A	C2-N3	2.01	1.37	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	4	7	4SU	C4-N3-C2	-8.21	119.37	127.34
6	5	37	T6A	N6-C10-N11	6.04	122.20	113.76
6	5	37	T6A	C5-C4-N3	-5.74	119.26	126.75
5	4	7	4SU	C5-C4-N3	5.42	119.72	114.69
6	5	37	T6A	N3-C2-N1	-5.37	120.20	128.60
6	5	37	T6A	C4-C5-C6	5.07	120.74	116.81
5	4	7	4SU	N3-C2-N1	4.10	120.33	114.89
6	5	37	T6A	N9-C8-N7	-4.05	108.37	113.91
6	5	34	U8U	O4-C4-C5	-3.92	119.12	124.96
6	5	37	T6A	N3-C4-N9	3.53	132.90	127.08
6	5	37	T6A	C2-N3-C4	3.51	120.03	111.75
6	5	34	U8U	C5-C4-N3	3.49	119.88	114.97
5	4	7	4SU	C5-C4-S4	-3.37	120.12	124.47
6	5	20	H2U	C5-C4-N3	-3.28	112.96	116.65
6	5	17	H2U	C5-C4-N3	-3.27	112.98	116.65
6	5	16	H2U	C5-C4-N3	-3.07	113.20	116.65
5	4	7	4SU	O2-C2-N1	-2.97	118.84	122.79
6	5	37	T6A	C5-N7-C8	2.95	107.69	103.51
6	5	37	T6A	O10-C10-N6	-2.91	118.71	123.62
6	5	34	U8U	C1'-N1-C6	-2.60	116.79	121.12
5	4	32	OMC	C1'-N1-C2	2.26	123.45	118.42

There are no chirality outliers.

All (17) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms
6	5	17	H2U	O4'-C1'-N1-C6
6	5	20	H2U	O4'-C1'-N1-C6
6	5	37	T6A	N11-C12-C14-O14
6	5	37	T6A	C13-C12-C14-O14
6	5	37	T6A	C13-C12-C14-C15
6	5	37	T6A	N11-C12-C14-C15
6	5	16	H2U	C4'-C5'-O5'-P
6	5	37	T6A	C13-C12-N11-C10
6	5	17	H2U	O4'-C1'-N1-C2
6	5	20	H2U	O4'-C1'-N1-C2
6	5	37	T6A	N11-C12-C13-ODA
6	5	17	H2U	O4'-C4'-C5'-O5'
5	4	32	OMC	C2'-C1'-N1-C2
6	5	20	H2U	O4'-C4'-C5'-O5'
6	5	20	H2U	C2'-C1'-N1-C2
6	5	16	H2U	C3'-C4'-C5'-O5'
6	5	17	H2U	C2'-C1'-N1-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	5	34	U8U	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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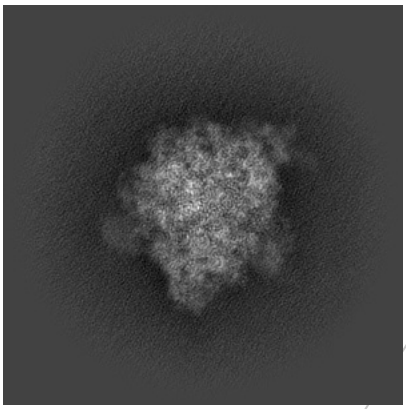
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-82632. These allow visual inspection of the internal detail of the map and identification of artifacts.

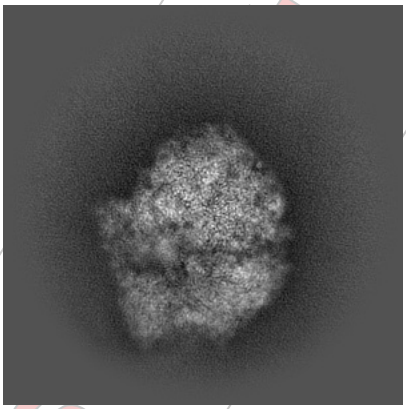
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

