Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 10:40 AM JST

PDB ID	:	44IJ / pdb_000044ij
EMDB ID	:	EMD-82633
Title	:	Structural basis of ribosomal RNA modification of 70S
Deposited on	:	2026-07-30
Resolution	:	2.08 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
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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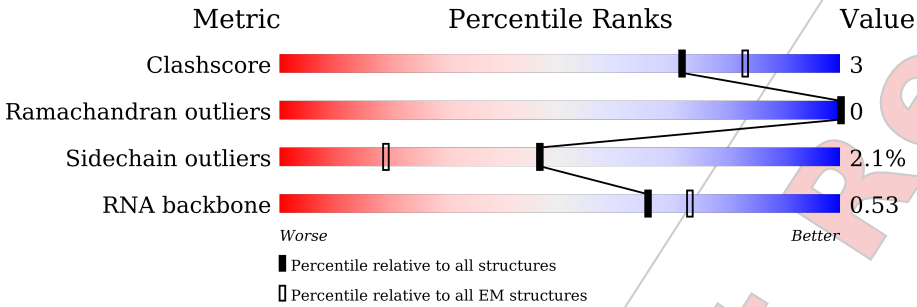
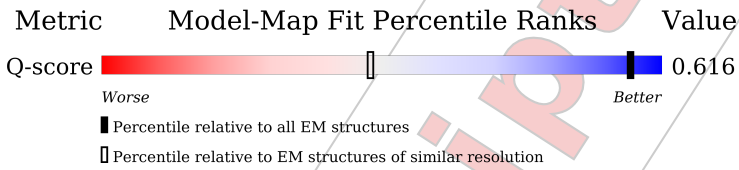
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.08 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	1976 (1.58 - 2.58)

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	73% 21% • 5%
2	1	120	80% 20%
3	2	1542	71% 25% • •

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Mol	Chain	Length	Quality of chain
4	A	273	92% 7%
5	B	209	92% 7%
6	C	201	93% 7%
7	D	179	75% 22%
8	E	177	85% 12%
9	F	149	62% 89% 11%
10	G	142	92% 8%
11	H	123	96%
12	I	144	85% 14%
13	J	136	88% 12%
14	K	127	88% 5% 7%
15	L	117	86% 13%
16	M	115	94% 5%
17	N	118	88% 10%
18	O	103	91% 8%
19	P	110	93% 7%
20	Q	100	85% 8% 7%
21	R	104	88% 9%
22	S	94	97%
23	T	85	86% 12%
24	U	78	95%
25	V	63	84% 11% 5%
26	W	59	86% 8%
27	X	70	17% 77% 9% 14%
28	a	57	84% 12%

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Mol	Chain	Length	Quality of chain
29	b	55	85% 7% 7%
30	c	46	91% 9%
31	d	65	95%
32	e	38	89% 11%
33	f	241	10% 75% 17% 7%
34	g	233	76% 12% 12%
35	h	206	85% 15%
36	i	167	79% 14% 7%
37	j	131	70% 11% 19%
38	k	179	14% 66% 18% 16%
39	l	130	92% 8%
40	m	130	5% 74% 22%
41	n	103	16% 75% 20%
42	o	129	78% 13% 9%
43	p	124	92% 7%
44	q	118	76% 19%
45	r	101	83% 16%
46	s	89	88% 10%
47	t	82	90% 10%
48	u	84	85% 11% 5%
49	v	75	77% 11% 12%
50	w	92	7% 73% 13% 14%
51	x	87	87% 11%
52	y	71	34% 89% 10%

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2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 139174 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 protein called Large ribosomal subunit protein uL2.

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

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

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- Molecule 7 is a protein called 50S ribosomal protein L5.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L9.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 27 is a protein called 50S ribosomal protein L31.

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

- Molecule 28 is a protein called 50S ribosomal protein L32.

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

- Molecule 29 is a protein called 50S ribosomal protein L33.

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

- Molecule 30 is a protein called 50S ribosomal protein L34.

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

- Molecule 31 is a protein called 50S ribosomal protein L35.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

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

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

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

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

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

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

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

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

- Molecule 37 is a protein called Small ribosomal subunit protein bS6, non-modified isoform.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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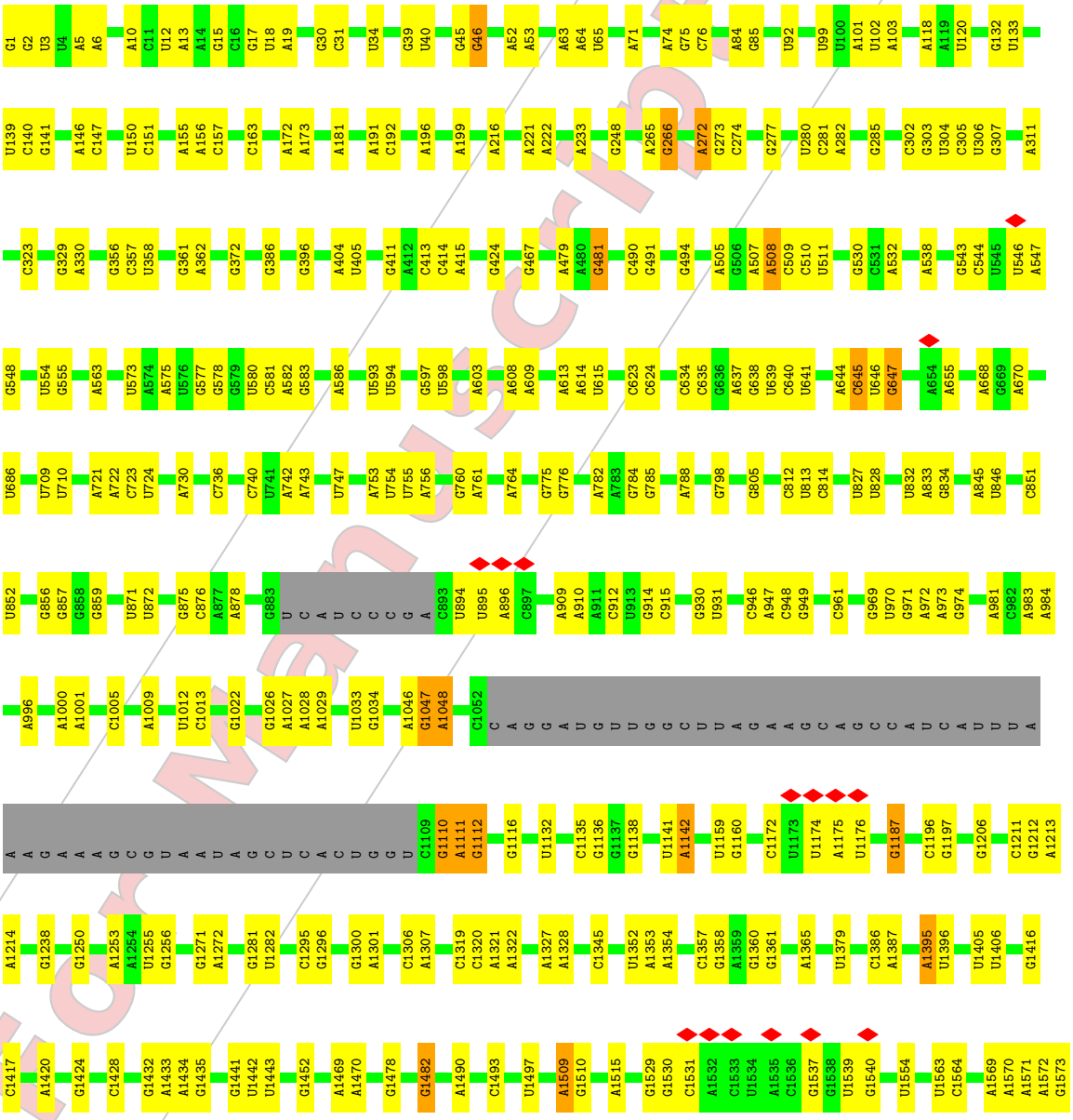
3 Residue-property plots (i)

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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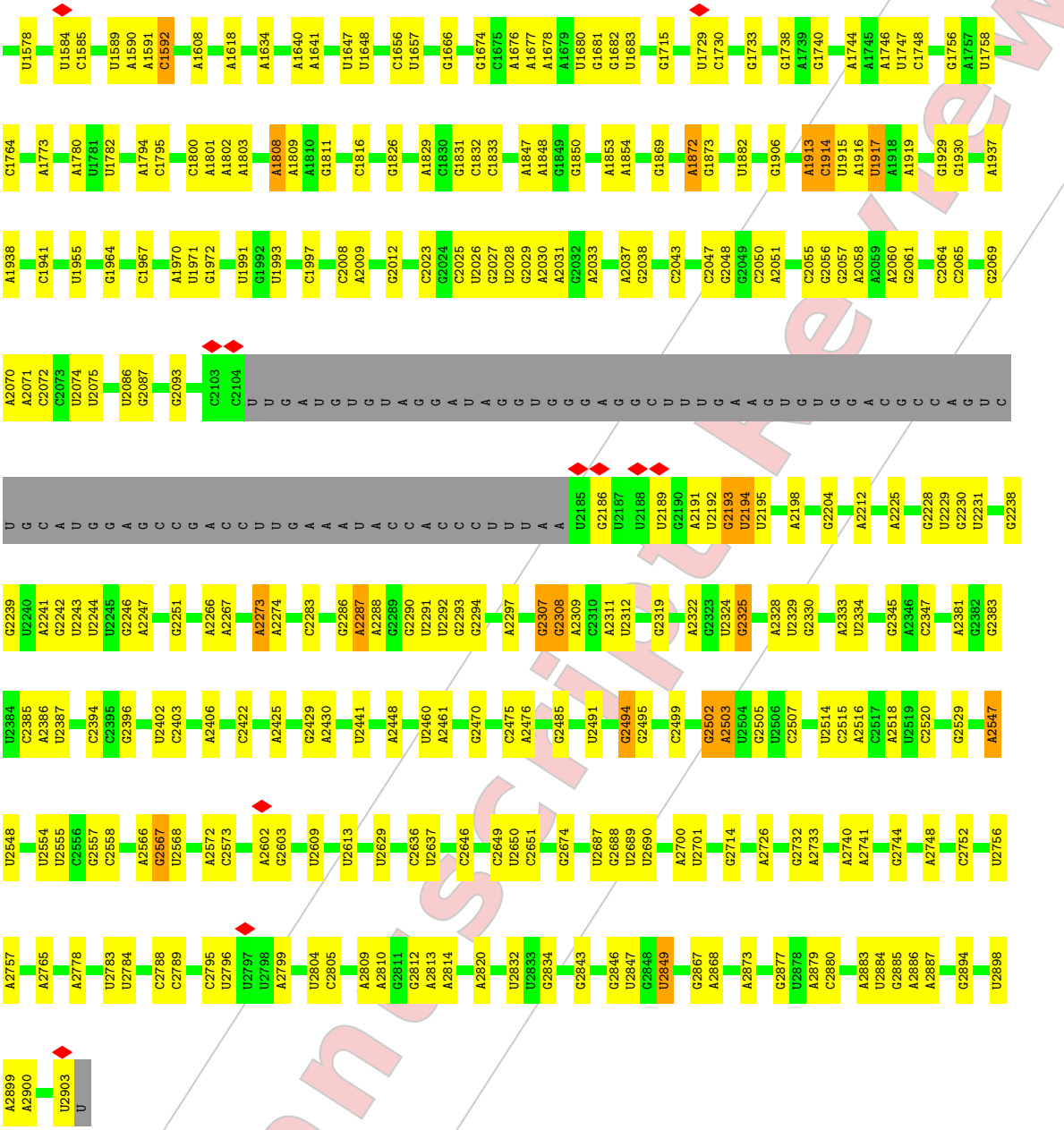
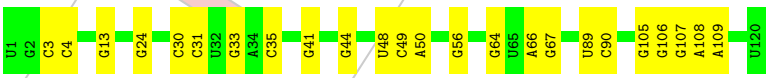


• Molecule 2: 5S rRNA

Chain 1:

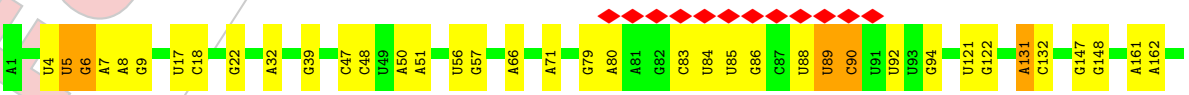




• Molecule 3: 16S rRNA

Chain 2:





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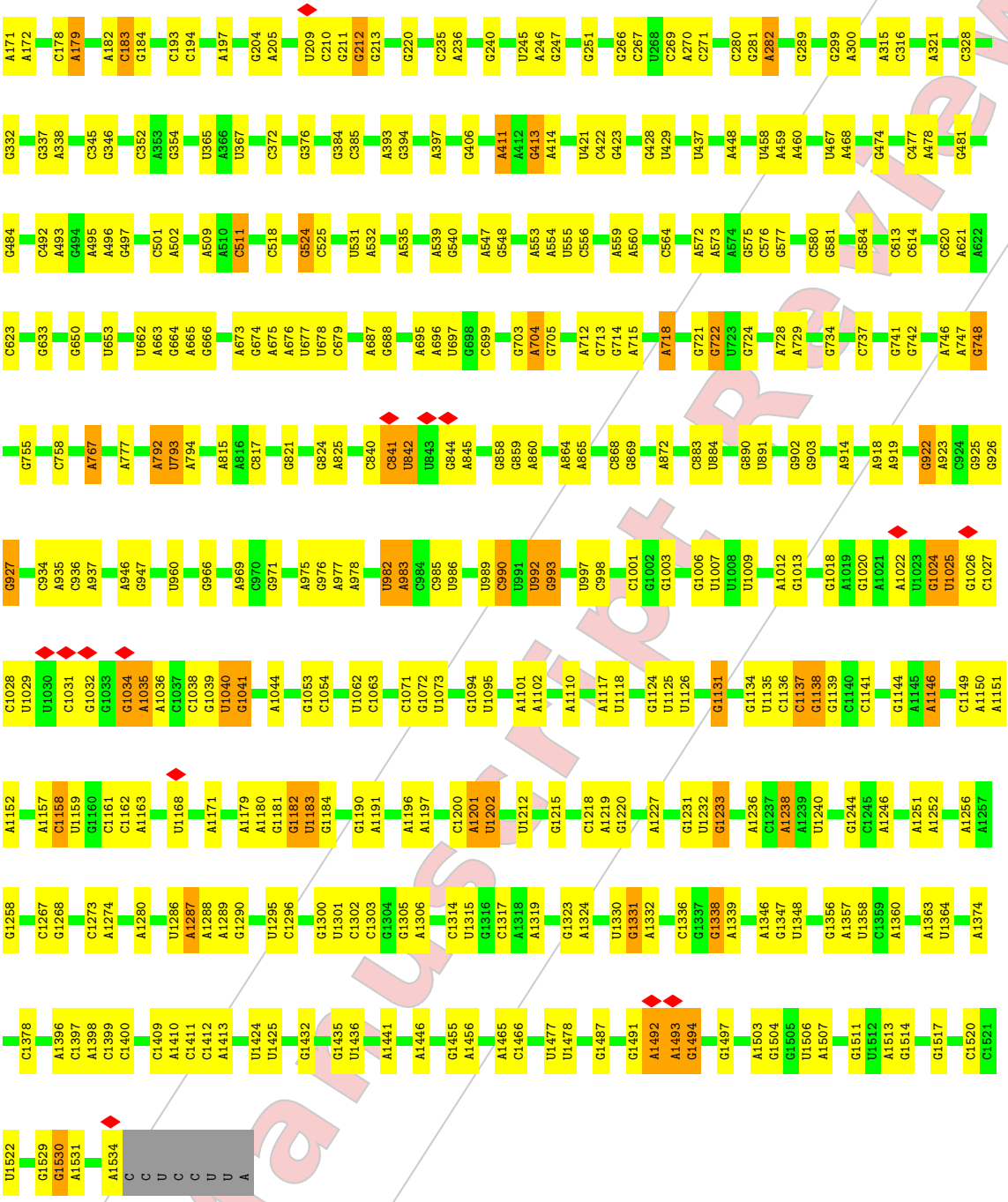
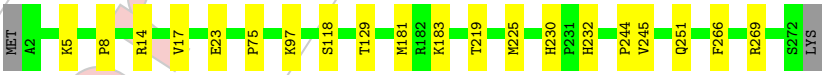


• Molecule 4: Large ribosomal subunit protein uL2

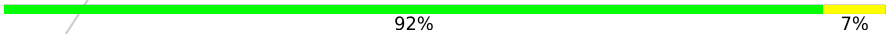
Chain A:





• Molecule 5: 50S ribosomal protein L3

Chain B:



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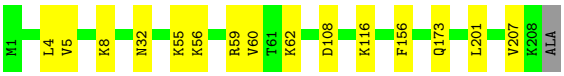
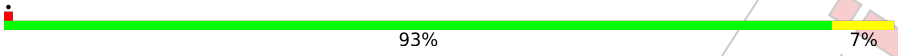


• Molecule 6: 50S ribosomal protein L4

Chain C:

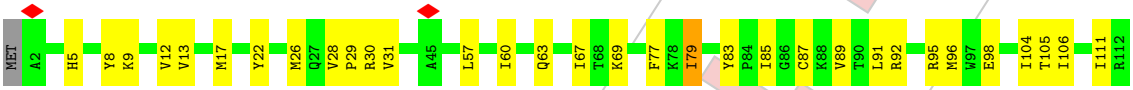


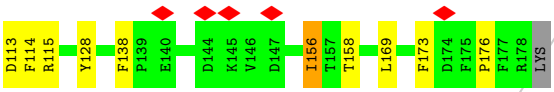


• Molecule 7: 50S ribosomal protein L5

Chain D:



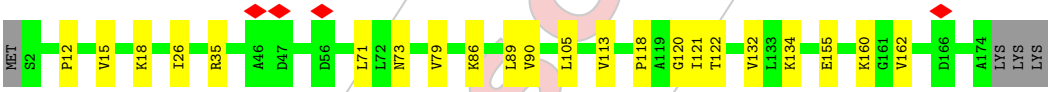




• Molecule 8: 50S ribosomal protein L6

Chain E:

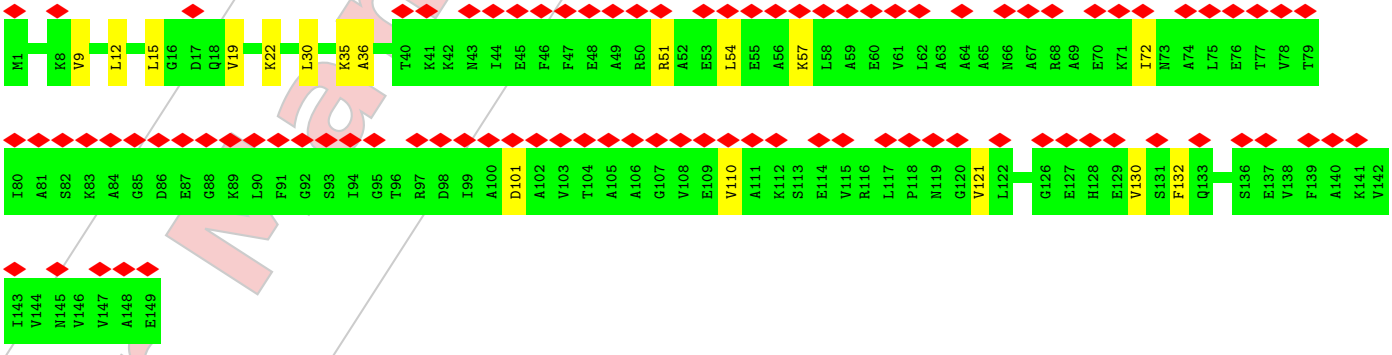




• Molecule 9: 50S ribosomal protein L9

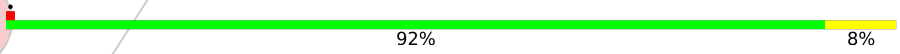
Chain F:





• Molecule 10: 50S ribosomal protein L13

Chain G:



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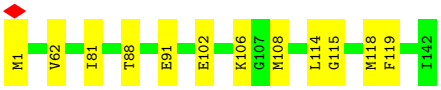
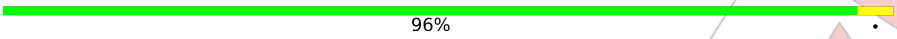
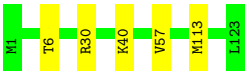


• Molecule 11: 50S ribosomal protein L14

Chain H:





• Molecule 12: 50S ribosomal protein L15

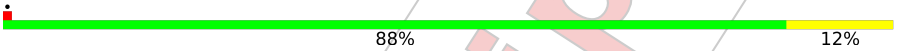
Chain I:

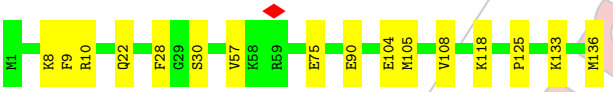




• Molecule 13: 50S ribosomal protein L16

Chain J:





• Molecule 14: 50S ribosomal protein L17

Chain K:





• Molecule 15: 50S ribosomal protein L18

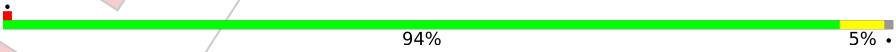
Chain L:





• Molecule 16: 50S ribosomal protein L19

Chain M:





• Molecule 17: 50S ribosomal protein L20

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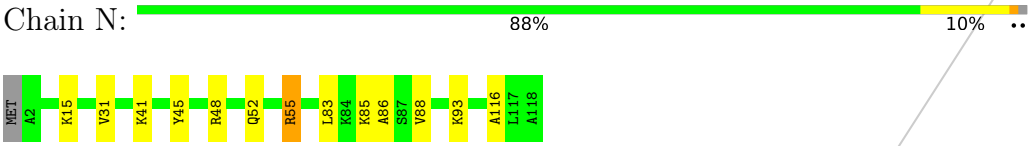
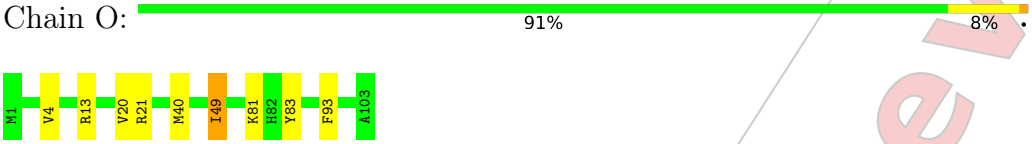
Chain N:



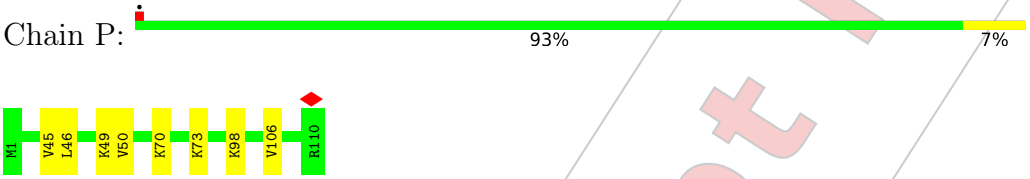
• Molecule 18: 50S ribosomal protein L21

Chain O:



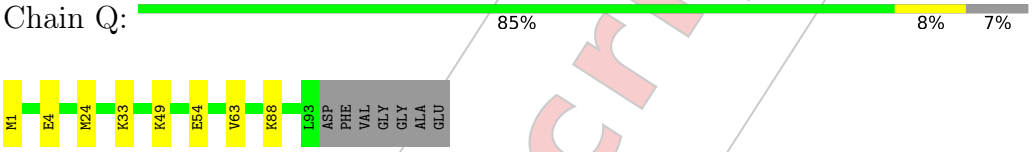
• Molecule 19: 50S ribosomal protein L22

Chain P:



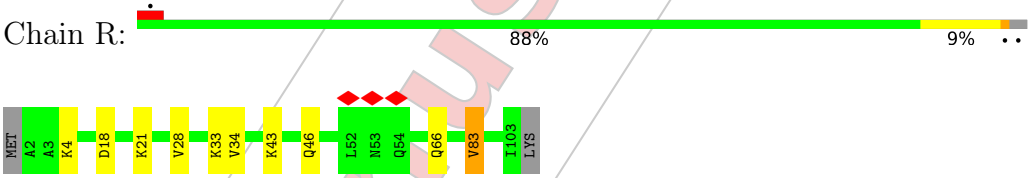
• Molecule 20: 50S ribosomal protein L23

Chain Q:



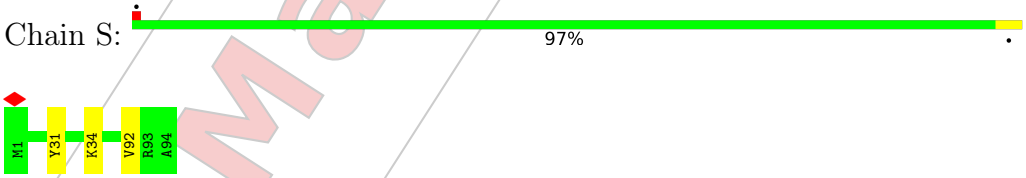
• Molecule 21: 50S ribosomal protein L24

Chain R:



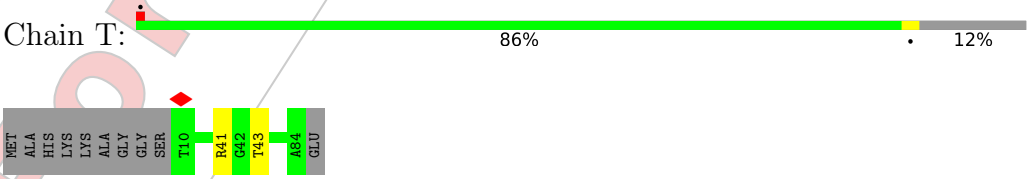
• Molecule 22: 50S ribosomal protein L25

Chain S:



• Molecule 23: 50S ribosomal protein L27

Chain T:



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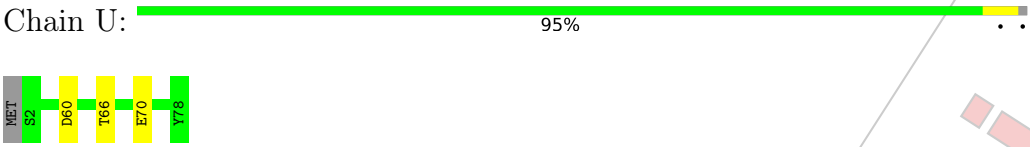
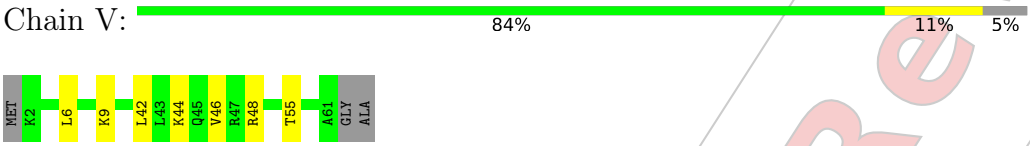
• Molecule 24: 50S ribosomal protein L28

Chain U:



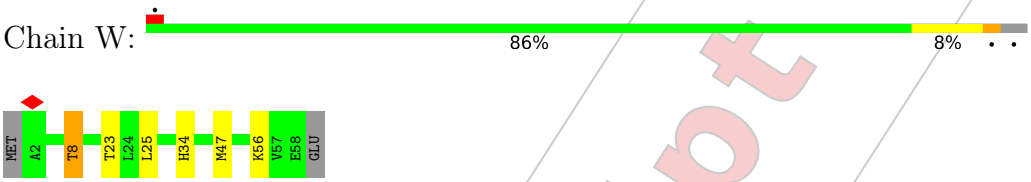
• Molecule 25: 50S ribosomal protein L29

Chain V:



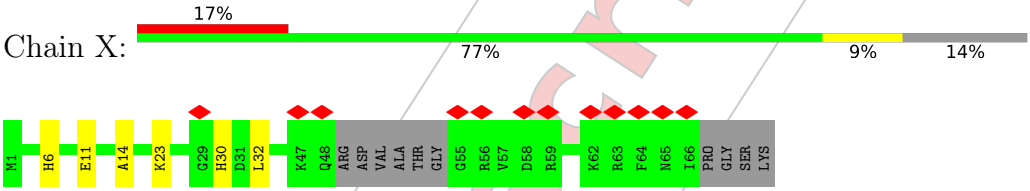
• Molecule 26: 50S ribosomal protein L30

Chain W:



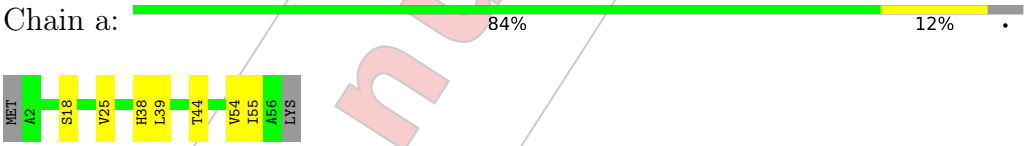
• Molecule 27: 50S ribosomal protein L31

Chain X:



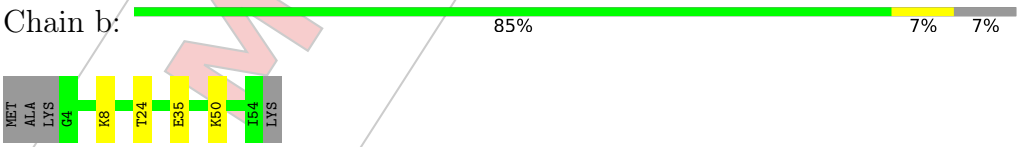
• Molecule 28: 50S ribosomal protein L32

Chain a:



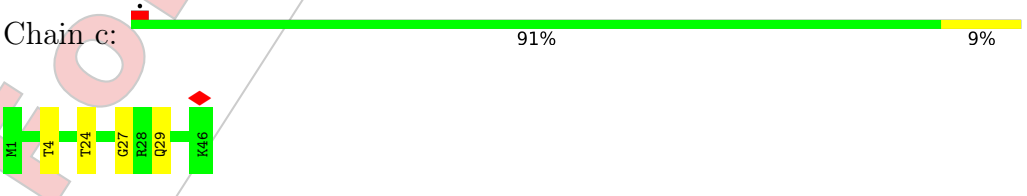
• Molecule 29: 50S ribosomal protein L33

Chain b:



• Molecule 30: 50S ribosomal protein L34

Chain c:



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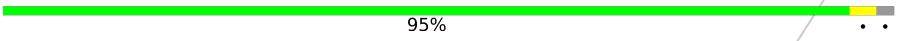
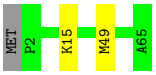
• Molecule 31: 50S ribosomal protein L35

Chain d:

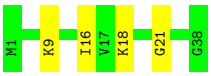




• Molecule 32: 50S ribosomal protein L36

Chain e:

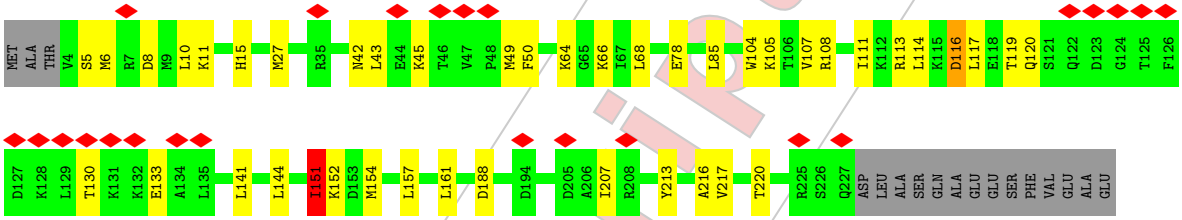




• Molecule 33: 30S ribosomal protein S2

Chain f:

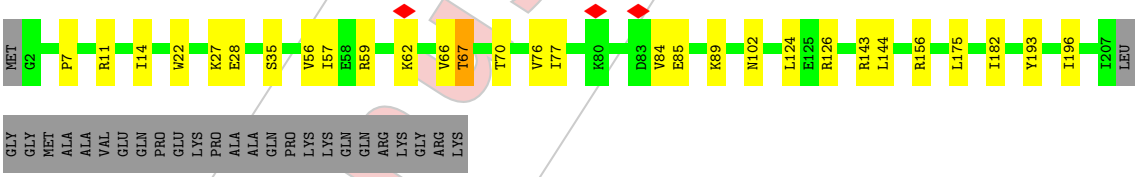




• Molecule 34: 30S ribosomal protein S3

Chain g:

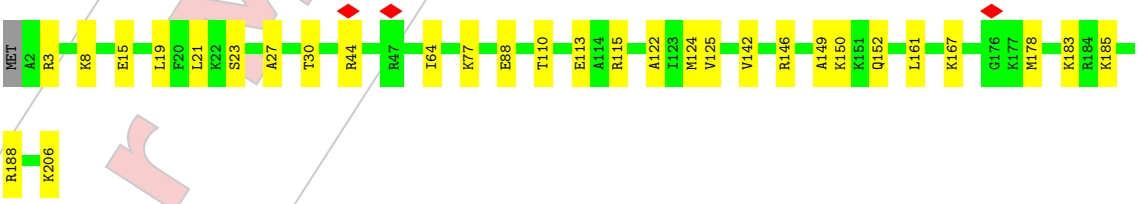




• Molecule 35: 30S ribosomal protein S4

Chain h:





• Molecule 36: 30S ribosomal protein S5

Chain i:



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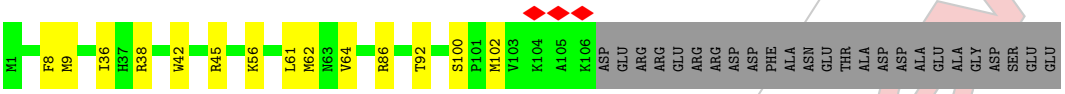
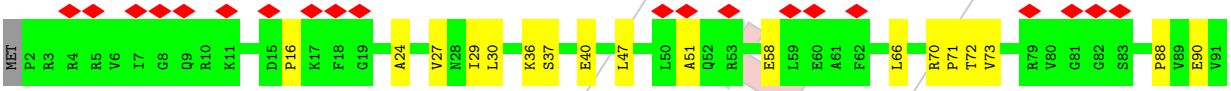
• Molecule 37: Small ribosomal subunit protein bS6, non-modified isoform