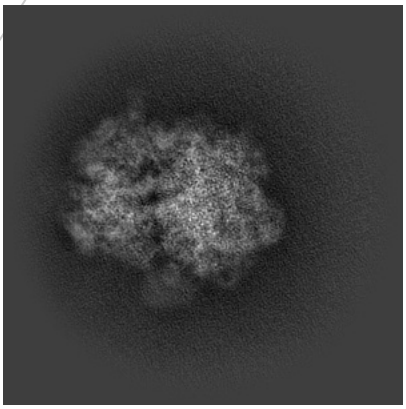
6.1.1 Primary map



X

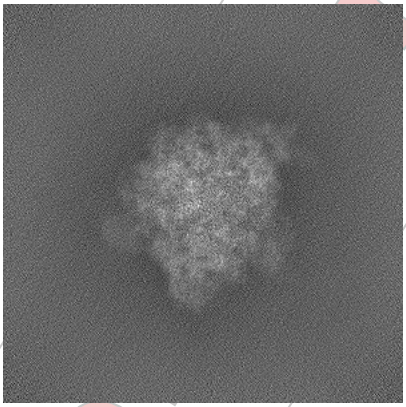


Y

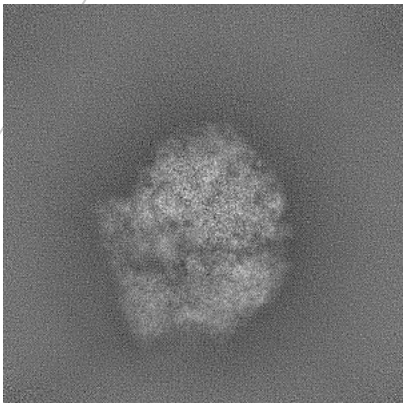


Z

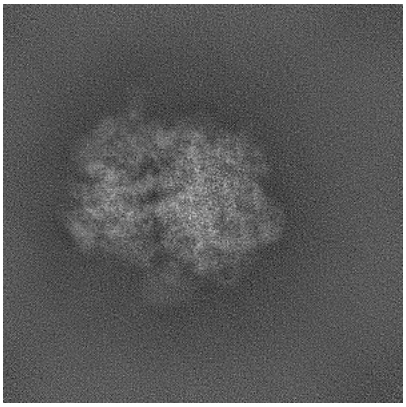
6.1.2 Raw map



X



Y



Z

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

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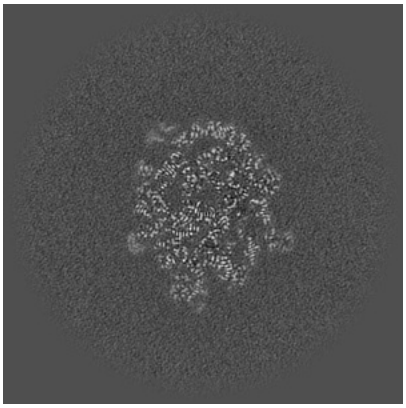
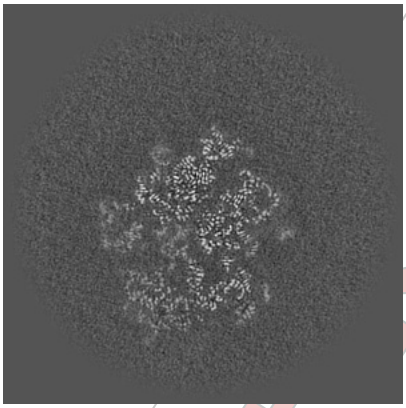
6.2 Central slices (i)

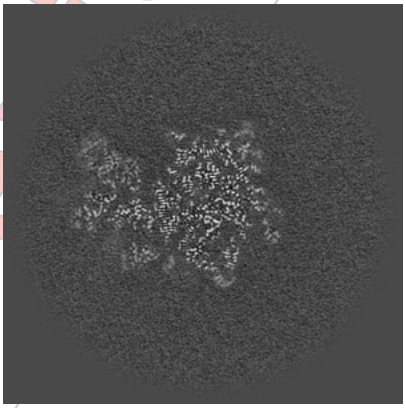
6.2.1 Primary map



X Index: 240

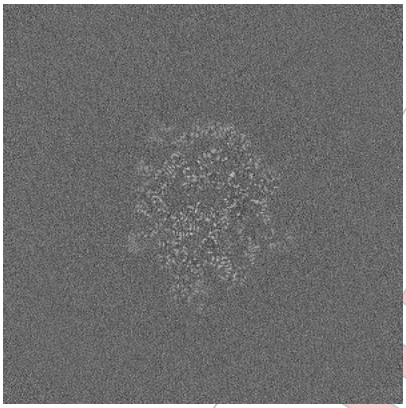


Y Index: 240

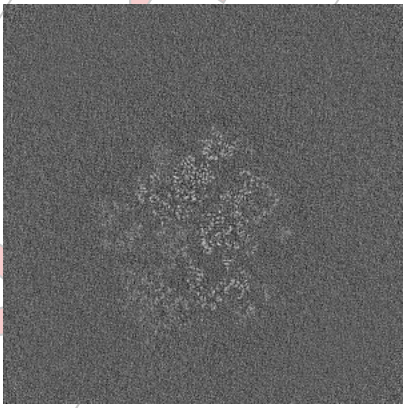


Z Index: 240

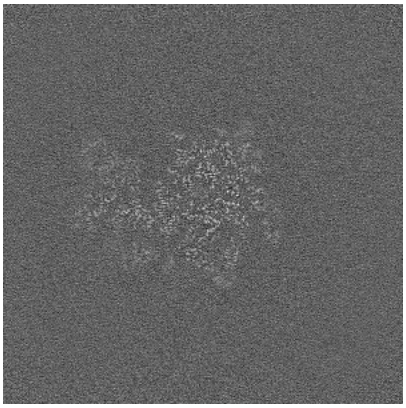
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

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

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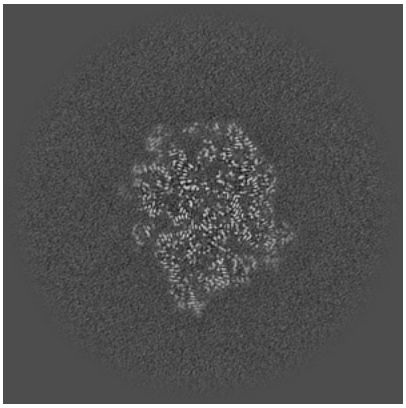
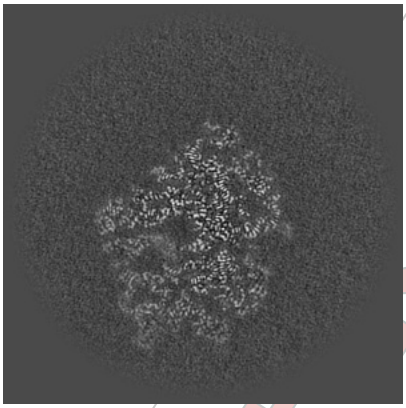
6.3 Largest variance slices (i)