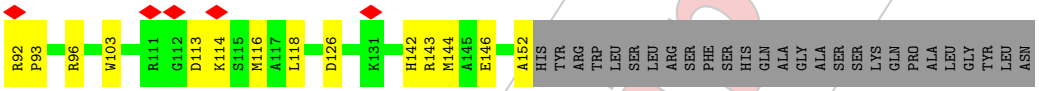




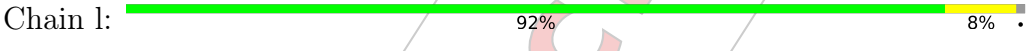
• Molecule 38: 30S ribosomal protein S7

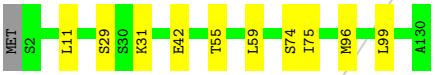




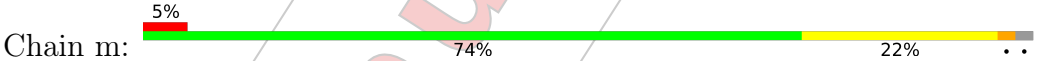


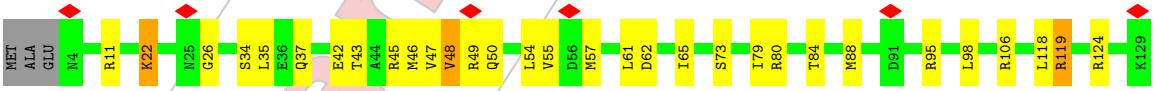
• Molecule 39: 30S ribosomal protein S8





• Molecule 40: 30S ribosomal protein S9

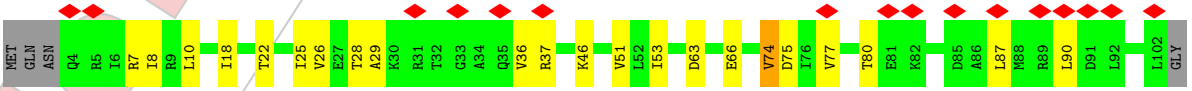






• Molecule 41: 30S ribosomal protein S10





• Molecule 42: 30S ribosomal protein S11

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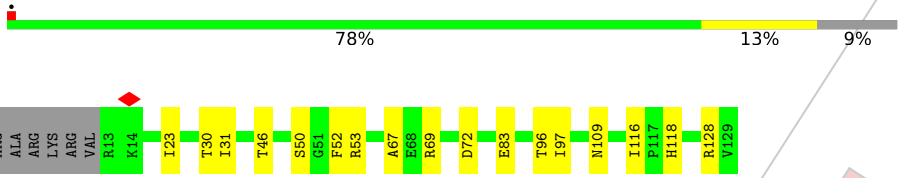
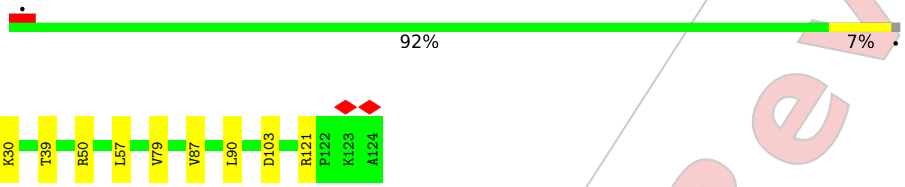
Chain o:



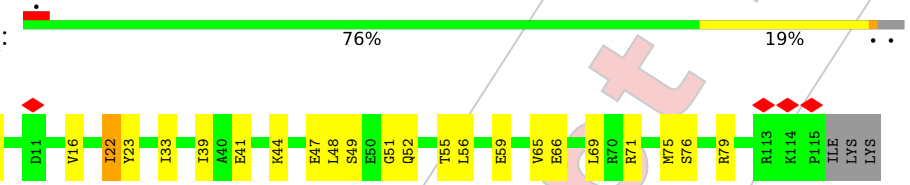
• Molecule 43: 30S ribosomal protein S12

Chain p:



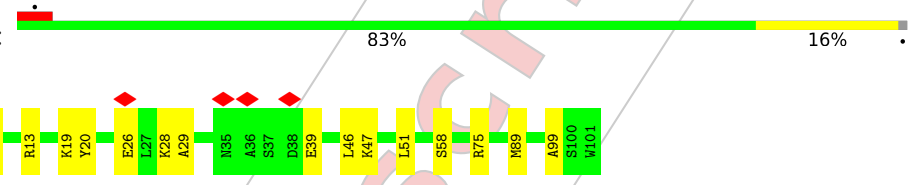
• Molecule 44: 30S ribosomal protein S13

Chain q:



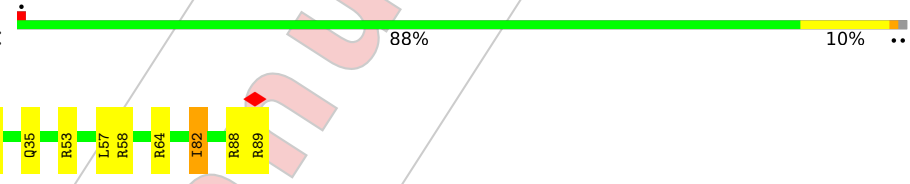
• Molecule 45: 30S ribosomal protein S14

Chain r:



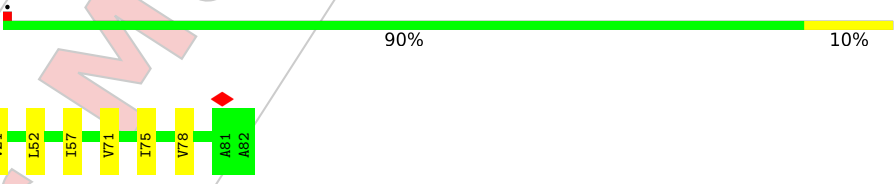
• Molecule 46: 30S ribosomal protein S15

Chain s:



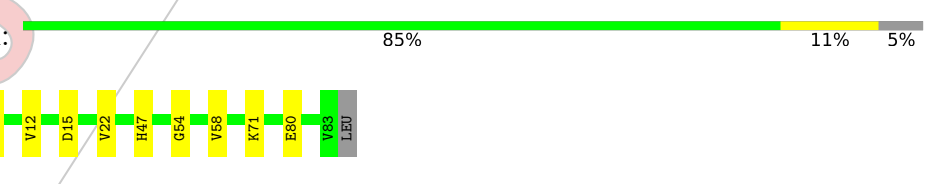
• Molecule 47: 30S ribosomal protein S16

Chain t:



• Molecule 48: 30S ribosomal protein S17

Chain u:



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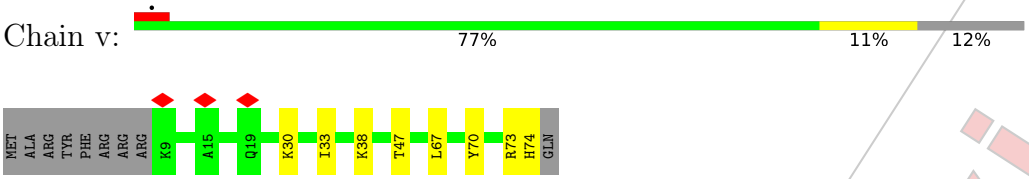
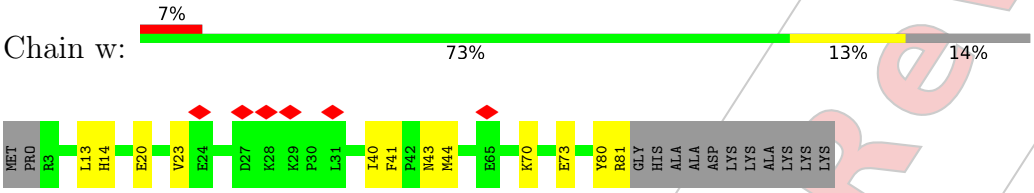
• Molecule 49: 30S ribosomal protein S18

Chain v:



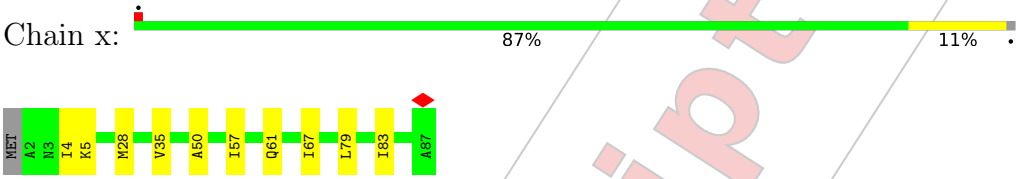
• Molecule 50: 30S ribosomal protein S19

Chain w:



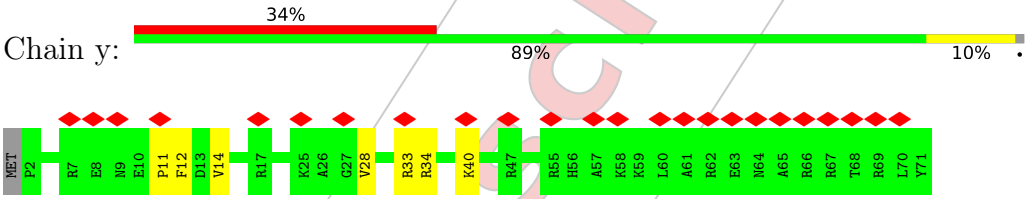
• Molecule 51: 30S ribosomal protein S20

Chain x:



• Molecule 52: 30S ribosomal protein S21

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	133854	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	0.630	Depositor
Minimum map value	-0.179	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	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 (i)

5.1 Standard geometry (i)

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	0.13	0/66326	0.31	0/103471
2	1	0.13	0/2869	0.26	0/4474
3	2	0.14	0/36859	0.33	0/57501
4	A	0.15	0/2121	0.40	0/2852
5	B	0.13	0/1580	0.34	0/2127
6	C	0.13	0/1571	0.34	0/2113
7	D	0.19	0/1434	0.47	0/1926
8	E	0.14	0/1315	0.38	0/1783
9	F	0.14	0/1122	0.40	0/1515
10	G	0.13	0/1152	0.32	0/1551
11	H	0.14	0/956	0.36	0/1279
12	I	0.14	0/1062	0.40	0/1413
13	J	0.17	0/1093	0.40	0/1460
14	K	0.14	0/958	0.35	0/1281
15	L	0.17	0/902	0.47	0/1209
16	M	0.14	0/929	0.37	0/1242
17	N	0.16	0/960	0.32	0/1278
18	O	0.14	0/829	0.39	0/1107
19	P	0.13	0/864	0.37	0/1156
20	Q	0.15	0/744	0.42	0/994
21	R	0.35	0/787	0.52	2/1051 (0.2%)
22	S	0.14	0/766	0.40	0/1025
23	T	0.12	0/579	0.36	0/767
24	U	0.14	0/635	0.37	0/848
25	V	0.15	0/492	0.34	0/655
26	W	0.12	0/443	0.28	0/593
27	X	0.25	0/488	0.50	0/649
28	a	0.11	0/440	0.32	0/588
29	b	0.12	0/424	0.35	0/565
30	c	0.11	0/380	0.34	0/498
31	d	0.13	0/513	0.37	0/676
32	e	0.16	0/303	0.41	0/397
33	f	0.16	0/1784	0.50	1/2403 (0.0%)
34	g	0.16	0/1651	0.42	0/2225

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Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	h	0.15	0/1665	0.40	0/2227
36	i	0.16	0/1157	0.42	0/1557
37	j	0.14	0/881	0.37	0/1189
38	k	0.16	0/1195	0.41	0/1602
39	l	0.16	0/989	0.42	0/1326
40	m	0.17	0/1034	0.40	0/1375
41	n	0.16	0/805	0.43	0/1089
42	o	0.15	0/893	0.40	0/1205
43	p	0.14	0/969	0.41	0/1300
44	q	0.16	0/892	0.48	0/1193
45	r	0.16	0/817	0.40	0/1088
46	s	0.17	0/722	0.40	0/964
47	t	0.16	0/659	0.46	0/884
48	u	0.16	0/657	0.45	0/881
49	v	0.13	0/553	0.36	0/742
50	w	0.15	0/652	0.43	0/877
51	x	0.20	0/676	0.36	0/895
52	y	0.11	0/598	0.27	0/792
All	All	0.14	0/151145	0.34	3/225858 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
27	X	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	R	46	GLN	CB-CA-C	-5.41	101.43	110.19
21	R	46	GLN	N-CA-CB	5.16	118.84	110.42
33	f	151	ILE	N-CA-C	-5.08	108.02	112.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	X	30	HIS	Sidechain