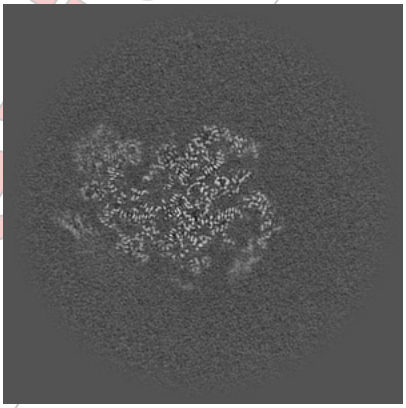
6.3.1 Primary map



X Index: 232

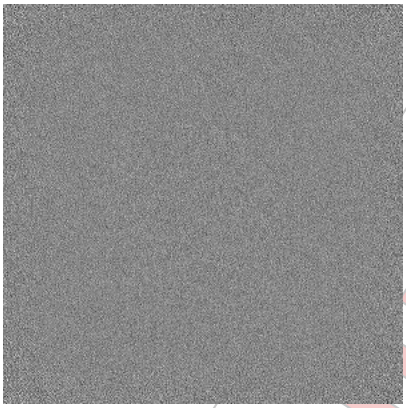


Y Index: 225

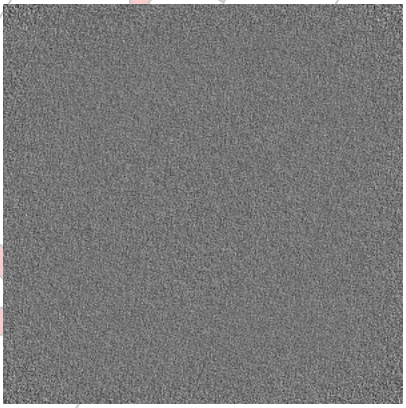


Z Index: 263

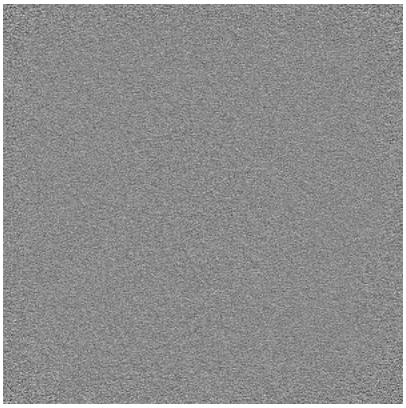
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

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

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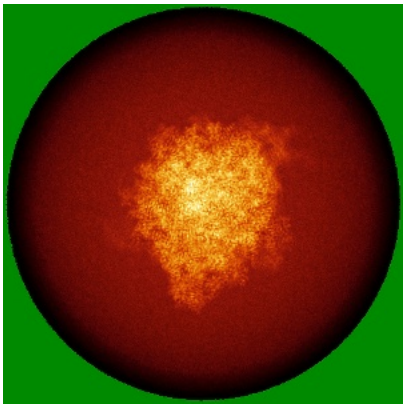
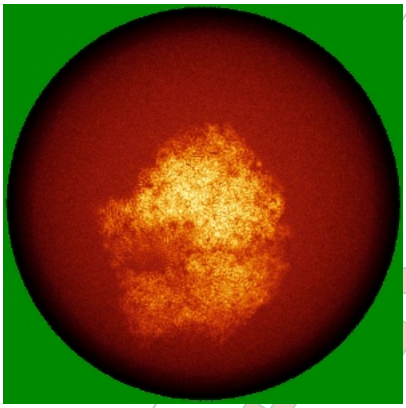
6.4 Orthogonal standard-deviation projections (False-color)

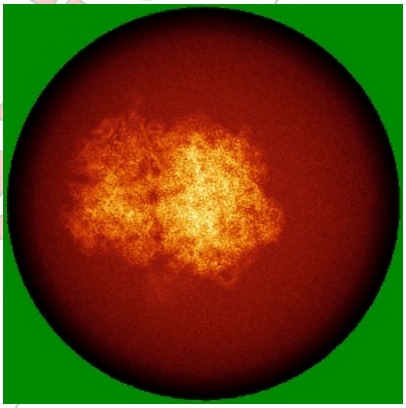
6.4.1 Primary map



X

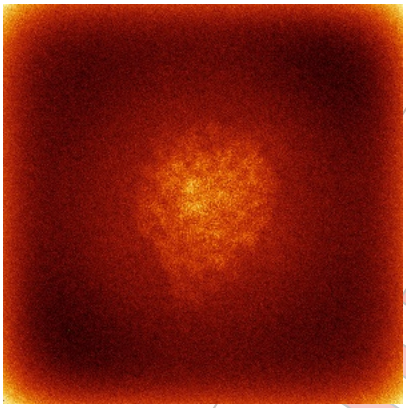


Y

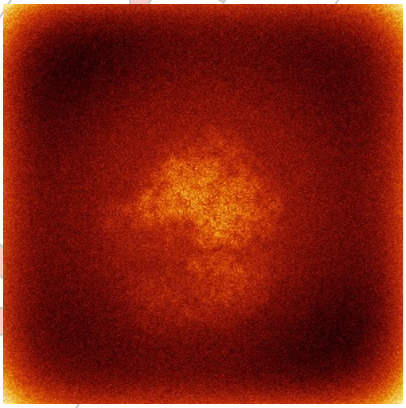


Z

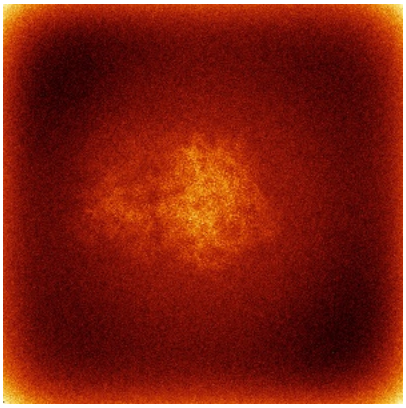
6.4.2 Raw map



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.

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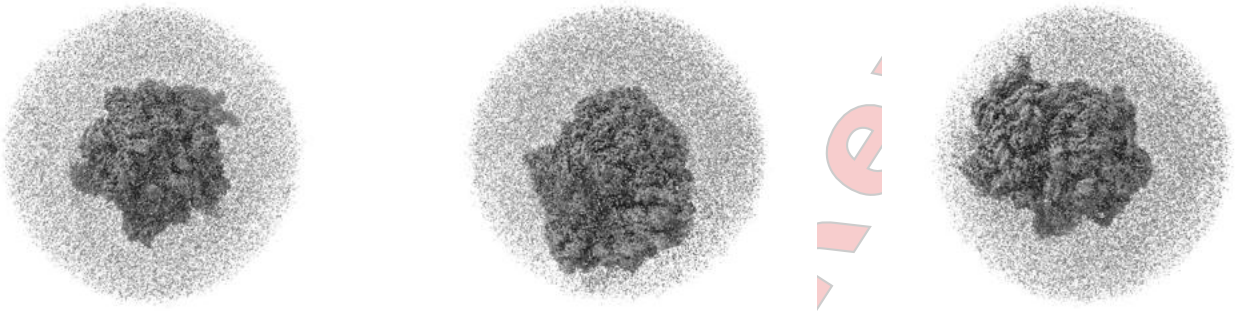
6.5 Orthogonal surface views (i)

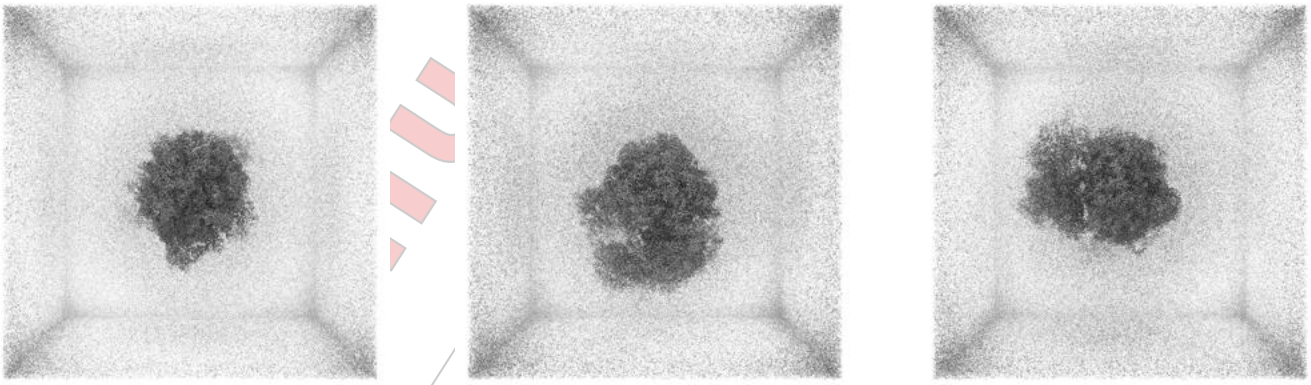
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. 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



X Y Z

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.

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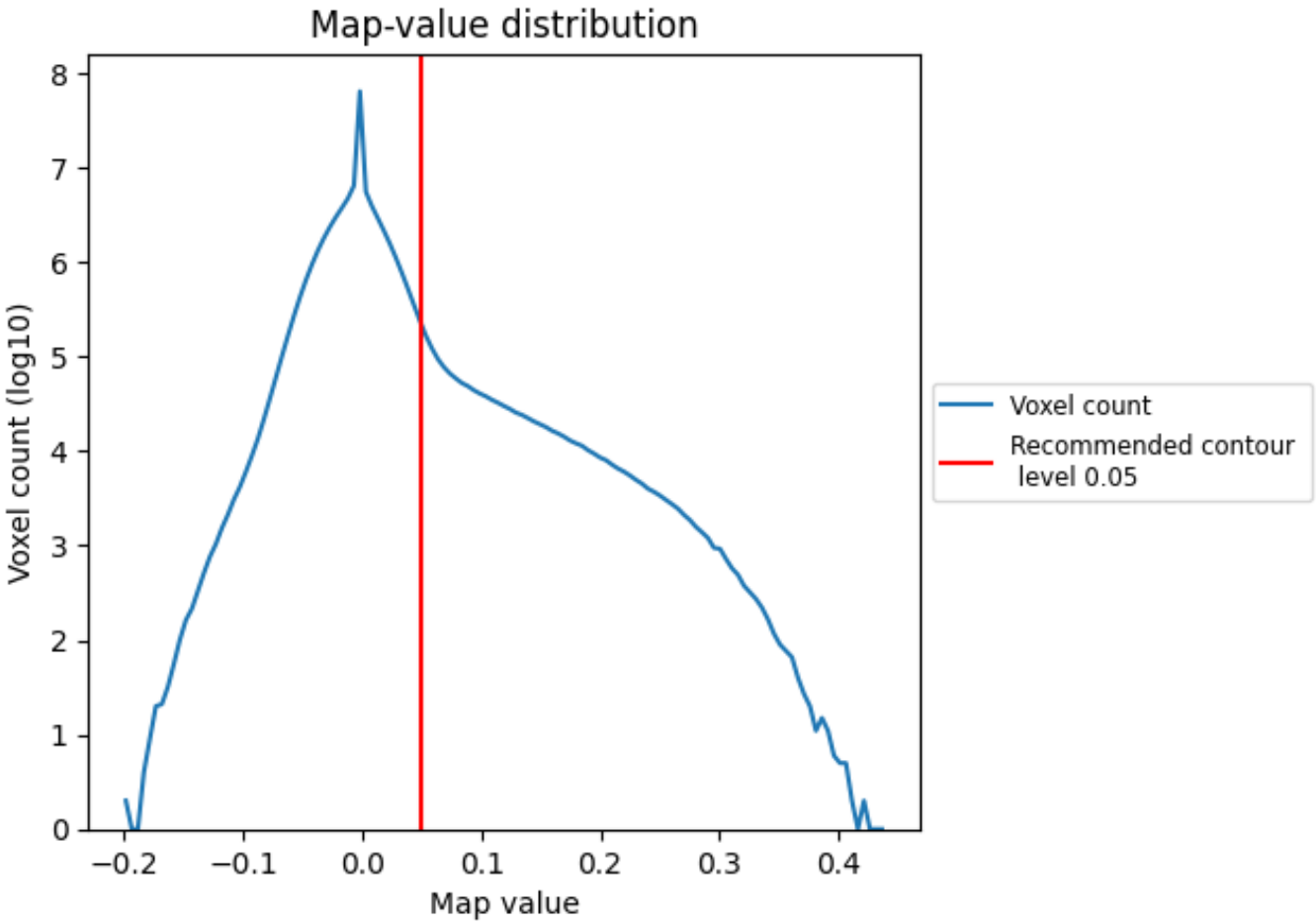
7 Map analysis

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

7.1 Map-value distribution



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.