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5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59219	0	29790	255	0
2	1	2566	0	1302	7	0
3	2	32917	0	16564	170	0
4	A	2082	0	2154	11	0
5	B	1559	0	1611	8	0
6	C	1552	0	1619	10	0
7	D	1410	0	1444	25	0
8	E	1295	0	1332	12	0
9	F	1111	0	1148	9	0
10	G	1129	0	1162	10	0
11	H	947	0	1023	3	0
12	I	1053	0	1129	14	0
13	J	1074	0	1157	9	0
14	K	945	0	989	3	0
15	L	892	0	923	9	0
16	M	917	0	962	4	0
17	N	947	0	1019	7	0
18	O	816	0	839	5	0
19	P	857	0	922	5	0
20	Q	738	0	807	4	0
21	R	779	0	831	4	0
22	S	753	0	780	1	0
23	T	572	0	593	2	0
24	U	625	0	652	1	0
25	V	491	0	523	4	0
26	W	439	0	482	4	0
27	X	480	0	482	3	0
28	a	434	0	445	4	0
29	b	417	0	451	2	0
30	c	377	0	418	2	0
31	d	504	0	572	2	0
32	e	302	0	343	2	0
33	f	1753	0	1780	26	0
34	g	1624	0	1696	19	0
35	h	1643	0	1707	16	0
36	i	1144	0	1185	10	0
37	j	862	0	864	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	k	1181	0	1238	28	0
39	l	979	0	1031	5	0
40	m	1022	0	1070	20	0
41	n	795	0	836	13	0
42	o	877	0	887	12	0
43	p	955	0	1016	4	0
44	q	883	0	941	14	0
45	r	805	0	844	12	0
46	s	714	0	734	7	0
47	t	649	0	666	4	0
48	u	648	0	691	3	0
49	v	544	0	565	5	0
50	w	637	0	665	7	0
51	x	670	0	719	6	0
52	y	590	0	629	5	0
All	All	139174	0	94232	789	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 (789) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1847:A:HO2'	1:0:1848:A:H8	1.07	0.92
13:J:105:MET:HE2	13:J:108:VAL:HG21	1.58	0.86
38:k:93:PRO:HA	38:k:96:ARG:HD3	1.59	0.84
3:2:1182:G:H4'	3:2:1183:U:H5'	1.61	0.82
18:O:40:MET:HG3	18:O:49:ILE:HG22	1.63	0.80
33:f:114:LEU:HB2	33:f:144:LEU:HD22	1.64	0.79
3:2:1009:U:H3	3:2:1018:G:H22	1.30	0.79
3:2:1013:G:H21	3:2:1219:A:H1'	1.47	0.79
6:C:97:ASN:HB2	6:C:100:MET:HG2	1.64	0.79
13:J:57:VAL:HG11	13:J:105:MET:HE1	1.64	0.78
3:2:673:A:H2'	3:2:674:G:C8	2.21	0.76
1:0:2324:U:H3'	1:0:2325:G:H5"	1.68	0.74
8:E:89:LEU:HD22	8:E:162:VAL:HG22	1.68	0.73
3:2:1003:G:N7	3:2:1034:G:N2	2.38	0.71
36:i:34:THR:HG22	36:i:52:LYS:HG2	1.73	0.71
20:Q:54:GLU:HB3	20:Q:88:LYS:HG3	1.73	0.70
34:g:77:ILE:HD13	34:g:84:VAL:HG21	1.74	0.69
44:q:49:SER:HB3	44:q:52:GLN:HE22	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:q:71:ARG:O	44:q:75:MET:HG2	1.92	0.69
42:o:50:SER:HA	42:o:69:ARG:HH12	1.56	0.69
3:2:492:C:H2'	3:2:493:A:C8	2.27	0.69
5:B:55:LYS:HD3	5:B:60:VAL:HG22	1.74	0.69
28:a:54:VAL:HG23	28:a:55:ILE:HG12	1.75	0.69
3:2:1003:G:C5	3:2:1034:G:N2	2.61	0.69
1:0:2796:U:H3	1:0:2799:A:H61	1.40	0.68
15:L:51:ALA:HB3	15:L:78:VAL:HG13	1.75	0.67
9:F:12:LEU:HD12	9:F:19:VAL:HG21	1.75	0.67
1:0:272:A:H2'	1:0:273:G:H8	1.59	0.67
3:2:1492:A:H2'	3:2:1493:A:C8	2.30	0.67
1:0:856:G:H2'	1:0:857:G:C8	2.30	0.67
3:2:675:A:H4'	49:v:73:ARG:HH12	1.60	0.67
38:k:72:THR:HA	38:k:96:ARG:HH12	1.60	0.67
40:m:45:ARG:O	40:m:48:VAL:HG12	1.95	0.66
3:2:946:A:H2'	3:2:947:G:C8	2.31	0.66
3:2:673:A:H2'	3:2:674:G:H8	1.59	0.66
1:0:2246:G:H2'	1:0:2247:A:H8	1.59	0.66
3:2:1356:G:H2'	3:2:1357:A:C8	2.31	0.66
3:2:147:G:H2'	3:2:148:G:C8	2.30	0.66
3:2:511:C:H4'	35:h:44:ARG:HH22	1.60	0.65
40:m:88:MET:HE1	40:m:95:ARG:HA	1.78	0.65
9:F:9:VAL:HG21	9:F:12:LEU:HG	1.77	0.65
7:D:105:THR:HG22	7:D:106:ILE:HD12	1.77	0.64
3:2:922:G:H2'	3:2:923:A:C8	2.32	0.64
1:0:1802:A:H2'	1:0:1803:A:C8	2.32	0.64
7:D:31:VAL:HA	7:D:158:THR:HG22	1.79	0.64
3:2:990:C:H5	3:2:1215:G:H1	1.43	0.64
3:2:662:U:H2'	3:2:663:A:C8	2.32	0.64
7:D:95:ARG:HA	7:D:98:GLU:HG3	1.80	0.64
49:v:30:LYS:HD2	49:v:33:ILE:HD11	1.77	0.64
24:U:66:THR:O	24:U:70:GLU:HG2	1.98	0.64
33:f:6:MET:HE1	33:f:10:LEU:HD12	1.80	0.64
40:m:55:VAL:HG23	40:m:57:MET:H	1.62	0.63
1:0:1916:A:H2'	1:0:1917:U:C6	2.32	0.63
3:2:718:A:H2	49:v:38:LYS:HE3	1.64	0.63
3:2:728:A:H2'	3:2:729:A:C8	2.34	0.63
1:0:2070:A:H2'	1:0:2071:A:H8	1.64	0.63
34:g:175:LEU:HD23	34:g:182:ILE:HD13	1.80	0.63
10:G:102:GLU:HG2	10:G:119:PHE:HZ	1.64	0.63
4:A:118:SER:HB2	4:A:129:THR:HB	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:g:57:ILE:HG12	34:g:66:VAL:HG23	1.81	0.62
3:2:1158:C:H5	3:2:1181:G:H1	1.47	0.62
1:0:1028:A:H2'	1:0:1029:A:C8	2.35	0.62
33:f:104:TRP:HA	33:f:107:VAL:HG22	1.82	0.62
1:0:1913:A:H61	3:2:1492:A:H1'	1.62	0.62
38:k:92:ARG:O	38:k:96:ARG:HG3	2.00	0.62
7:D:91:LEU:HD13	7:D:96:MET:HA	1.81	0.62
1:0:2809:A:H2'	1:0:2810:A:C8	2.35	0.62
3:2:714:G:H2'	3:2:715:A:C8	2.34	0.62
3:2:269:C:H2'	3:2:270:A:H8	1.64	0.62
3:2:1071:C:H2'	3:2:1072:G:H8	1.64	0.62
20:Q:4:GLU:OE1	20:Q:49:LYS:HE3	1.99	0.62
3:2:688:G:H1	3:2:699:C:H5	1.46	0.62
41:n:7:ARG:HG2	41:n:75:ASP:HB3	1.82	0.61
46:s:53:ARG:O	46:s:57:LEU:HD22	2.00	0.61
1:0:581:C:H2'	1:0:582:A:H8	1.65	0.61
3:2:1491:G:H2'	3:2:1492:A:O4'	2.01	0.61
1:0:172:A:H2'	1:0:173:A:H8	1.65	0.61
37:j:42:TRP:CE2	37:j:102:MET:HG3	2.36	0.61
12:I:78:ARG:HG2	12:I:113:ALA:HB3	1.81	0.61
42:o:116:ILE:HD11	52:y:28:VAL:HG13	1.83	0.61
3:2:17:U:H2'	3:2:18:C:C6	2.36	0.61
1:0:1916:A:H2'	1:0:1917:U:H6	1.66	0.61
42:o:50:SER:HA	42:o:69:ARG:NH1	2.16	0.60
7:D:111:ILE:HG13	7:D:114:PHE:HB2	1.82	0.60
1:0:2070:A:H2'	1:0:2071:A:C8	2.36	0.60
4:A:75:PRO:HG2	4:A:97:LYS:HD3	1.82	0.60
3:2:1162:C:H2'	3:2:1163:A:H8	1.67	0.60
35:h:88:GLU:HG2	35:h:188:ARG:HD3	1.84	0.60
44:q:23:TYR:HE1	44:q:69:LEU:HD12	1.65	0.60
21:R:28:VAL:HG22	21:R:34:VAL:HG12	1.84	0.59
3:2:1238:A:N7	3:2:1303:C:H1'	2.17	0.59
45:r:89:MET:HE2	45:r:89:MET:HA	1.83	0.59
3:2:746:A:H2'	3:2:747:A:C8	2.38	0.59
3:2:337:G:H2'	3:2:338:A:C8	2.38	0.59
38:k:66:LEU:HB3	38:k:70:ARG:HH21	1.68	0.59
37:j:38:ARG:HH11	37:j:61:LEU:HD21	1.68	0.59
3:2:539:A:H2'	3:2:540:G:C8	2.38	0.58
36:i:131:THR:HG22	36:i:131:THR:O	2.03	0.58
1:0:1141:U:H4'	1:0:1142:A:O4'	2.03	0.58
1:0:2898:U:H2'	1:0:2899:A:H8	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:26:MET:HE3	7:D:30:ARG:HH21	1.69	0.58
3:2:1218:C:H2'	3:2:1219:A:C8	2.39	0.58
1:0:2071:A:H2'	1:0:2072:C:C6	2.39	0.58
8:E:118:PRO:HG2	8:E:121:ILE:HD13	1.86	0.58
1:0:2193:G:H2'	1:0:2194:U:C6	2.38	0.58
8:E:122:THR:HG23	8:E:134:LYS:HE2	1.85	0.58
3:2:1358:U:OP1	45:r:75:ARG:HG3	2.04	0.57
44:q:39:ILE:HD11	44:q:56:LEU:HD21	1.86	0.57
7:D:67:ILE:HD13	7:D:87:CYS:HB3	1.85	0.57
21:R:4:LYS:HG2	21:R:83:VAL:HG22	1.85	0.57
1:0:191:A:H2'	1:0:192:C:H6	1.69	0.57
1:0:981:A:H8	1:0:2027:G:H21	1.51	0.57
3:2:1040:U:H2'	3:2:1041:G:H8	1.69	0.57
3:2:1305:G:H1'	3:2:1332:A:N6	2.20	0.57
1:0:832:U:H2'	1:0:833:A:H8	1.70	0.57
44:q:51:GLY:O	44:q:55:THR:HG23	2.04	0.57
3:2:56:U:H2'	3:2:57:G:H8	1.69	0.57
3:2:458:U:H2'	3:2:459:A:H8	1.70	0.57
33:f:111:ILE:HD11	33:f:151:ILE:HG22	1.86	0.57
1:0:1746:A:H2'	1:0:1747:U:C6	2.40	0.57
41:n:28:THR:HG21	41:n:90:LEU:HD22	1.85	0.57
1:0:172:A:H2'	1:0:173:A:C8	2.39	0.57
1:0:2813:A:H2'	1:0:2814:A:H8	1.70	0.56
38:k:72:THR:HG23	38:k:73:VAL:HG22	1.87	0.56
50:w:41:PHE:H	50:w:44:MET:HE1	1.70	0.56
1:0:1138:G:H21	10:G:108:MET:HE2	1.69	0.56
1:0:1:G:H2'	1:0:2:G:H8	1.68	0.56
1:0:1000:A:H2'	1:0:1001:A:C8	2.40	0.56
1:0:1048:A:H62	1:0:1110:G:H21	1.51	0.56
3:2:1040:U:H2'	3:2:1041:G:C8	2.40	0.56
44:q:5:ALA:HB2	44:q:22:ILE:HD12	1.88	0.56
1:0:1808:A:H3'	1:0:1809:A:C8	2.40	0.56
1:0:2246:G:H2'	1:0:2247:A:C8	2.39	0.56
3:2:1251:A:H2'	3:2:1252:A:C8	2.40	0.56
18:O:4:VAL:HG22	18:O:13:ARG:HG3	1.87	0.56
10:G:114:LEU:HG	10:G:118:MET:HE2	1.88	0.56
52:y:33:ARG:HH21	52:y:34:ARG:HB2	1.71	0.56
3:2:713:G:H2'	3:2:714:G:C8	2.40	0.55
1:0:1469:A:H2'	1:0:1470:A:C8	2.41	0.55
34:g:156:ARG:HH11	34:g:193:TYR:HB3	1.72	0.55
3:2:946:A:H2'	3:2:947:G:H8	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:5:U:H4'	3:2:6:G:O5'	2.06	0.55
3:2:1477:U:H2'	3:2:1478:U:C6	2.42	0.55
38:k:51:ALA:HB2	38:k:58:GLU:HG3	1.87	0.55
40:m:47:VAL:HA	40:m:50:GLN:HG3	1.89	0.55
3:2:1218:C:H2'	3:2:1219:A:H8	1.71	0.55
41:n:29:ALA:HB1	41:n:36:VAL:HG11	1.88	0.55
1:0:2193:G:H2'	1:0:2194:U:H6	1.70	0.55
17:N:41:LYS:HE2	17:N:45:TYR:CZ	2.41	0.55
1:0:742:A:H2'	1:0:743:A:C8	2.41	0.55
1:0:1572:A:H2'	1:0:1573:G:H8	1.71	0.55
3:2:1360:A:C8	45:r:58:SER:HB3	2.42	0.55
33:f:68:LEU:HD11	33:f:151:ILE:HD11	1.88	0.55
1:0:742:A:H2'	1:0:743:A:H8	1.72	0.55
1:0:272:A:H2'	1:0:273:G:C8	2.42	0.55
1:0:581:C:H2'	1:0:582:A:C8	2.42	0.55
1:0:2812:G:H2'	1:0:2813:A:C8	2.42	0.55
3:2:1356:G:H2'	3:2:1357:A:H8	1.72	0.55
3:2:1323:G:H2'	3:2:1324:A:C8	2.43	0.54
26:W:8:THR:HG23	26:W:56:LYS:HG3	1.88	0.54
1:0:1:G:H2'	1:0:2:G:C8	2.43	0.54
33:f:49:MET:HE2	33:f:49:MET:HA	1.89	0.54
1:0:1802:A:H2'	1:0:1803:A:H8	1.73	0.54
7:D:57:LEU:HA	7:D:60:ILE:HG22	1.89	0.54
44:q:48:LEU:HD22	44:q:52:GLN:OE1	2.08	0.54
1:0:1915:U:H2'	1:0:1916:A:O4'	2.07	0.54
1:0:2194:U:H2'	1:0:2195:U:H6	1.72	0.54
33:f:8:ASP:HA	33:f:11:LYS:HB2	1.89	0.54
51:x:35:VAL:HG11	51:x:79:LEU:HD13	1.89	0.54
1:0:76:C:O2'	25:V:55:THR:HG21	2.07	0.54
3:2:1493:A:H2'	3:2:1494:G:H8	1.71	0.54
47:t:52:LEU:HD12	47:t:57:ILE:HD11	1.89	0.54
1:0:273:G:H2'	1:0:274:C:C6	2.43	0.54
1:0:2273:A:H2'	1:0:2274:A:C8	2.43	0.54
42:o:31:ILE:HG12	42:o:46:THR:HG22	1.90	0.54
46:s:35:GLN:HA	46:s:35:GLN:OE1	2.08	0.54
3:2:1149:C:H2'	3:2:1150:A:H8	1.73	0.53
12:I:30:THR:HG22	12:I:33:ARG:H	1.73	0.53
41:n:37:ARG:HH22	41:n:77:VAL:HG22	1.73	0.53
1:0:1432:G:H2'	1:0:1433:A:C8	2.43	0.53
3:2:997:U:H2'	3:2:998:C:O4'	2.08	0.53
3:2:1530:G:H2'	3:2:1531:A:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:s:58:ARG:HH11	46:s:58:ARG:HG3	1.72	0.53
3:2:1314:C:H2'	3:2:1315:U:C6	2.44	0.53
37:j:45:ARG:O	37:j:56:LYS:HA	2.09	0.53
38:k:72:THR:HG22	38:k:142:HIS:NE2	2.23	0.53
38:k:88:PRO:HG2	38:k:152:ALA:HB2	1.90	0.53
5:B:56:LYS:HD2	5:B:59:ARG:HG3	1.90	0.53
7:D:60:ILE:HD11	7:D:138:PHE:CD1	2.44	0.53
1:0:721:A:H2'	1:0:722:A:C8	2.43	0.53
1:0:1353:A:H2'	1:0:1354:A:C8	2.44	0.53
1:0:947:A:H2'	1:0:948:C:C6	2.44	0.53
3:2:411:A:C4	3:2:413:G:H1'	2.43	0.53
1:0:2515:C:H2'	1:0:2516:A:H8	1.74	0.53
1:0:2557:G:H2'	1:0:2558:C:C6	2.44	0.53
3:2:767:A:H8	3:2:1511:G:H21	1.56	0.53
3:2:539:A:H2'	3:2:540:G:H8	1.73	0.52
3:2:1038:C:H2'	3:2:1039:G:H8	1.74	0.52
44:q:22:ILE:HD11	44:q:65:VAL:HG21	1.90	0.52
3:2:1273:C:H2'	3:2:1274:A:O4'	2.10	0.52
3:2:1412:C:H2'	3:2:1413:A:C8	2.44	0.52
32:e:18:LYS:HE2	32:e:21:GLY:HA2	1.90	0.52
34:g:77:ILE:HA	34:g:84:VAL:HG23	1.90	0.52
39:l:29:SER:HA	39:l:59:LEU:HD22	1.91	0.52
3:2:718:A:C2	49:v:38:LYS:HE3	2.44	0.52
3:2:1038:C:H2'	3:2:1039:G:C8	2.45	0.52
3:2:1287:A:H2'	3:2:1288:A:C8	2.45	0.52
37:j:8:PHE:HE1	37:j:62:MET:HE2	1.74	0.52
1:0:1187:G:H5'	18:O:83:TYR:CE1	2.45	0.52
44:q:44:LYS:HB2	44:q:47:GLU:HG2	1.92	0.52
3:2:664:G:H22	3:2:741:G:H1	1.58	0.52
1:0:645:C:H2'	1:0:647:G:N7	2.25	0.52
1:0:1048:A:H1'	1:0:1112:G:H21	1.74	0.52
3:2:269:C:H2'	3:2:270:A:C8	2.43	0.52
3:2:695:A:H2'	3:2:696:A:C8	2.44	0.52
38:k:114:LYS:HB2	38:k:118:LEU:HD13	1.91	0.52
3:2:1151:A:HO2'	3:2:1152:A:H8	1.55	0.52
49:v:70:TYR:HB2	49:v:74:HIS:NE2	2.25	0.51
1:0:1405:U:H2'	1:0:1406:U:C6	2.46	0.51
1:0:1914:C:H41	3:2:1409:C:H4'	1.74	0.51
42:o:97:ILE:HG22	52:y:12:PHE:HZ	1.74	0.51
1:0:2241:A:H2'	1:0:2242:G:C8	2.44	0.51
38:k:144:MET:HA	38:k:144:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:191:A:H2'	1:0:192:C:C6	2.46	0.51
1:0:479:A:N3	1:0:481:G:H5"	2.25	0.51
1:0:593:U:H2'	1:0:594:U:C6	2.45	0.51
1:0:639:U:H2'	1:0:640:C:H6	1.75	0.51
1:0:1530:G:H2'	1:0:1531:C:C6	2.46	0.51
1:0:1853:A:H2'	1:0:1854:A:C8	2.45	0.51
7:D:8:TYR:HA	7:D:12:VAL:HG12	1.93	0.51
4:A:183:LYS:HZ3	4:A:266:PHE:HA	1.76	0.51
3:2:553:A:H2'	3:2:554:A:H8	1.75	0.51
25:V:42:LEU:O	25:V:46:VAL:HG23	2.11	0.51
3:2:674:G:H21	42:o:118:HIS:HB2	1.76	0.51
36:i:15:LEU:HA	36:i:37:THR:HG22	1.92	0.51
45:r:19:LYS:HG2	45:r:20:TYR:CD1	2.45	0.51
36:i:36:LEU:HD22	36:i:134:ILE:HG13	1.93	0.50
1:0:5:A:H2'	1:0:6:A:C8	2.46	0.50
4:A:8:PRO:HB3	4:A:14:ARG:HG3	1.92	0.50
40:m:26:GLY:HA2	40:m:61:LEU:O	2.10	0.50
44:q:16:VAL:HB	44:q:41:GLU:HG3	1.92	0.50
17:N:86:ALA:HB2	17:N:116:ALA:HB2	1.94	0.50
50:w:40:ILE:HA	50:w:44:MET:HE1	1.93	0.50
3:2:1491:G:H3'	3:2:1492:A:C8	2.46	0.50
1:0:2243:U:H2'	1:0:2244:U:C6	2.46	0.50
3:2:524:G:H2'	3:2:525:C:C6	2.47	0.50
43:p:87:VAL:HG11	43:p:90:LEU:HD12	1.93	0.50
51:x:35:VAL:HG22	51:x:50:ALA:HB1	1.93	0.50
1:0:2291:U:H2'	1:0:2292:U:C6	2.46	0.50
39:l:11:LEU:HD22	39:l:75:ILE:HD11	1.94	0.50
40:m:80:ARG:O	40:m:84:THR:HG22	2.11	0.50
51:x:28:MET:HE1	51:x:67:ILE:HG21	1.94	0.50
1:0:1677:A:H2'	1:0:1678:A:H8	1.77	0.50
1:0:1914:C:H2'	1:0:1915:U:O4'	2.12	0.50
3:2:477:C:H2'	3:2:478:A:C8	2.46	0.50
3:2:1305:G:H22	3:2:1331:G:H2'	1.77	0.50
8:E:86:LYS:HE3	8:E:132:VAL:HG22	1.92	0.50
19:P:73:LYS:HB2	19:P:106:VAL:HB	1.93	0.50
1:0:1047:G:H21	1:0:1111:A:N6	2.10	0.50
1:0:1677:A:H2'	1:0:1678:A:C8	2.47	0.50
2:1:66:A:H61	2:1:107:G:H2'	1.77	0.50
9:F:110:VAL:HG11	9:F:132:PHE:HE2	1.76	0.50
1:0:2334:U:C4	15:L:16:ARG:HD3	2.47	0.49
10:G:88:THR:OG1	10:G:91:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:33:ARG:HB3	15:L:34:HIS:CD2	2.47	0.49
40:m:22:LYS:HG3	40:m:62:ASP:HB2	1.94	0.49
47:t:71:VAL:O	47:t:75:ILE:HG13	2.12	0.49
8:E:73:ASN:C	8:E:73:ASN:HD22	2.19	0.49
9:F:110:VAL:HG11	9:F:132:PHE:CE2	2.47	0.49
3:2:56:U:H2'	3:2:57:G:C8	2.48	0.49
3:2:337:G:H2'	3:2:338:A:H8	1.77	0.49
3:2:1137:C:H1'	3:2:1138:G:C2	2.47	0.49
11:H:40:LYS:HE3	11:H:57:VAL:HG12	1.94	0.49
38:k:72:THR:HA	38:k:96:ARG:NH1	2.27	0.49
1:0:305:C:H2'	1:0:306:U:C6	2.48	0.49
39:l:96:MET:HE2	39:l:99:LEU:HB2	1.94	0.49
41:n:66:GLU:HB3	45:r:99:ALA:HB2	1.92	0.49
1:0:639:U:H2'	1:0:640:C:C6	2.47	0.49
15:L:74:VAL:O	15:L:78:VAL:HG22	2.13	0.49
42:o:67:ALA:HB2	42:o:96:THR:HG23	1.95	0.49
1:0:1028:A:H2'	1:0:1029:A:H8	1.78	0.49
3:2:1493:A:H2'	3:2:1494:G:C8	2.47	0.49
34:g:70:THR:HG21	34:g:76:VAL:HG21	1.95	0.49
50:w:20:GLU:HA	50:w:23:VAL:HG12	1.95	0.49
1:0:608:A:H2'	1:0:609:A:C8	2.48	0.49
15:L:11:ALA:O	15:L:15:ARG:HG3	2.13	0.49
34:g:143:ARG:NH1	34:g:144:LEU:HD21	2.28	0.49
37:j:36:ILE:HD13	37:j:64:VAL:HG12	1.95	0.49
1:0:2898:U:H2'	1:0:2899:A:C8	2.46	0.48
45:r:46:LEU:HD22	50:w:13:LEU:HB2	1.95	0.48
33:f:216:ALA:O	33:f:220:THR:HG22	2.13	0.48
35:h:3:ARG:HD2	35:h:115:ARG:HH21	1.77	0.48
1:0:64:A:H2'	1:0:65:U:C6	2.48	0.48
15:L:56:LYS:O	15:L:60:GLU:HG3	2.12	0.48
33:f:130:THR:HB	33:f:133:GLU:HB2	1.96	0.48
1:0:2554:U:H2'	1:0:2555:U:O2	2.14	0.48
4:A:245:VAL:HG12	4:A:251:GLN:HA	1.95	0.48
12:I:79:LEU:HG	12:I:112:LEU:HA	1.96	0.48
33:f:15:HIS:HB3	33:f:43:LEU:HD11	1.95	0.48
34:g:56:VAL:CG2	34:g:67:THR:HG23	2.44	0.48
40:m:45:ARG:O	40:m:49:ARG:HG2	2.13	0.48
1:0:760:G:H2'	1:0:761:A:O4'	2.13	0.48
1:0:1306:C:H2'	1:0:1307:A:H8	1.79	0.48
1:0:2649:C:H2'	1:0:2650:U:H6	1.78	0.48
3:2:580:C:H2'	3:2:581:G:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:922:G:H2'	3:2:923:A:H8	1.77	0.48
33:f:152:LYS:HB3	33:f:152:LYS:NZ	2.29	0.48
47:t:75:ILE:HA	47:t:78:VAL:HG12	1.95	0.48
1:0:871:U:H2'	1:0:872:U:C6	2.49	0.48
1:0:1386:C:H2'	1:0:1387:A:C8	2.49	0.48
1:0:1482:G:H1'	1:0:1509:A:H61	1.77	0.48
1:0:1794:A:H2'	1:0:1795:C:C6	2.48	0.48
1:0:2051:A:H8	1:0:2051:A:OP2	1.97	0.48
1:0:2228:G:H2'	1:0:2229:U:C6	2.48	0.48
1:0:2834:G:H2'	1:0:2879:A:H61	1.79	0.48
6:C:23:PHE:CE1	12:I:1:MET:HE2	2.48	0.48
10:G:1:MET:HE1	17:N:93:LYS:HE2	1.96	0.48
22:S:31:TYR:O	22:S:92:VAL:HA	2.13	0.48
3:2:728:A:H2'	3:2:729:A:H8	1.76	0.48
7:D:128:TYR:HB3	7:D:156:ILE:HG23	1.96	0.48
12:I:74:THR:HG22	12:I:107:PHE:HB2	1.95	0.48
13:J:30:SER:HA	13:J:133:LYS:HE2	1.95	0.48
1:0:356:G:H2'	1:0:357:C:C6	2.49	0.48
1:0:2311:A:N3	7:D:85:ILE:HD11	2.28	0.48
1:0:2809:A:H2'	1:0:2810:A:H8	1.79	0.48
3:2:384:G:H2'	3:2:385:C:C6	2.49	0.48
3:2:458:U:H2'	3:2:459:A:C8	2.48	0.48
40:m:11:ARG:HB3	40:m:106:ARG:HH11	1.79	0.48
1:0:155:A:H2'	1:0:156:A:C8	2.49	0.47
1:0:2740:A:H2'	1:0:2741:A:C8	2.49	0.47
7:D:8:TYR:HB2	7:D:173:PHE:HZ	1.79	0.47
1:0:2286:G:H4'	1:0:2287:A:O4'	2.14	0.47
1:0:2700:A:H2'	1:0:2701:U:C6	2.48	0.47
7:D:5:HIS:CE1	7:D:9:LYS:HZ1	2.32	0.47
8:E:105:LEU:HB2	8:E:113:VAL:HB	1.97	0.47
14:K:79:LEU:HD23	14:K:83:LEU:HD12	1.96	0.47
33:f:213:TYR:O	33:f:217:VAL:HG23	2.14	0.47
34:g:124:LEU:HD13	34:g:196:ILE:HG21	1.96	0.47
1:0:832:U:H2'	1:0:833:A:C8	2.50	0.47
1:0:1539:U:H2'	1:0:1540:G:H8	1.79	0.47
5:B:156:PHE:CE1	10:G:81:ILE:HD13	2.50	0.47
6:C:111:GLU:HB3	12:I:1:MET:HE3	1.94	0.47
1:0:2030:A:C2	1:0:2499:C:H5"	2.49	0.47
3:2:131:A:H2'	3:2:132:C:C6	2.50	0.47
3:2:1233:G:H5'	40:m:119:ARG:HH12	1.79	0.47
5:B:108:ASP:OD1	5:B:173:GLN:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:30:LEU:HD12	38:k:30:LEU:O	2.14	0.47
41:n:22:THR:O	41:n:26:VAL:HG23	2.14	0.47
1:0:1589:U:H2'	1:0:1590:A:H8	1.79	0.47
3:2:1491:G:H2'	3:2:1492:A:C8	2.50	0.47
20:Q:24:MET:O	20:Q:24:MET:HE3	2.13	0.47
28:a:38:HIS:HB3	28:a:44:THR:HG22	1.96	0.47
33:f:114:LEU:HB2	33:f:144:LEU:CD2	2.39	0.47
39:l:31:LYS:HB2	39:l:31:LYS:HE3	1.59	0.47
1:0:668:A:H2'	1:0:670:A:H62	1.80	0.47
1:0:1196:C:H2'	1:0:1197:G:H8	1.79	0.47
1:0:1746:A:H2'	1:0:1747:U:H6	1.78	0.47
3:2:864:A:H2'	3:2:865:A:C8	2.50	0.47
7:D:104:ILE:HD11	7:D:176:PRO:HD3	1.96	0.47
34:g:67:THR:HB	34:g:102:ASN:HB2	1.97	0.47
41:n:8:ILE:HB	41:n:74:VAL:HG23	1.96	0.47
2:1:66:A:N6	2:1:107:G:H2'	2.30	0.47
3:2:1330:U:H2'	3:2:1331:G:O4'	2.15	0.47
8:E:120:GLY:C	8:E:121:ILE:HD12	2.40	0.47
18:O:21:ARG:HD2	18:O:93:PHE:CG	2.49	0.47
1:0:851:C:H2'	1:0:852:U:C6	2.50	0.47
1:0:1047:G:N2	1:0:1111:A:N6	2.63	0.47
3:2:8:A:N7	35:h:206:LYS:HA	2.30	0.47
21:R:18:ASP:OD1	21:R:21:LYS:HD2	2.14	0.47
23:T:41:ARG:HA	23:T:41:ARG:HD3	1.61	0.47
36:i:115:LEU:HD13	36:i:123:VAL:HG11	1.96	0.47
1:0:45:G:H5'	1:0:46:G:OP1	2.14	0.47
1:0:414:C:H2'	1:0:415:A:H8	1.80	0.47
1:0:2064:C:H2'	1:0:2065:C:H6	1.80	0.47
3:2:1162:C:H2'	3:2:1163:A:C8	2.49	0.47
40:m:11:ARG:HB3	40:m:106:ARG:NH1	2.29	0.47