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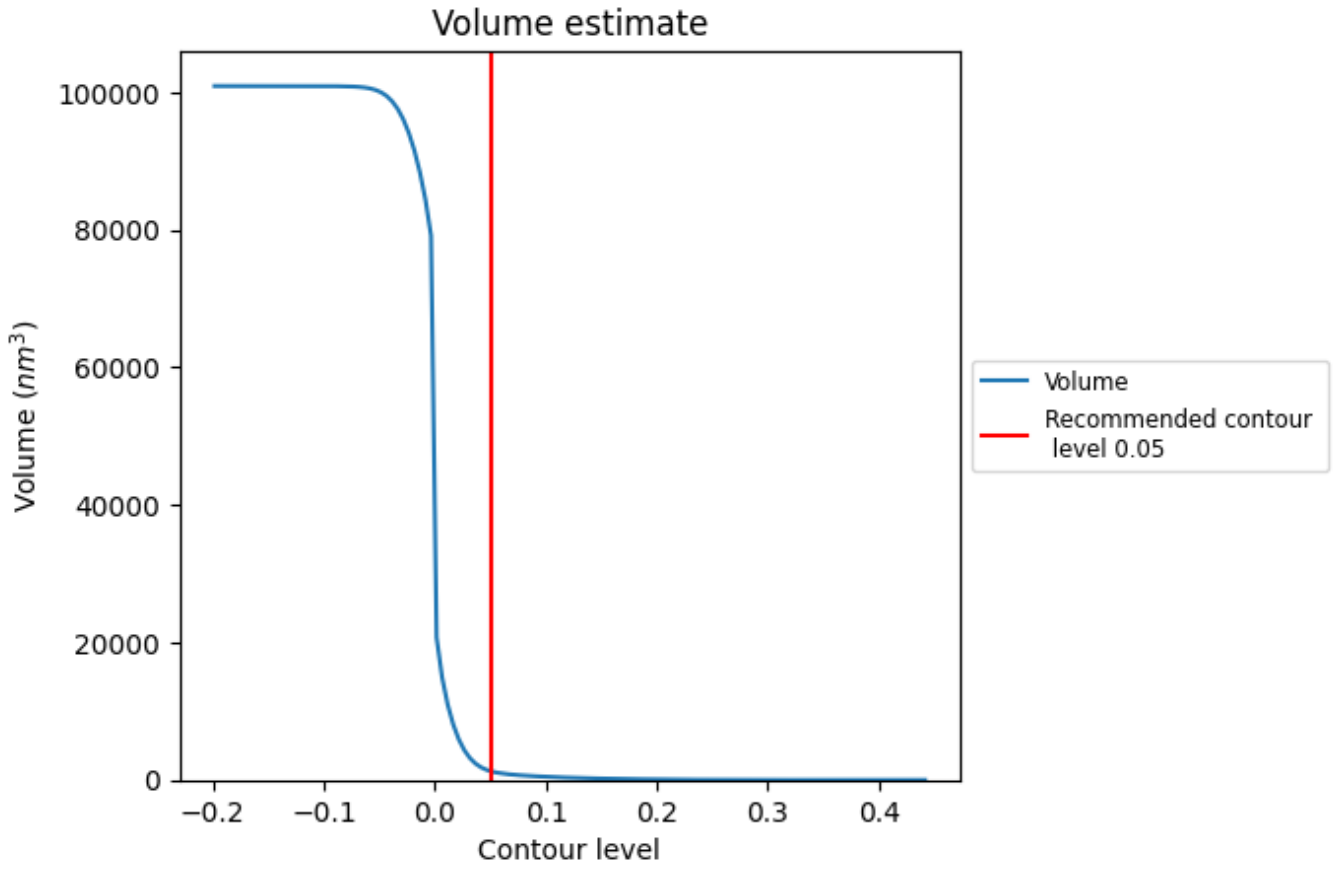
7.2 Volume estimate