1:0:2230:G:H2'	1:0:2231:U:C6	2.51	0.46
2:1:106:G:H2'	2:1:107:G:O4'	2.15	0.46
9:F:35:LYS:HE3	9:F:35:LYS:HB2	1.76	0.46
20:Q:1:MET:HB3	20:Q:1:MET:HE3	1.76	0.46
1:0:413:C:H2'	1:0:414:C:H6	1.80	0.46
1:0:577:G:H2'	1:0:578:G:C8	2.51	0.46
4:A:5:LYS:HD2	4:A:17:VAL:HG22	1.97	0.46
37:j:9:MET:SD	37:j:86:ARG:HB3	2.56	0.46
41:n:53:ILE:HG21	41:n:63:ASP:OD1	2.15	0.46
1:0:645:C:O2'	1:0:646:U:H5"	2.16	0.46
1:0:1572:A:H2'	1:0:1573:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2266:A:H4'	1:0:2267:A:N3	2.30	0.46
3:2:1062:U:H2'	3:2:1063:C:C6	2.51	0.46
5:B:116:LYS:HA	14:K:1:MET:HE3	1.96	0.46
6:C:146:VAL:HG12	6:C:185:LYS:HB2	1.98	0.46
1:0:30:G:H2'	1:0:31:C:H6	1.81	0.46
1:0:1386:C:H2'	1:0:1387:A:H8	1.79	0.46
1:0:2494:G:C2	1:0:2495:G:C8	3.03	0.46
3:2:1338:G:H2'	3:2:1339:A:C8	2.50	0.46
15:L:56:LYS:HD3	15:L:57:ALA:H	1.80	0.46
33:f:6:MET:HE3	33:f:6:MET:C	2.39	0.46
1:0:12:U:H2'	1:0:12:U:O2	2.15	0.46
1:0:2025:C:H2'	1:0:2026:U:C6	2.50	0.46
1:0:2567:G:H2'	1:0:2568:U:C6	2.51	0.46
3:2:1149:C:H2'	3:2:1150:A:C8	2.50	0.46
21:R:33:LYS:HE2	21:R:66:GLN:NE2	2.31	0.46
1:0:930:G:H1'	26:W:25:LEU:HD11	1.97	0.46
1:0:1321:A:C4	1:0:1322:A:C8	3.03	0.46
36:i:37:THR:HG21	36:i:64:MET:HE2	1.98	0.46
1:0:150:U:H2'	1:0:151:C:C6	2.51	0.46
3:2:1201:A:H4'	3:2:1202:U:H5'	1.96	0.46
33:f:66:LYS:HE3	33:f:154:MET:HG2	1.98	0.46
33:f:68:LEU:HB3	33:f:161:LEU:HD12	1.98	0.46
1:0:580:U:H2'	1:0:581:C:C6	2.51	0.46
3:2:1492:A:H2'	3:2:1493:A:H8	1.80	0.46
5:B:8:LYS:HB2	5:B:201:LEU:HD11	1.98	0.46
34:g:85:GLU:O	34:g:89:LYS:HG3	2.16	0.46
36:i:81:LEU:HG	36:i:147:MET:SD	2.56	0.46
38:k:37:SER:HA	38:k:40:GLU:HG2	1.98	0.46
41:n:10:LEU:HD11	41:n:25:ILE:HD12	1.97	0.46
42:o:52:PHE:O	42:o:53:ARG:HD2	2.16	0.46
1:0:1295:C:C2	1:0:1296:G:C8	3.04	0.46
3:2:1144:G:N2	3:2:1146:A:H62	2.13	0.46
12:I:132:ARG:HG3	12:I:142:ILE:HD11	1.98	0.46
38:k:71:PRO:HG3	38:k:103:TRP:CZ3	2.51	0.46
38:k:146:GLU:HA	38:k:146:GLU:OE1	2.15	0.46
48:u:15:ASP:OD2	48:u:54:GLY:HA2	2.16	0.46
51:x:57:ILE:O	51:x:61:GLN:HG2	2.16	0.46
1:0:1138:G:N2	10:G:108:MET:HE2	2.31	0.46
45:r:9:ARG:O	45:r:13:ARG:HG3	2.15	0.46
47:t:4:ILE:HG12	47:t:21:VAL:HG22	1.98	0.46
1:0:1353:A:H2'	1:0:1354:A:H8	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1469:A:H2'	1:0:1470:A:H8	1.79	0.45
3:2:696:A:H2'	3:2:697:U:H6	1.81	0.45
3:2:792:A:H4'	3:2:793:U:O5'	2.16	0.45
3:2:1492:A:H2'	3:2:1493:A:O4'	2.15	0.45
6:C:130:LYS:HD2	6:C:130:LYS:HA	1.75	0.45
38:k:24:ALA:O	38:k:27:VAL:HG12	2.17	0.45
40:m:34:SER:OG	40:m:37:GLN:HG3	2.16	0.45
51:x:79:LEU:O	51:x:83:ILE:HG12	2.16	0.45
1:0:1794:A:H2'	1:0:1795:C:H6	1.81	0.45
1:0:2064:C:H2'	1:0:2065:C:C6	2.51	0.45
1:0:2345:G:N3	1:0:2381:A:H2'	2.32	0.45
3:2:393:A:C2	3:2:394:G:C8	3.04	0.45
7:D:17:MET:HE1	7:D:22:TYR:O	2.16	0.45
7:D:115:ARG:HD3	7:D:115:ARG:N	2.31	0.45
35:h:19:LEU:HD22	35:h:64:ILE:HG13	1.98	0.45
52:y:11:PRO:HB2	52:y:14:VAL:HG23	1.99	0.45
1:0:30:G:H2'	1:0:31:C:C6	2.51	0.45
3:2:1295:U:H2'	3:2:1296:C:C6	2.51	0.45
14:K:1:MET:HE2	14:K:3:HIS:CE1	2.52	0.45
38:k:71:PRO:HG3	38:k:103:TRP:HZ3	1.81	0.45
42:o:83:GLU:HG2	42:o:109:ASN:HB2	1.97	0.45
1:0:554:U:H2'	1:0:555:G:O4'	2.17	0.45
1:0:2194:U:H2'	1:0:2195:U:C6	2.50	0.45
1:0:2547:A:H2'	1:0:2548:U:C6	2.51	0.45
3:2:992:U:H4'	3:2:993:G:O5'	2.16	0.45
10:G:102:GLU:HG2	10:G:119:PHE:CZ	2.49	0.45
1:0:582:A:H2'	1:0:583:G:H8	1.80	0.45
1:0:1196:C:H2'	1:0:1197:G:C8	2.51	0.45
23:T:43:THR:O	23:T:43:THR:HG23	2.17	0.45
36:i:88:VAL:HG22	36:i:93:ARG:HG2	1.98	0.45
40:m:119:ARG:H	40:m:119:ARG:HG2	1.60	0.45
1:0:1441:G:H2'	1:0:1442:U:C6	2.52	0.45
3:2:978:A:C4	3:2:1319:A:C2	3.03	0.45
17:N:83:LEU:HD22	17:N:88:VAL:HG21	1.97	0.45
33:f:113:ARG:HA	33:f:116:ASP:OD2	2.16	0.45
33:f:117:LEU:HB3	33:f:141:LEU:HD12	1.99	0.45
1:0:2813:A:H2'	1:0:2814:A:C8	2.52	0.45
3:2:89:U:H4'	3:2:90:C:O5'	2.15	0.45
27:X:11:GLU:OE2	27:X:23:LYS:HB3	2.16	0.45
48:u:47:HIS:HB2	48:u:71:LYS:HE3	1.99	0.45
1:0:17:G:H2'	1:0:18:U:H6	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:29:PRO:HB2	7:D:169:LEU:HD12	1.99	0.45
19:P:45:VAL:O	19:P:49:LYS:HG3	2.17	0.45
35:h:23:SER:HB2	35:h:161:LEU:HD21	1.99	0.45
1:0:721:A:H2'	1:0:722:A:H8	1.82	0.45
1:0:851:C:H2'	1:0:852:U:H6	1.81	0.45
1:0:1047:G:N2	1:0:1111:A:C5	2.85	0.45
1:0:1442:U:H2'	1:0:1443:U:C6	2.52	0.45
3:2:204:G:C4	3:2:205:A:C8	3.04	0.45
3:2:555:U:H2'	3:2:556:C:C6	2.52	0.45
35:h:27:ALA:HB3	35:h:30:THR:HG23	1.97	0.45
1:0:64:A:H2'	1:0:65:U:H6	1.81	0.45
1:0:507:A:H5"	1:0:508:A:H3'	1.99	0.45
1:0:1869:G:H21	1:0:1872:A:H2	1.65	0.45
12:I:19:LEU:HD12	12:I:27:LEU:HD13	1.99	0.45
17:N:48:ARG:HE	17:N:48:ARG:HB3	1.58	0.45
33:f:116:ASP:HA	33:f:119:THR:HG22	2.00	0.45
33:f:117:LEU:O	33:f:120:GLN:HG3	2.17	0.45
1:0:2086:U:H2'	1:0:2087:G:C8	2.52	0.44
1:0:2674:G:H4'	11:H:30:ARG:HD2	1.98	0.44
1:0:2795:C:H2'	1:0:2796:U:C6	2.52	0.44
5:B:5:VAL:H	5:B:32:ASN:HD21	1.65	0.44
9:F:30:LEU:HB3	9:F:36:ALA:HB3	1.99	0.44
38:k:72:THR:HG22	38:k:142:HIS:CE1	2.51	0.44
40:m:118:LEU:HD22	40:m:124:ARG:HB3	1.99	0.44
1:0:2191:A:H2'	1:0:2192:U:C6	2.52	0.44
3:2:868:C:H2'	3:2:869:G:O4'	2.17	0.44
3:2:1144:G:H21	3:2:1146:A:H62	1.65	0.44
3:2:1513:A:H2'	3:2:1514:G:C8	2.53	0.44
50:w:43:ASN:OD1	50:w:43:ASN:C	2.60	0.44
1:0:17:G:H2'	1:0:18:U:C6	2.51	0.44
1:0:1433:A:O2'	1:0:1434:A:H5'	2.16	0.44
1:0:1570:A:H2'	1:0:1571:A:C8	2.52	0.44
1:0:2329:U:H2'	1:0:2330:G:C8	2.52	0.44
2:1:48:U:H2'	2:1:49:C:C6	2.52	0.44
1:0:18:U:H2'	1:0:19:A:H8	1.82	0.44
1:0:2074:U:H2'	1:0:2075:U:C6	2.52	0.44
38:k:27:VAL:HG21	38:k:40:GLU:OE1	2.18	0.44
44:q:23:TYR:CE1	44:q:69:LEU:HD12	2.50	0.44
1:0:146:A:H2'	1:0:147:C:C6	2.53	0.44
1:0:543:G:H2'	1:0:544:C:H6	1.82	0.44
1:0:634:C:H2'	1:0:635:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2047:C:H2'	1:0:2048:G:H8	1.82	0.44
34:g:11:ARG:HA	34:g:14:ILE:HD12	2.00	0.44
38:k:24:ALA:HA	38:k:27:VAL:HG12	1.99	0.44
38:k:90:GLU:H	38:k:90:GLU:CD	2.25	0.44
3:2:161:A:H2'	3:2:162:A:C8	2.53	0.44
6:C:139:LYS:HB2	6:C:139:LYS:HE3	1.67	0.44
7:D:5:HIS:CE1	7:D:9:LYS:NZ	2.85	0.44
34:g:156:ARG:HD3	34:g:193:TYR:HB3	2.00	0.44
36:i:162:GLU:HG2	36:i:163:GLU:OE1	2.17	0.44
3:2:553:A:H2'	3:2:554:A:C8	2.51	0.44
1:0:973:A:H5"	18:O:81:LYS:HD2	1.99	0.44
1:0:2485:G:O3'	13:J:125:PRO:HB3	2.17	0.44
3:2:722:G:H2'	3:2:722:G:N3	2.32	0.44
4:A:183:LYS:HB2	4:A:183:LYS:NZ	2.33	0.44
25:V:6:LEU:HD23	25:V:9:LYS:NZ	2.32	0.44
52:y:40:LYS:HE3	52:y:40:LYS:HB3	1.62	0.44
1:0:52:A:H2'	1:0:53:A:C8	2.52	0.44
1:0:623:C:H2'	1:0:624:C:H6	1.82	0.44
1:0:2050:C:H2'	1:0:2051:A:C8	2.53	0.44
1:0:2783:U:H2'	1:0:2784:U:H6	1.83	0.44
3:2:676:A:H2'	3:2:677:U:H6	1.82	0.44
41:n:8:ILE:HD11	41:n:87:LEU:HD21	2.00	0.44
1:0:638:G:H2'	1:0:639:U:C6	2.52	0.43
1:0:2241:A:H2'	1:0:2242:G:H8	1.83	0.43
1:0:2328:A:H2'	1:0:2329:U:C6	2.52	0.43
1:0:2649:C:H2'	1:0:2650:U:C6	2.53	0.43
3:2:1435:G:H2'	3:2:1436:U:C6	2.53	0.43
29:b:35:GLU:HG2	29:b:50:LYS:HG3	1.99	0.43
1:0:833:A:H2'	1:0:834:G:C8	2.53	0.43
1:0:909:A:H2'	1:0:912:C:H5	1.82	0.43
1:0:2394:C:H5"	12:I:63:LYS:HE2	2.01	0.43
1:0:2899:A:H2'	1:0:2900:A:C8	2.53	0.43
3:2:1465:A:H2'	3:2:1466:C:C6	2.53	0.43
4:A:183:LYS:NZ	4:A:266:PHE:HA	2.33	0.43
40:m:35:LEU:CD1	40:m:48:VAL:HG11	2.47	0.43
45:r:28:LYS:HZ1	45:r:47:LYS:HG3	1.83	0.43
1:0:948:C:H2'	1:0:949:G:H8	1.83	0.43
1:0:1590:A:H2'	1:0:1591:A:H8	1.82	0.43
3:2:162:A:O5'	3:2:162:A:H8	2.01	0.43
15:L:88:LYS:HE3	15:L:116:GLN:HG3	1.99	0.43
48:u:58:VAL:HB	48:u:80:GLU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1360:G:N7	1:0:1361:G:C8	2.87	0.43
3:2:1003:G:C6	3:2:1034:G:N2	2.86	0.43
13:J:8:LYS:HG2	13:J:9:PHE:CD2	2.52	0.43
33:f:45:LYS:HG2	33:f:50:PHE:HB2	2.00	0.43
1:0:150:U:H2'	1:0:151:C:H6	1.84	0.43
1:0:788:A:H1'	30:c:4:THR:HG21	1.99	0.43
1:0:813:U:H2'	1:0:814:C:C6	2.53	0.43
1:0:969:G:H2'	1:0:970:U:C6	2.53	0.43
1:0:2788:C:H2'	1:0:2789:C:C6	2.54	0.43
3:2:936:C:C2	3:2:937:A:C8	3.06	0.43
1:0:52:A:H2'	1:0:53:A:H8	1.83	0.43
1:0:132:G:H2'	1:0:133:U:C6	2.54	0.43
1:0:1405:U:H2'	1:0:1406:U:H6	1.82	0.43
1:0:1831:G:H2'	1:0:1832:C:C6	2.54	0.43
1:0:2243:U:H2'	1:0:2244:U:H6	1.83	0.43
1:0:2307:G:H4'	1:0:2308:G:O5'	2.18	0.43
3:2:674:G:H2'	3:2:675:A:H8	1.84	0.43
4:A:181:MET:HE3	4:A:269:ARG:HH22	1.83	0.43
6:C:23:PHE:HE1	12:I:1:MET:HE2	1.84	0.43
43:p:79:VAL:O	43:p:103:ASP:HB3	2.18	0.43
3:2:147:G:H2'	3:2:148:G:H8	1.81	0.43
3:2:501:C:H2'	3:2:502:A:C8	2.53	0.43
3:2:501:C:H2'	3:2:502:A:H8	1.83	0.43
3:2:704:A:C4	3:2:705:G:C8	3.07	0.43
3:2:1288:A:H2'	3:2:1289:A:C8	2.54	0.43
7:D:77:PHE:HB2	7:D:79:ILE:HG12	2.00	0.43
8:E:35:ARG:HD3	8:E:71:LEU:HD23	2.01	0.43
25:V:44:LYS:O	25:V:48:ARG:HG2	2.19	0.43
31:d:49:MET:HE3	31:d:49:MET:HB3	1.82	0.43
33:f:64:LYS:HG3	33:f:64:LYS:O	2.19	0.43
3:2:212:G:C4	3:2:213:G:C8	3.07	0.43
13:J:28:PHE:HB2	13:J:104:GLU:OE2	2.18	0.43
40:m:54:LEU:HD23	40:m:98:LEU:HD23	2.00	0.43
1:0:1047:G:N2	1:0:1111:A:C6	2.85	0.43
1:0:1213:A:H2'	1:0:1214:A:C8	2.54	0.43
3:2:824:G:H2'	3:2:825:A:H8	1.84	0.43
3:2:1131:G:H2'	3:2:1131:G:N3	2.34	0.43
9:F:130:VAL:HG23	9:F:132:PHE:HE1	1.84	0.43
34:g:62:LYS:HA	34:g:62:LYS:HD3	1.86	0.43
35:h:122:ALA:HA	35:h:146:ARG:HD3	2.00	0.43
38:k:47:LEU:HD23	38:k:47:LEU:HA	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:s:8:THR:O	46:s:12:VAL:HG23	2.19	0.43
51:x:79:LEU:HD23	51:x:79:LEU:HA	1.88	0.43
1:0:2700:A:H2'	1:0:2701:U:H6	1.84	0.43
3:2:235:C:H2'	3:2:236:A:H8	1.84	0.43
3:2:1072:G:H2'	3:2:1073:U:C6	2.54	0.43
3:2:1157:A:C2	3:2:1181:G:C4	3.07	0.43
30:c:24:THR:HG23	30:c:27:GLY:H	1.84	0.43
35:h:8:LYS:HG3	35:h:21:LEU:HD13	2.01	0.43
35:h:124:MET:HE3	35:h:124:MET:HB2	1.92	0.43
38:k:143:ARG:NH1	38:k:146:GLU:HB3	2.34	0.43
40:m:35:LEU:HD11	40:m:48:VAL:HG11	2.01	0.43
1:0:39:G:H2'	1:0:40:U:C6	2.53	0.42
1:0:2386:A:H2'	1:0:2387:U:C6	2.53	0.42
3:2:178:C:N3	3:2:179:A:C2	2.87	0.42
3:2:246:A:C2	3:2:282:A:C5	3.07	0.42
3:2:792:A:H1'	3:2:793:U:OP2	2.19	0.42
3:2:1314:C:H2'	3:2:1315:U:H6	1.82	0.42
6:C:130:LYS:HB2	6:C:133:LEU:HD12	2.00	0.42
26:W:8:THR:HA	26:W:34:HIS:O	2.19	0.42
38:k:16:PRO:HB3	40:m:42:GLU:HB3	2.01	0.42
44:q:65:VAL:HG13	44:q:66:GLU:N	2.34	0.42
45:r:5:SER:O	45:r:9:ARG:HG3	2.19	0.42
1:0:510:C:C2	1:0:511:U:C6	3.07	0.42
1:0:623:C:H2'	1:0:624:C:C6	2.54	0.42
1:0:2037:A:H2'	1:0:2038:G:C8	2.54	0.42
1:0:2514:U:H2'	1:0:2515:C:C6	2.54	0.42
1:0:2812:G:H2'	1:0:2813:A:H8	1.82	0.42
34:g:56:VAL:HG23	34:g:67:THR:HG23	2.00	0.42
1:0:18:U:H2'	1:0:19:A:C8	2.54	0.42
1:0:2650:U:H2'	1:0:2651:C:H6	1.84	0.42
1:0:2804:U:H2'	1:0:2805:C:H6	1.84	0.42
32:e:9:LYS:NZ	32:e:16:ILE:HD12	2.34	0.42
38:k:113:ASP:HB3	38:k:118:LEU:HD22	2.01	0.42
40:m:65:ILE:HG23	40:m:79:ILE:HD11	1.99	0.42
41:n:37:ARG:NH2	41:n:77:VAL:HG22	2.34	0.42
1:0:155:A:H2'	1:0:156:A:H8	1.83	0.42
3:2:1071:C:H2'	3:2:1072:G:C8	2.48	0.42
3:2:1396:A:H4'	3:2:1397:C:H5"	2.02	0.42
35:h:125:VAL:HA	35:h:142:VAL:O	2.20	0.42
40:m:43:THR:O	40:m:46:MET:HG2	2.20	0.42
3:2:459:A:H2'	3:2:460:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:13:VAL:HG13	7:D:28:VAL:HG21	2.02	0.42
34:g:27:LYS:HB3	34:g:28:GLU:OE1	2.19	0.42
44:q:33:ILE:HG23	44:q:59:GLU:HG2	2.00	0.42
45:r:20:TYR:CE2	45:r:51:LEU:HD22	2.54	0.42
1:0:597:G:H2'	1:0:598:U:C6	2.54	0.42
1:0:2502:G:H5'	1:0:2503:A:C5'	2.50	0.42
1:0:2687:U:H2'	1:0:2688:G:O4'	2.19	0.42
19:P:70:LYS:HB2	19:P:70:LYS:HE2	1.85	0.42
1:0:357:C:H2'	1:0:358:U:C6	2.55	0.42
3:2:299:G:H2'	3:2:300:A:C8	2.54	0.42
10:G:106:LYS:HE3	10:G:106:LYS:HB2	1.90	0.42
12:I:121:THR:HA	12:I:141:LYS:O	2.19	0.42
35:h:110:THR:O	35:h:113:GLU:HB2	2.20	0.42
38:k:36:LYS:HG3	38:k:40:GLU:OE2	2.20	0.42
1:0:634:C:H2'	1:0:635:C:H6	1.84	0.42
1:0:1159:U:C2	1:0:1160:G:C8	3.07	0.42
1:0:2028:U:H2'	1:0:2029:G:C8	2.54	0.42
3:2:918:A:H2'	3:2:919:A:C8	2.55	0.42
3:2:925:G:C2	3:2:927:G:C8	3.08	0.42
6:C:149:ILE:HB	6:C:188:MET:HG2	2.01	0.42
38:k:143:ARG:HD2	38:k:143:ARG:HA	1.84	0.42
43:p:30:LYS:HB3	43:p:57:LEU:HD12	2.00	0.42
46:s:64:ARG:HH11	46:s:89:ARG:NH1	2.18	0.42
1:0:709:U:H2'	1:0:710:U:C6	2.55	0.42
1:0:1913:A:N6	3:2:1493:A:H1'	2.35	0.42
8:E:12:PRO:HD2	8:E:15:VAL:HG21	2.02	0.42
1:0:753:A:H2'	1:0:754:U:H6	1.84	0.42
1:0:755:U:H2'	1:0:756:A:C8	2.55	0.42
1:0:1747:U:H2'	1:0:1748:C:C6	2.55	0.42
3:2:270:A:H2'	3:2:271:C:C6	2.55	0.42
3:2:747:A:H2'	3:2:748:G:O4'	2.20	0.42
3:2:1522:U:H5"	42:o:128:ARG:HH22	1.84	0.42
7:D:69:LYS:HE3	7:D:69:LYS:HB2	1.77	0.42
12:I:55:MET:HA	12:I:56:PRO:HD3	1.91	0.42
16:M:24:ASP:HB2	16:M:88:ARG:O	2.19	0.42
19:P:46:LEU:O	19:P:50:VAL:HG23	2.20	0.42
1:0:1327:A:H2'	1:0:1328:A:O4'	2.20	0.41
1:0:2460:U:C2	1:0:2461:A:C8	3.09	0.41
1:0:2846:G:H2'	1:0:2847:U:C6	2.55	0.41
3:2:437:U:H5"	35:h:152:GLN:OE1	2.20	0.41
3:2:1455:G:H2'	3:2:1456:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:108:ILE:HA	12:I:1:MET:HE1	2.02	0.41
17:N:52:GLN:HA	17:N:55:ARG:HD3	2.01	0.41
50:w:80:TYR:CD1	50:w:81:ARG:HG2	2.55	0.41
1:0:265:A:H4'	1:0:266:G:OP1	2.21	0.41
3:2:1024:G:H4'	3:2:1025:U:O5'	2.20	0.41
13:J:57:VAL:HG11	13:J:105:MET:CE	2.41	0.41
1:0:1281:G:H2'	1:0:1282:U:C6	2.55	0.41
1:0:1640:A:H2'	1:0:1641:A:H8	1.85	0.41
31:d:15:LYS:HD3	31:d:15:LYS:HA	1.93	0.41
33:f:157:LEU:HD23	33:f:157:LEU:HA	1.90	0.41
50:w:70:LYS:O	50:w:73:GLU:HG3	2.20	0.41
1:0:306:U:H2'	1:0:307:G:O4'	2.21	0.41
1:0:582:A:H2'	1:0:583:G:C8	2.56	0.41
1:0:2849:U:H4'	1:0:2868:A:C2	2.55	0.41
3:2:1513:A:H2'	3:2:1514:G:H8	1.85	0.41
10:G:115:GLY:HA2	10:G:118:MET:HE3	2.01	0.41
3:2:1410:A:H2'	3:2:1411:C:C6	2.55	0.41
5:B:4:LEU:HD23	5:B:4:LEU:HA	1.94	0.41
13:J:75:GLU:HB2	13:J:90:GLU:HG3	2.02	0.41
29:b:8:LYS:HG3	29:b:24:THR:HG22	2.02	0.41
41:n:46:LYS:HB2	41:n:46:LYS:HE3	1.64	0.41
3:2:678:U:H2'	3:2:679:C:H6	1.86	0.41
7:D:113:ASP:OD1	7:D:115:ARG:HD2	2.21	0.41
9:F:51:ARG:HG2	9:F:54:LEU:HD23	2.02	0.41
16:M:114:LEU:HD23	16:M:114:LEU:HA	1.87	0.41
17:N:15:LYS:HB3	17:N:15:LYS:HE2	1.71	0.41
26:W:23:THR:HG23	26:W:47:MET:HG2	2.02	0.41
35:h:161:LEU:HD12	35:h:161:LEU:O	2.20	0.41
46:s:82:ILE:HD13	46:s:82:ILE:HA	1.86	0.41
46:s:88:ARG:HA	46:s:88:ARG:NE	2.35	0.41
1:0:2:G:H2'	1:0:3:U:C6	2.55	0.41
1:0:84:A:H4'	1:0:85:G:O5'	2.21	0.41
1:0:1591:A:H2'	1:0:1592:C:C6	2.55	0.41
1:0:1656:C:H2'	1:0:1657:U:H6	1.85	0.41
1:0:1682:G:H2'	1:0:1683:U:C6	2.56	0.41
3:2:859:G:H2'	3:2:860:A:C8	2.56	0.41
3:2:1491:G:H3'	3:2:1492:A:H8	1.83	0.41
7:D:63:GLN:HB2	27:X:6:HIS:CE1	2.56	0.41
33:f:42:ASN:O	33:f:43:LEU:HB2	2.21	0.41
34:g:35:SER:HB3	34:g:59:ARG:HH22	1.86	0.41
35:h:178:MET:O	35:h:178:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1357:C:H2'	1:0:1358:G:O4'	2.20	0.41
1:0:1563:U:H2'	1:0:1564:C:C6	2.56	0.41
1:0:2636:C:H2'	1:0:2637:U:C6	2.55	0.41
2:1:49:C:H2'	2:1:50:A:C8	2.56	0.41
3:2:841:C:H3'	3:2:842:U:H4'	2.01	0.41
8:E:18:LYS:HB3	8:E:18:LYS:HE2	1.69	0.41
34:g:7:PRO:O	34:g:11:ARG:HG3	2.20	0.41
45:r:26:GLU:HA	45:r:29:ALA:HB3	2.03	0.41
1:0:640:C:H2'	1:0:641:U:H6	1.86	0.41
1:0:875:G:H2'	1:0:876:C:C6	2.56	0.41
1:0:971:G:H2'	1:0:972:A:O4'	2.20	0.41
1:0:2012:G:OP1	19:P:98:LYS:HD2	2.20	0.41
2:1:30:C:H2'	2:1:31:C:H5'	2.02	0.41
3:2:902:G:H2'	3:2:903:G:H8	1.86	0.41
3:2:1134:G:H2'	3:2:1135:U:O4'	2.20	0.41
8:E:90:VAL:HG12	8:E:160:LYS:HA	2.03	0.41
12:I:111:ILE:HG22	12:I:128:THR:HG21	2.02	0.41
28:a:39:LEU:HD23	28:a:39:LEU:HA	1.88	0.41
33:f:207:ILE:HD13	33:f:207:ILE:HA	1.88	0.41
35:h:149:ALA:O	35:h:152:GLN:HG3	2.20	0.41
42:o:23:ILE:HG12	42:o:96:THR:HG21	2.03	0.41
42:o:72:ASP:OD1	42:o:72:ASP:O	2.37	0.41
1:0:15:G:H4'	28:a:18:SER:HB3	2.02	0.41
3:2:1240:U:O4	38:k:116:MET:HE2	2.21	0.41
16:M:11:GLU:H	16:M:11:GLU:HG2	1.66	0.41
36:i:151:GLU:OE2	36:i:161:VAL:HG21	2.21	0.41
1:0:2290:G:H2'	1:0:2291:U:C6	2.56	0.40
3:2:182:A:O2'	3:2:183:C:H5'	2.21	0.40
4:A:232:HIS:NE2	4:A:244:PRO:HA	2.36	0.40
8:E:155:GLU:H	8:E:155:GLU:HG3	1.72	0.40
15:L:83:LEU:HD23	15:L:83:LEU:HA	1.91	0.40
34:g:22:TRP:HB3	34:g:59:ARG:HB2	2.03	0.40
43:p:50:ARG:HD2	43:p:90:LEU:HD11	2.02	0.40
1:0:156:A:H2'	1:0:157:C:C6	2.57	0.40
1:0:303:G:H2'	1:0:304:U:C6	2.56	0.40
1:0:723:C:H2'	1:0:724:U:O4'	2.21	0.40
1:0:1319:C:O2'	1:0:1320:C:H5'	2.22	0.40
3:2:171:A:H2'	3:2:172:A:C8	2.57	0.40
3:2:193:C:H2'	3:2:194:C:C6	2.57	0.40
3:2:459:A:H2'	3:2:460:A:C8	2.56	0.40
3:2:712:A:H2'	3:2:713:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:985:C:H2'	3:2:986:U:C6	2.56	0.40
3:2:1035:A:H2'	3:2:1035:A:N3	2.35	0.40
3:2:1219:A:H2'	3:2:1220:G:C8	2.56	0.40
4:A:225:MET:CE	4:A:230:HIS:HB2	2.51	0.40
7:D:114:PHE:C	7:D:115:ARG:HD3	2.47	0.40
16:M:24:ASP:OD1	16:M:24:ASP:C	2.64	0.40
27:X:14:ALA:HA	27:X:32:LEU:O	2.22	0.40
44:q:5:ALA:C	44:q:7:ILE:H	2.30	0.40
45:r:19:LYS:HG2	45:r:20:TYR:CE1	2.56	0.40
1:0:1666:G:O3'	11:H:6:THR:HG23	2.21	0.40
1:0:1680:U:H2'	1:0:1681:G:O4'	2.21	0.40
1:0:2329:U:H2'	1:0:2330:G:H8	1.86	0.40
1:0:2804:U:H2'	1:0:2805:C:C6	2.56	0.40
3:2:982:U:H4'	3:2:983:A:O5'	2.21	0.40
33:f:27:MET:HE2	33:f:188:ASP:O	2.21	0.40
41:n:87:LEU:HD12	41:n:87:LEU:HA	1.90	0.40
1:0:755:U:H2'	1:0:756:A:H8	1.85	0.40
1:0:1048:A:H1'	1:0:1112:G:N2	2.35	0.40
1:0:2008:C:H2'	1:0:2009:A:H8	1.87	0.40
1:0:2057:G:H2'	1:0:2058:A:H8	1.87	0.40
1:0:2093:G:H5'	9:F:22:LYS:HD2	2.03	0.40
2:1:3:C:H2'	2:1:4:C:C6	2.57	0.40
3:2:1424:U:H2'	3:2:1425:U:C6	2.57	0.40
13:J:136:MET:HE2	13:J:136:MET:HB3	2.00	0.40
39:l:42:GLU:HA	39:l:42:GLU:OE1	2.21	0.40
1:0:644:A:H2'	1:0:645:C:O4'	2.22	0.40
1:0:1395:A:O2'	1:0:1396:U:H5"	2.20	0.40
1:0:2292:U:H2'	1:0:2293:G:C8	2.56	0.40
3:2:613:C:H2'	3:2:614:C:C6	2.56	0.40
3:2:620:C:H2'	3:2:621:A:C8	2.56	0.40
3:2:859:G:H2'	3:2:860:A:H8	1.84	0.40
3:2:883:C:O2'	3:2:884:U:H5'	2.21	0.40
3:2:1231:G:H2'	3:2:1232:U:C6	2.55	0.40