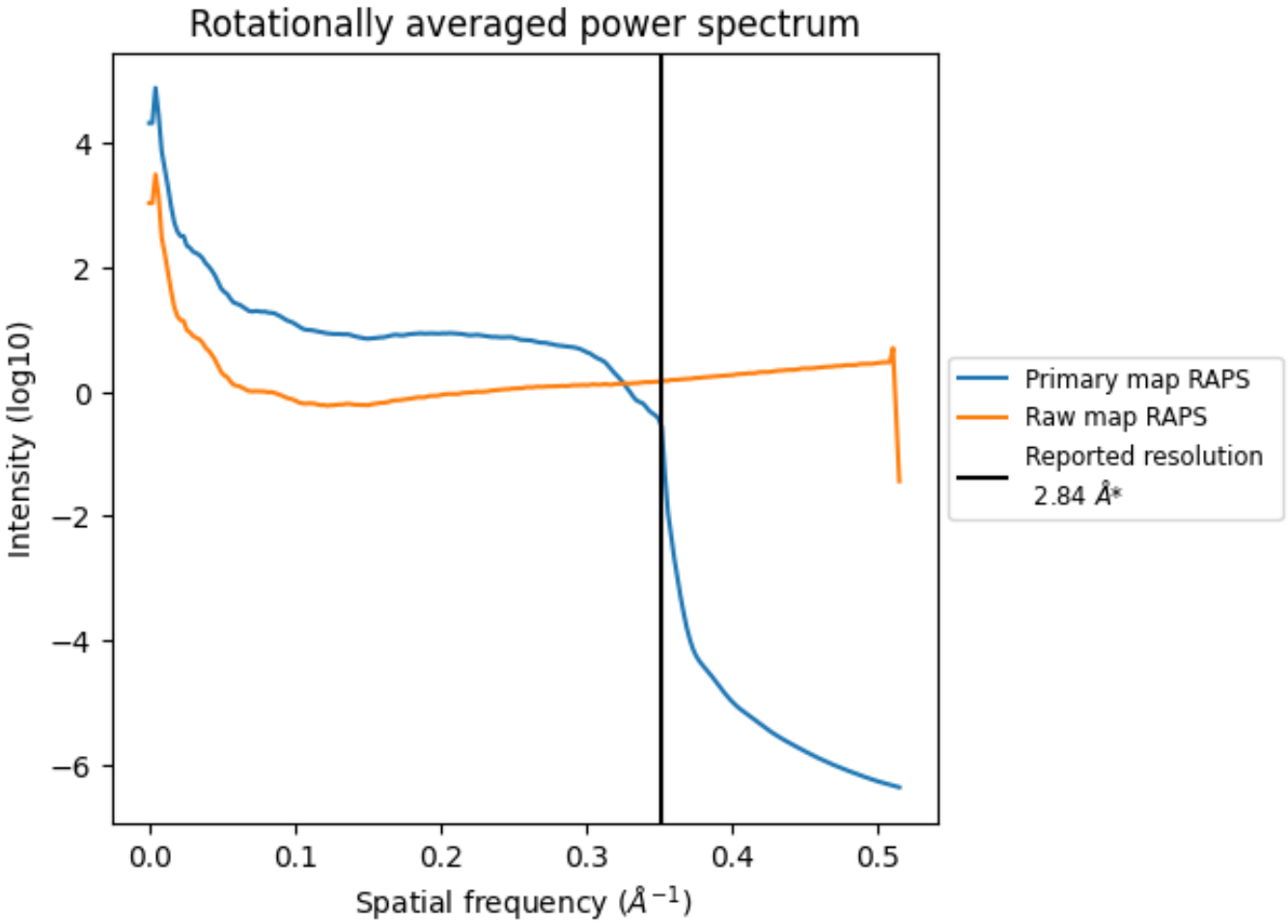


The volume at the recommended contour level is 1294 nm^3; this corresponds to an approximate mass of 1169 kDa.

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.

For Manus

7.3 Rotationally averaged power spectrum (i)



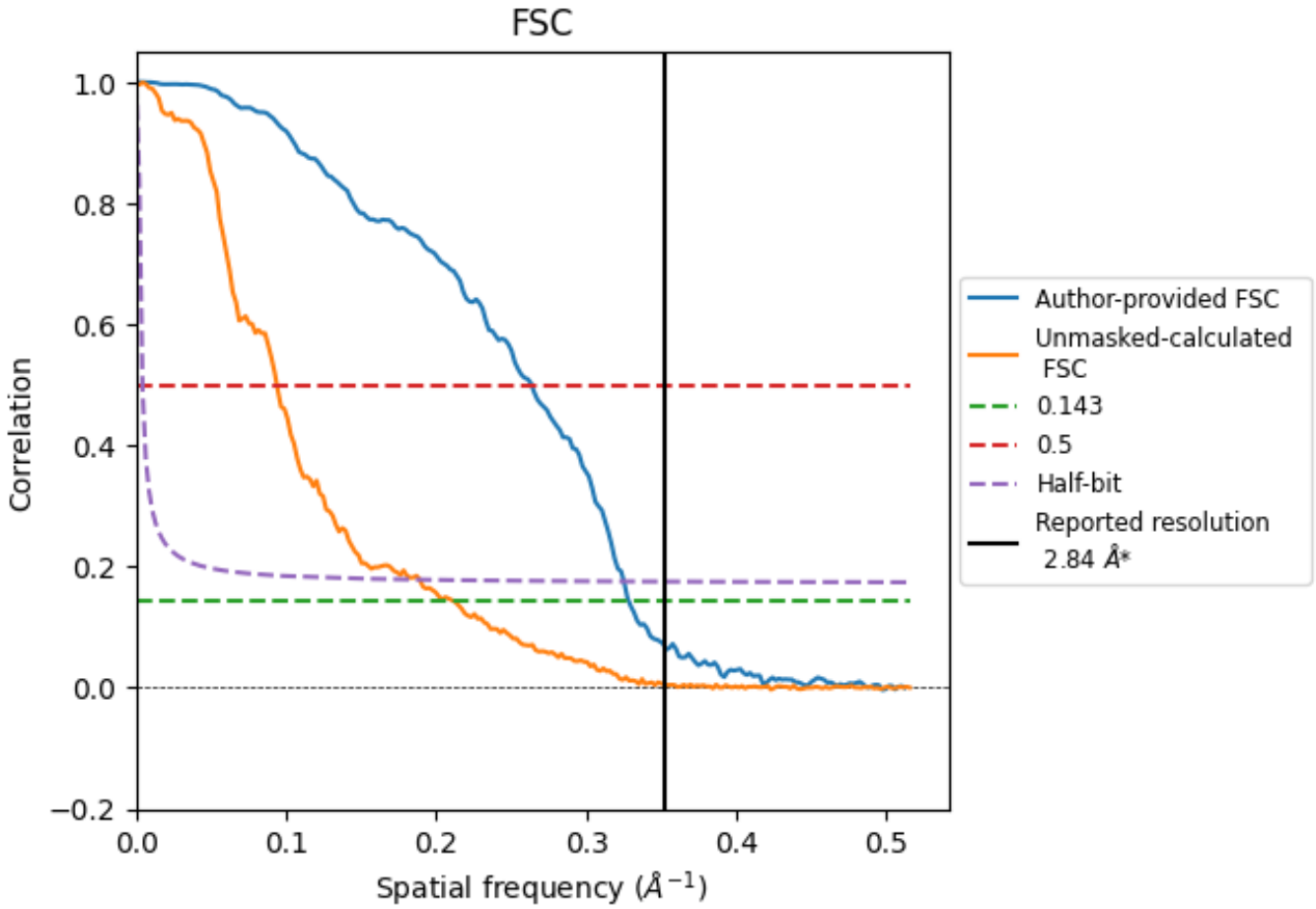
*Reported resolution corresponds to spatial frequency of 0.352 Å^{-1}