There are no symmetry-related clashes.

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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	
4	A	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
5	B	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
6	C	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
7	D	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
8	E	171/177 (97%)	165 (96%)	6 (4%)	0	100	100
9	F	147/149 (99%)	141 (96%)	6 (4%)	0	100	100
10	G	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
11	H	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
12	I	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
13	J	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
14	K	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
15	L	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
16	M	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
17	N	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
18	O	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
19	P	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
20	Q	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
21	R	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
22	S	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
23	T	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
24	U	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
25	V	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
26	W	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
27	X	56/70 (80%)	51 (91%)	5 (9%)	0	100	100
28	a	53/57 (93%)	53 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	b	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
30	c	44/46 (96%)	44 (100%)	0	0	100	100
31	d	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
32	e	36/38 (95%)	36 (100%)	0	0	100	100
33	f	222/241 (92%)	207 (93%)	15 (7%)	0	100	100
34	g	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
35	h	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
36	i	153/167 (92%)	146 (95%)	7 (5%)	0	100	100
37	j	104/131 (79%)	103 (99%)	1 (1%)	0	100	100
38	k	149/179 (83%)	141 (95%)	8 (5%)	0	100	100
39	l	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
40	m	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
41	n	97/103 (94%)	93 (96%)	4 (4%)	0	100	100
42	o	115/129 (89%)	110 (96%)	5 (4%)	0	100	100
43	p	121/124 (98%)	115 (95%)	6 (5%)	0	100	100
44	q	112/118 (95%)	103 (92%)	9 (8%)	0	100	100
45	r	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
46	s	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
47	t	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
48	u	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
49	v	64/75 (85%)	64 (100%)	0	0	100	100
50	w	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
51	x	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
52	y	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
All	All	5581/5909 (94%)	5399 (97%)	182 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	216/218 (99%)	214 (99%)	2 (1%)	70	77
5	B	164/164 (100%)	162 (99%)	2 (1%)	63	70
6	C	165/165 (100%)	162 (98%)	3 (2%)	51	58
7	D	148/150 (99%)	143 (97%)	5 (3%)	32	34
8	E	134/138 (97%)	132 (98%)	2 (2%)	57	64
9	F	114/114 (100%)	109 (96%)	5 (4%)	25	25
10	G	116/116 (100%)	115 (99%)	1 (1%)	70	77
11	H	104/104 (100%)	103 (99%)	1 (1%)	68	75
12	I	103/103 (100%)	101 (98%)	2 (2%)	50	56
13	J	109/109 (100%)	106 (97%)	3 (3%)	38	42
14	K	98/103 (95%)	96 (98%)	2 (2%)	48	54
15	L	86/87 (99%)	85 (99%)	1 (1%)	63	70
16	M	99/100 (99%)	97 (98%)	2 (2%)	48	54
17	N	89/90 (99%)	86 (97%)	3 (3%)	32	34
18	O	84/84 (100%)	82 (98%)	2 (2%)	43	47
19	P	93/93 (100%)	93 (100%)	0	100	100
20	Q	80/84 (95%)	78 (98%)	2 (2%)	42	46
21	R	83/85 (98%)	81 (98%)	2 (2%)	43	47
22	S	78/78 (100%)	77 (99%)	1 (1%)	61	68
23	T	57/63 (90%)	57 (100%)	0	100	100
24	U	67/68 (98%)	66 (98%)	1 (2%)	57	64
25	V	54/55 (98%)	54 (100%)	0	100	100
26	W	47/49 (96%)	46 (98%)	1 (2%)	47	52
27	X	55/62 (89%)	55 (100%)	0	100	100
28	a	46/48 (96%)	45 (98%)	1 (2%)	45	51
29	b	46/49 (94%)	46 (100%)	0	100	100
30	c	38/38 (100%)	37 (97%)	1 (3%)	40	45
31	d	51/52 (98%)	51 (100%)	0	100	100
32	e	34/34 (100%)	34 (100%)	0	100	100
33	f	186/199 (94%)	179 (96%)	7 (4%)	29	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	g	170/190 (90%)	168 (99%)	2 (1%)	63	70
35	h	172/173 (99%)	166 (96%)	6 (4%)	32	33
36	i	118/126 (94%)	113 (96%)	5 (4%)	26	26
37	j	92/112 (82%)	90 (98%)	2 (2%)	45	51
38	k	124/147 (84%)	122 (98%)	2 (2%)	55	62
39	l	104/105 (99%)	102 (98%)	2 (2%)	50	56
40	m	105/107 (98%)	101 (96%)	4 (4%)	29	30
41	n	87/90 (97%)	83 (95%)	4 (5%)	24	23
42	o	90/99 (91%)	89 (99%)	1 (1%)	65	73
43	p	103/104 (99%)	101 (98%)	2 (2%)	50	56
44	q	92/96 (96%)	89 (97%)	3 (3%)	33	35
45	r	83/84 (99%)	82 (99%)	1 (1%)	63	70
46	s	76/77 (99%)	75 (99%)	1 (1%)	61	68
47	t	65/65 (100%)	64 (98%)	1 (2%)	57	64
48	u	74/78 (95%)	71 (96%)	3 (4%)	27	27
49	v	57/65 (88%)	55 (96%)	2 (4%)	32	33
50	w	70/79 (89%)	69 (99%)	1 (1%)	59	66
51	x	65/66 (98%)	63 (97%)	2 (3%)	35	38
52	y	60/61 (98%)	60 (100%)	0	100	100
All	All	4651/4826 (96%)	4555 (98%)	96 (2%)	46	52

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	23	GLU
4	A	219	THR
5	B	62	LYS
5	B	207	VAL
6	C	46	GLN
6	C	74	LYS
6	C	164	LEU
7	D	79	ILE
7	D	83	TYR
7	D	89	VAL
7	D	92	ARG

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Mol	Chain	Res	Type
7	D	156	ILE
8	E	26	ILE
8	E	79	VAL
9	F	15	LEU
9	F	57	LYS
9	F	72	ILE
9	F	101	ASP
9	F	121	VAL
10	G	62	VAL
11	H	113	MET
12	I	78	ARG
12	I	122	VAL
13	J	10	ARG
13	J	22	GLN
13	J	118	LYS
14	K	15	SER
14	K	95	THR
15	L	100	HIS
16	M	7	GLN
16	M	12	GLN
17	N	31	VAL
17	N	55	ARG
17	N	85	LYS
18	O	20	VAL
18	O	49	ILE
20	Q	33	LYS
20	Q	63	VAL
21	R	43	LYS
21	R	83	VAL
22	S	34	LYS
24	U	60	ASP
26	W	8	THR
28	a	25	VAL
30	c	29	GLN
33	f	5	SER
33	f	78	GLU
33	f	85	LEU
33	f	105	LYS
33	f	108	ARG
33	f	116	ASP
33	f	151	ILE
34	g	67	THR

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Mol	Chain	Res	Type
34	g	126	ARG
35	h	15	GLU
35	h	77	LYS
35	h	150	LYS
35	h	167	LYS
35	h	183	LYS
35	h	185	LYS
36	i	11	LEU
36	i	22	SER
36	i	32	SER
36	i	72	ILE
36	i	117	VAL
37	j	92	THR
37	j	100	SER
38	k	29	ILE
38	k	126	ASP
39	l	55	THR
39	l	74	SER
40	m	22	LYS
40	m	48	VAL
40	m	73	SER
40	m	119	ARG
41	n	18	ILE
41	n	51	VAL
41	n	74	VAL
41	n	80	THR
42	o	30	THR
43	p	39	THR
43	p	121	ARG
44	q	22	ILE
44	q	76	SER
44	q	79	ARG
45	r	39	GLU
46	s	82	ILE
47	t	6	LEU
48	u	8	LEU
48	u	12	VAL
48	u	22	VAL
49	v	47	THR
49	v	67	LEU
50	w	14	HIS
51	x	4	ILE

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Mol	Chain	Res	Type
51	x	5	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	15	HIS
4	A	58	HIS
5	B	49	GLN
5	B	150	GLN
5	B	185	ASN
6	C	136	GLN
12	I	104	GLN
13	J	97	GLN
14	K	3	HIS
15	L	29	HIS
16	M	56	HIS
16	M	75	GLN
19	P	15	GLN
20	Q	91	GLN
21	R	46	GLN
25	V	15	ASN
28	a	38	HIS
30	c	26	ASN
31	d	24	HIS
33	f	122	GLN
34	g	6	HIS
34	g	185	ASN
35	h	126	ASN
35	h	136	GLN
35	h	164	GLN
36	i	121	HIS
36	i	132	ASN
38	k	68	ASN
38	k	130	ASN
42	o	22	HIS
42	o	118	HIS
43	p	112	GLN
51	x	3	ASN
51	x	61	GLN
51	x	82	GLN

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5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2754/2904 (94%)	318 (11%)	6 (0%)
2	1	119/120 (99%)	14 (11%)	0
3	2	1533/1542 (99%)	240 (15%)	31 (2%)
All	All	4406/4566 (96%)	572 (12%)	37 (0%)

All (572) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	10	A
1	0	13	A
1	0	34	U
1	0	46	G
1	0	63	A
1	0	71	A
1	0	74	A
1	0	75	G
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	120	U
1	0	139	U
1	0	140	C
1	0	141	G
1	0	163	C
1	0	181	A
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	280	U
1	0	281	C
1	0	282	A

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Mol	Chain	Res	Type
1	0	285	G
1	0	302	C
1	0	311	A
1	0	323	C
1	0	329	G
1	0	330	A
1	0	361	G
1	0	362	A
1	0	372	G
1	0	386	G
1	0	396	G
1	0	404	A
1	0	405	U
1	0	411	G
1	0	424	G
1	0	467	G
1	0	481	G
1	0	490	C
1	0	491	G
1	0	494	G
1	0	505	A
1	0	508	A
1	0	509	C
1	0	530	G
1	0	532	A
1	0	538	A
1	0	547	A
1	0	548	G
1	0	563	A
1	0	573	U
1	0	575	A
1	0	586	A
1	0	603	A
1	0	613	A
1	0	614	A
1	0	615	U
1	0	637	A
1	0	645	C
1	0	647	G
1	0	655	A
1	0	686	U
1	0	730	A

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Mol	Chain	Res	Type
1	0	736	C
1	0	740	C
1	0	747	U
1	0	764	A
1	0	775	G
1	0	776	G
1	0	782	A
1	0	784	G
1	0	785	G
1	0	798	G
1	0	805	G
1	0	812	C
1	0	827	U
1	0	828	U
1	0	845	A
1	0	846	U
1	0	859	G
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	931	U
1	0	946	C
1	0	961	C
1	0	974	G
1	0	983	A
1	0	984	A
1	0	996	A
1	0	1005	C
1	0	1009	A
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

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Mol	Chain	Res	Type
1	0	1048	A
1	0	1110	G
1	0	1111	A
1	0	1112	G
1	0	1116	G
1	0	1132	U
1	0	1135	C
1	0	1136	G
1	0	1142	A
1	0	1172	C
1	0	1174	U
1	0	1175	A
1	0	1176	U
1	0	1187	G
1	0	1206	G
1	0	1211	C
1	0	1212	G
1	0	1238	G
1	0	1250	G
1	0	1253	A
1	0	1255	U
1	0	1256	G
1	0	1271	G
1	0	1272	A
1	0	1300	G
1	0	1301	A
1	0	1345	C
1	0	1352	U
1	0	1365	A
1	0	1379	U
1	0	1395	A
1	0	1416	G
1	0	1417	C
1	0	1420	A
1	0	1424	G
1	0	1428	C
1	0	1435	G
1	0	1452	G
1	0	1478	G
1	0	1482	G
1	0	1490	A
1	0	1493	C

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Mol	Chain	Res	Type
1	0	1497	U
1	0	1509	A
1	0	1510	G
1	0	1515	A
1	0	1529	G
1	0	1537	G
1	0	1554	U
1	0	1569	A
1	0	1578	U
1	0	1584	U
1	0	1585	C
1	0	1592	C
1	0	1608	A
1	0	1618	A
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	1740	G
1	0	1744	A
1	0	1756	G
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	1826	G
1	0	1829	A
1	0	1833	C
1	0	1850	G
1	0	1872	A

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Mol	Chain	Res	Type
1	0	1873	G
1	0	1882	U
1	0	1906	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	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	2023	C
1	0	2031	A
1	0	2033	A
1	0	2043	C
1	0	2055	C
1	0	2056	G
1	0	2060	A
1	0	2061	G
1	0	2069	G
1	0	2186	G
1	0	2189	U
1	0	2194	U
1	0	2198	A
1	0	2204	G
1	0	2212	A
1	0	2225	A
1	0	2238	G
1	0	2239	G
1	0	2251	G
1	0	2273	A
1	0	2283	C

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Mol	Chain	Res	Type
1	0	2287	A
1	0	2288	A
1	0	2294	G
1	0	2297	A
1	0	2307	G
1	0	2308	G
1	0	2309	A
1	0	2312	U
1	0	2319	G
1	0	2322	A
1	0	2325	G
1	0	2333	A
1	0	2347	C
1	0	2383	G
1	0	2385	C
1	0	2396	G
1	0	2402	U
1	0	2403	C
1	0	2406	A
1	0	2422	C
1	0	2425	A
1	0	2429	G
1	0	2430	A
1	0	2441	U
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	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	2573	C

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Mol	Chain	Res	Type
1	0	2602	A
1	0	2603	G
1	0	2609	U
1	0	2613	U
1	0	2629	U
1	0	2646	C
1	0	2689	U
1	0	2690	U
1	0	2714	G
1	0	2726	A
1	0	2732	G
1	0	2733	A
1	0	2744	G
1	0	2748	A
1	0	2752	C
1	0	2757	A
1	0	2765	A
1	0	2778	A
1	0	2820	A
1	0	2832	U
1	0	2843	G
1	0	2849	U
1	0	2867	G
1	0	2873	A
1	0	2877	G
1	0	2880	C
1	0	2883	A
1	0	2884	U
1	0	2885	G
1	0	2886	A
1	0	2887	A
1	0	2894	G
1	0	2903	U
2	1	13	G
2	1	24	G
2	1	33	G
2	1	35	C
2	1	41	G
2	1	44	G
2	1	56	G
2	1	64	G
2	1	67	G