For Manu

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.352 Å^{-1}

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8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	3.05	3.80	3.08
Unmasked-calculated*	4.73	10.66	5.29

*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 4.73 differs from the reported value 2.84 by more than 10 %

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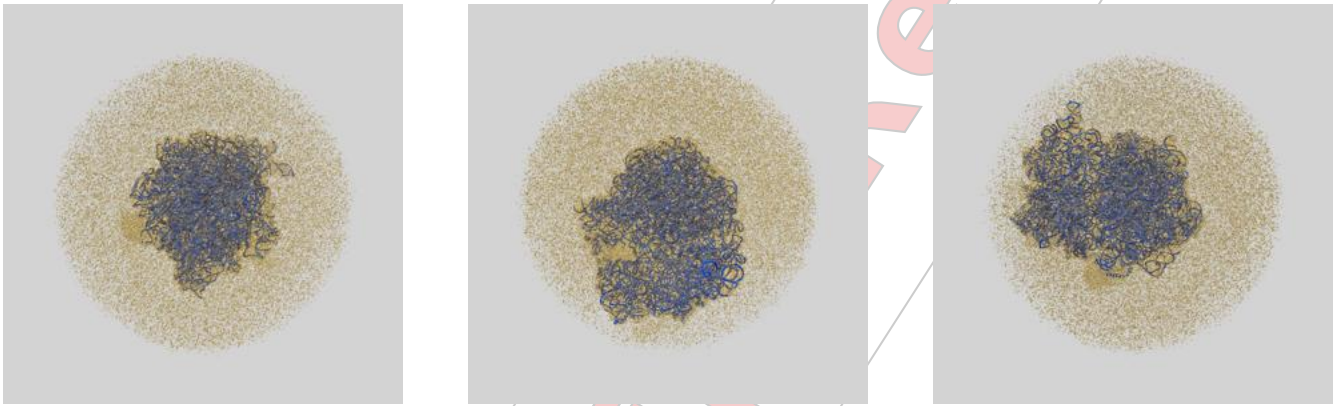
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-82632 and PDB model 44II. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

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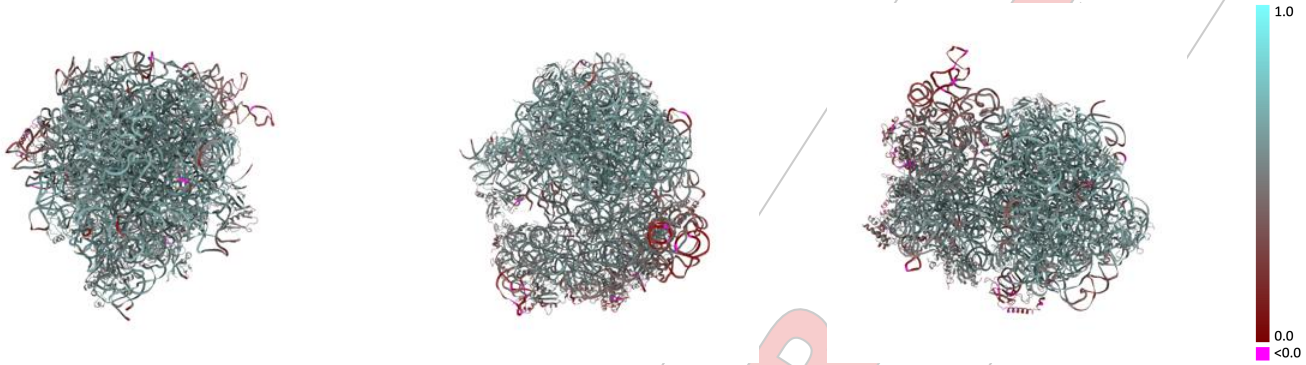
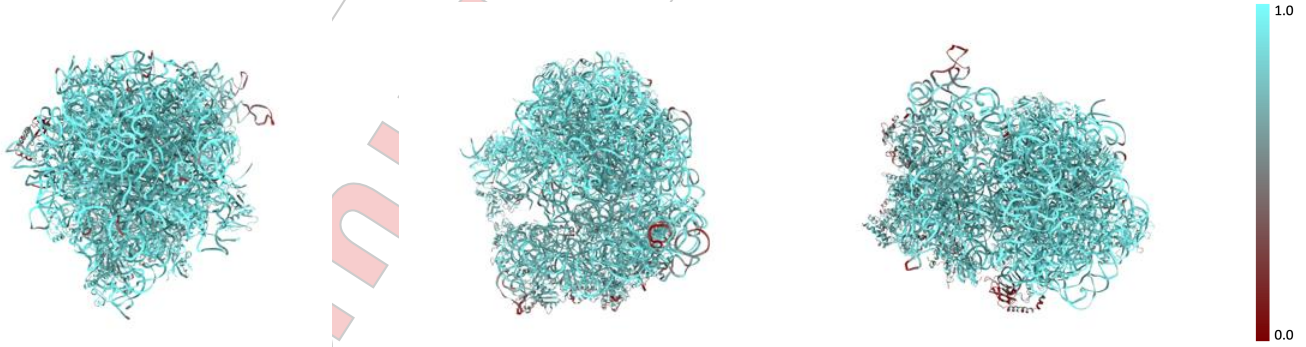
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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



X Y Z

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 (0.05).

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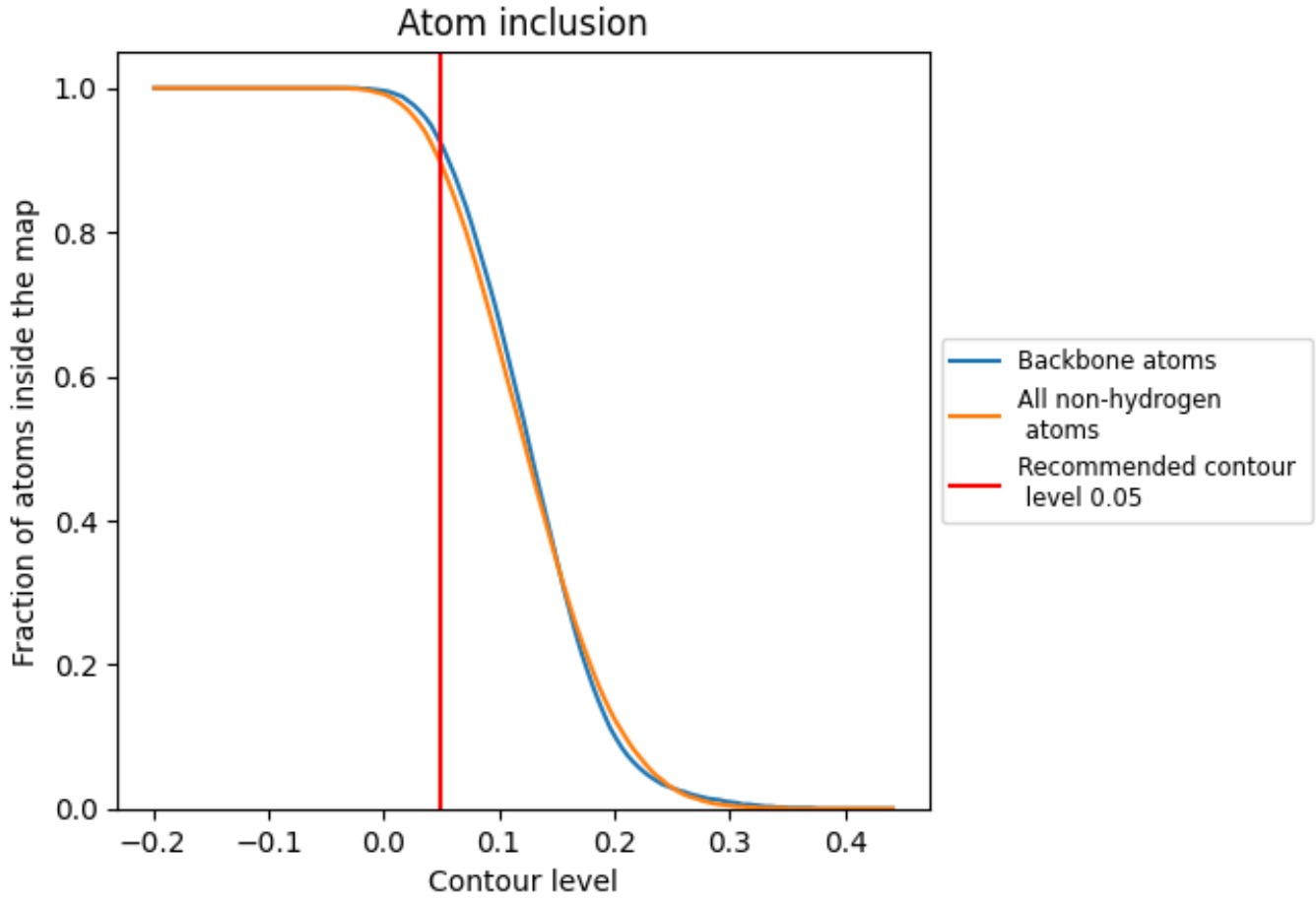
9.4 Atom inclusion



At the recommended contour level, 92% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

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9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8950	0.5400
0	0.9650	0.5870
1	0.9530	0.5630
2	0.8900	0.5000
3	0.8140	0.4920
4	0.8240	0.4600
5	0.8570	0.4900
A	0.9190	0.6000
B	0.9240	0.5960
C	0.8650	0.5560
D	0.7840	0.4860
E	0.8240	0.5030
F	0.3040	0.2580
G	0.9140	0.5870
H	0.8930	0.5880
I	0.9120	0.5880
J	0.9010	0.5840
K	0.9330	0.6000
L	0.8610	0.5370
M	0.8880	0.5810
N	0.9370	0.6060
O	0.9080	0.5840
P	0.8740	0.5720
Q	0.8460	0.5470
R	0.8590	0.5350
S	0.8770	0.5470
T	0.9100	0.5970
U	0.8850	0.5810
V	0.8390	0.5230
W	0.9060	0.5890
X	0.6810	0.3890
a	0.8990	0.5960
b	0.8700	0.5640
c	0.9180	0.6040
d	0.9250	0.6170



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Chain	Atom inclusion	Q-score
e	0.9180	0.5950
f	0.6710	0.4140
g	0.7650	0.4840
h	0.6350	0.3620
i	0.8480	0.5380
j	0.7890	0.4830
k	0.5660	0.3780
l	0.8440	0.5360
m	0.7370	0.4400
n	0.6120	0.3680
o	0.8010	0.5100
p	0.7780	0.5020
q	0.7560	0.4650
r	0.7830	0.4800
s	0.8200	0.4910
t	0.6810	0.3870
u	0.7580	0.4620
v	0.7930	0.4950
w	0.7470	0.4760
x	0.7340	0.3960
y	0.5500	0.3660

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