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Mol	Chain	Res	Type
2	1	89	U
2	1	90	C
2	1	105	G
2	1	108	A
2	1	109	A
3	2	4	U
3	2	6	G
3	2	7	A
3	2	9	G
3	2	22	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	71	A
3	2	80	A
3	2	83	C
3	2	84	U
3	2	85	U
3	2	86	G
3	2	88	U
3	2	90	C
3	2	92	U
3	2	94	G
3	2	121	U
3	2	122	G
3	2	131	A
3	2	179	A
3	2	183	C
3	2	184	G
3	2	197	A
3	2	209	U
3	2	210	C
3	2	211	G
3	2	212	G
3	2	220	G
3	2	240	G
3	2	245	U
3	2	247	G

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Mol	Chain	Res	Type
3	2	251	G
3	2	266	G
3	2	267	C
3	2	280	C
3	2	282	A
3	2	289	G
3	2	316	C
3	2	321	A
3	2	328	C
3	2	332	G
3	2	345	C
3	2	346	G
3	2	352	C
3	2	354	G
3	2	365	U
3	2	367	U
3	2	372	C
3	2	376	G
3	2	397	A
3	2	406	G
3	2	411	A
3	2	413	G
3	2	414	A
3	2	421	U
3	2	422	C
3	2	423	G
3	2	429	U
3	2	448	A
3	2	468	A
3	2	474	G
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	524	G
3	2	531	U
3	2	532	A
3	2	535	A
3	2	547	A

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Mol	Chain	Res	Type
3	2	548	G
3	2	559	A
3	2	560	A
3	2	564	C
3	2	572	A
3	2	573	A
3	2	576	C
3	2	577	G
3	2	584	G
3	2	623	C
3	2	633	G
3	2	650	G
3	2	653	U
3	2	665	A
3	2	666	G
3	2	687	A
3	2	703	G
3	2	704	A
3	2	718	A
3	2	721	G
3	2	722	G
3	2	724	G
3	2	734	G
3	2	737	C
3	2	742	G
3	2	748	G
3	2	755	G
3	2	758	C
3	2	767	A
3	2	777	A
3	2	792	A
3	2	793	U
3	2	794	A
3	2	815	A
3	2	817	C
3	2	821	G
3	2	840	C
3	2	841	C
3	2	842	U
3	2	844	G
3	2	845	A
3	2	858	G

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Mol	Chain	Res	Type
3	2	872	A
3	2	890	G
3	2	891	U
3	2	914	A
3	2	922	G
3	2	926	G
3	2	927	G
3	2	934	C
3	2	935	A
3	2	960	U
3	2	966	G
3	2	969	A
3	2	971	G
3	2	975	A
3	2	976	G
3	2	977	A
3	2	983	A
3	2	989	U
3	2	990	C
3	2	992	U
3	2	993	G
3	2	1001	C
3	2	1006	G
3	2	1007	U
3	2	1012	A
3	2	1020	G
3	2	1022	A
3	2	1025	U
3	2	1026	G
3	2	1027	C
3	2	1028	C
3	2	1029	U
3	2	1031	C
3	2	1032	G
3	2	1034	G
3	2	1035	A
3	2	1036	A
3	2	1041	G
3	2	1044	A
3	2	1053	G
3	2	1054	C
3	2	1094	G

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Mol	Chain	Res	Type
3	2	1095	U
3	2	1101	A
3	2	1102	A
3	2	1110	A
3	2	1117	A
3	2	1118	U
3	2	1124	G
3	2	1125	U
3	2	1126	U
3	2	1131	G
3	2	1136	C
3	2	1138	G
3	2	1139	G
3	2	1141	C
3	2	1146	A
3	2	1158	C
3	2	1159	U
3	2	1161	C
3	2	1168	U
3	2	1171	A
3	2	1180	A
3	2	1183	U
3	2	1184	G
3	2	1191	A
3	2	1196	A
3	2	1197	A
3	2	1200	C
3	2	1201	A
3	2	1202	U
3	2	1212	U
3	2	1227	A
3	2	1233	G
3	2	1236	A
3	2	1238	A
3	2	1244	G
3	2	1246	A
3	2	1256	A
3	2	1258	G
3	2	1268	G
3	2	1280	A
3	2	1286	U
3	2	1287	A

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Mol	Chain	Res	Type
3	2	1290	G
3	2	1300	G
3	2	1301	U
3	2	1302	C
3	2	1306	A
3	2	1317	C
3	2	1331	G
3	2	1336	C
3	2	1338	G
3	2	1346	A
3	2	1347	G
3	2	1348	U
3	2	1363	A
3	2	1364	U
3	2	1374	A
3	2	1378	C
3	2	1398	A
3	2	1400	C
3	2	1432	G
3	2	1441	A
3	2	1446	A
3	2	1487	G
3	2	1492	A
3	2	1493	A
3	2	1494	G
3	2	1497	G
3	2	1503	A
3	2	1504	G
3	2	1506	U
3	2	1507	A
3	2	1517	G
3	2	1520	C
3	2	1529	G
3	2	1530	G
3	2	1534	A

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	546	U
1	0	1026	G
1	0	1111	A

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Mol	Chain	Res	Type
1	0	2193	G
1	0	2307	G
1	0	2756	U
3	2	5	U
3	2	79	G
3	2	89	U
3	2	183	C
3	2	210	C
3	2	281	G
3	2	315	A
3	2	345	C
3	2	422	C
3	2	428	G
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	982	U
3	2	992	U
3	2	1024	G
3	2	1040	U
3	2	1053	G
3	2	1117	A
3	2	1137	C
3	2	1179	A
3	2	1182	G
3	2	1190	G
3	2	1201	A
3	2	1267	C
3	2	1347	G
3	2	1399	C

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

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

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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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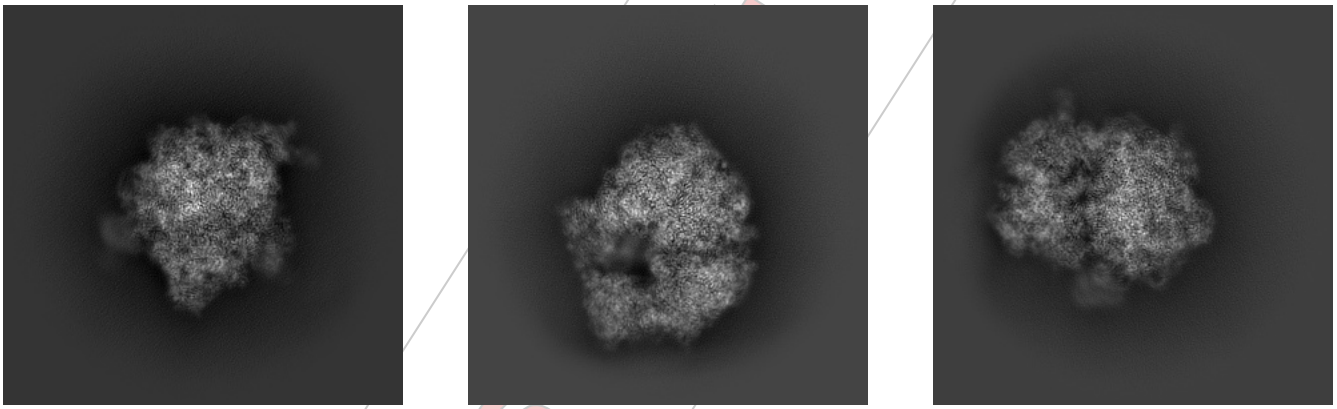
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-82633. 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.

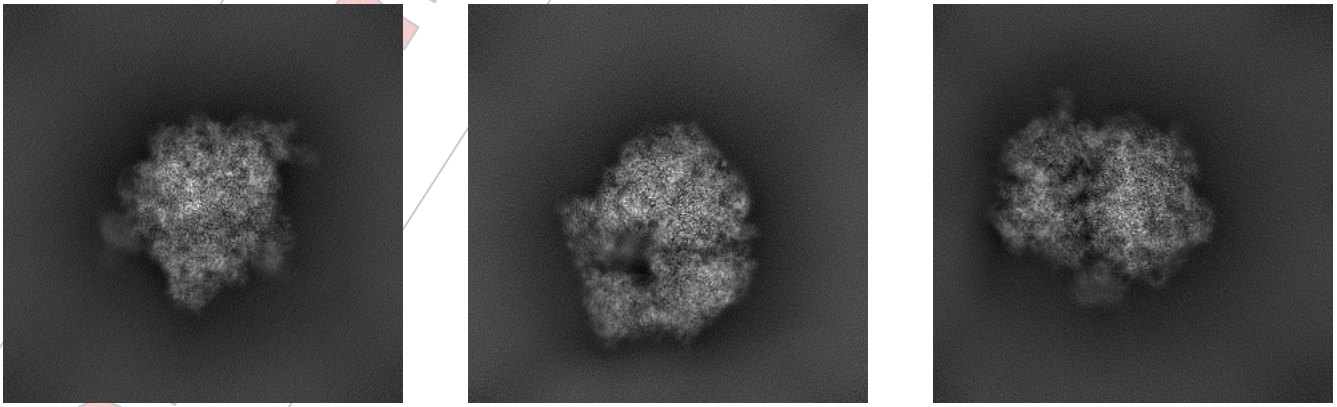
6.1 Orthogonal projections

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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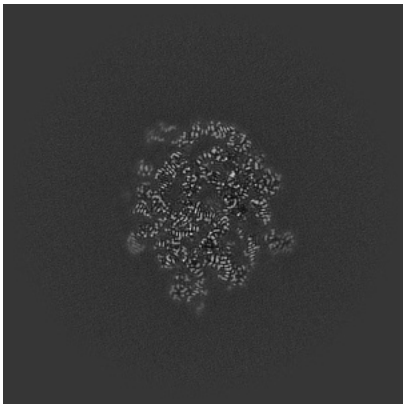
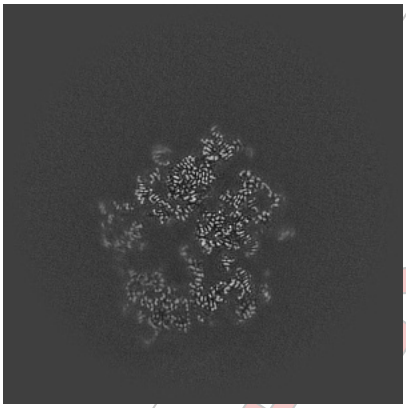
6.2 Central slices (i)

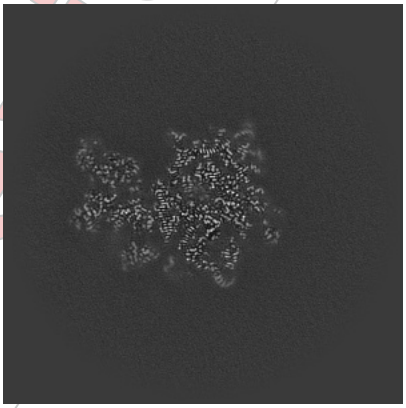
6.2.1 Primary map



X Index: 240

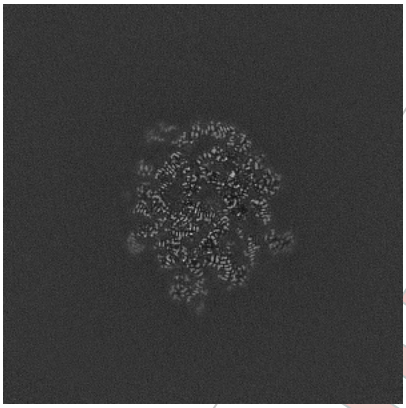


Y Index: 240

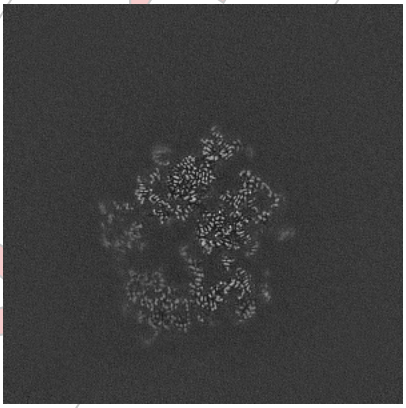


Z Index: 240

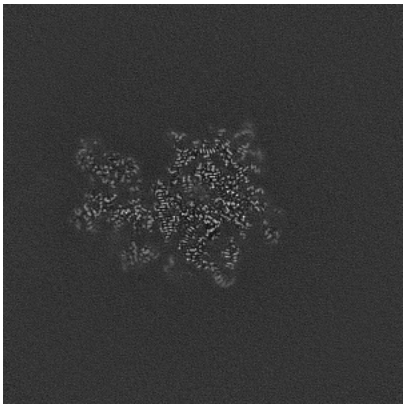
6.2.2 Raw map



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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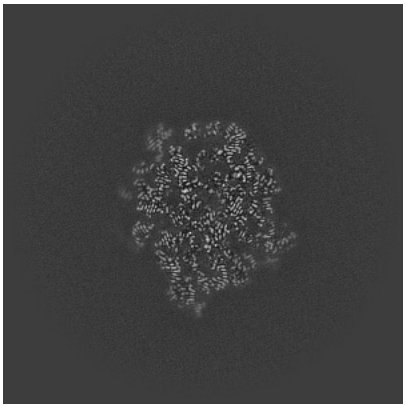
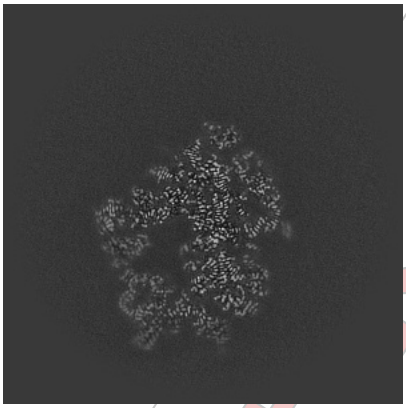
6.3 Largest variance slices (i)

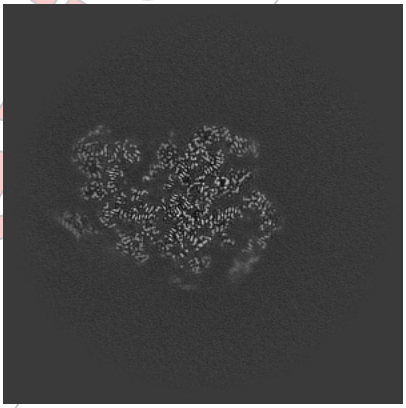
6.3.1 Primary map



X Index: 234

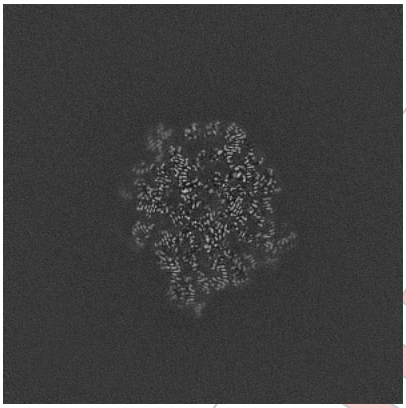


Y Index: 226

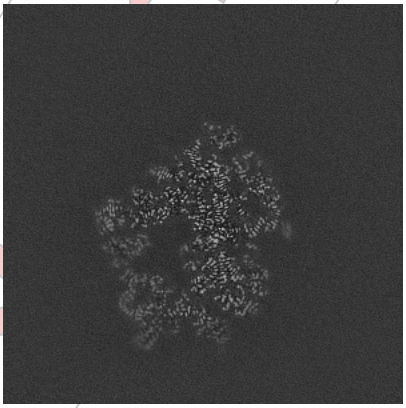


Z Index: 263

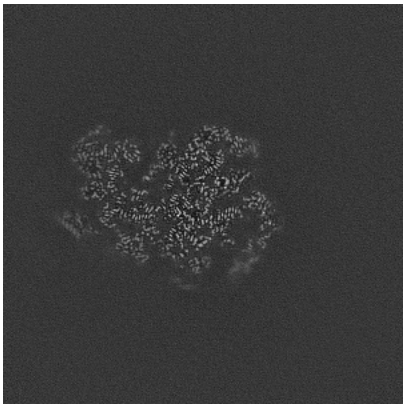
6.3.2 Raw map



X Index: 234



Y Index: 226



Z Index: 263

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

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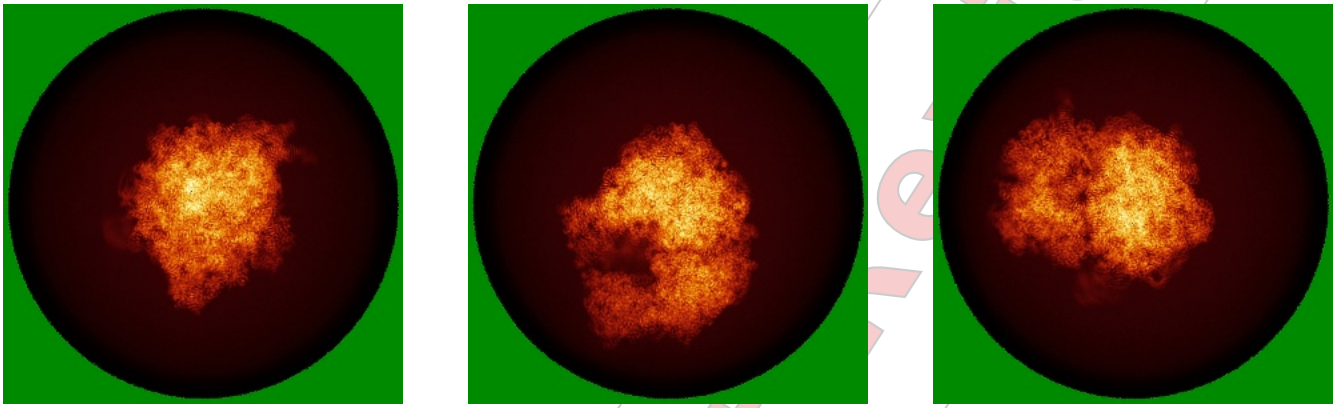
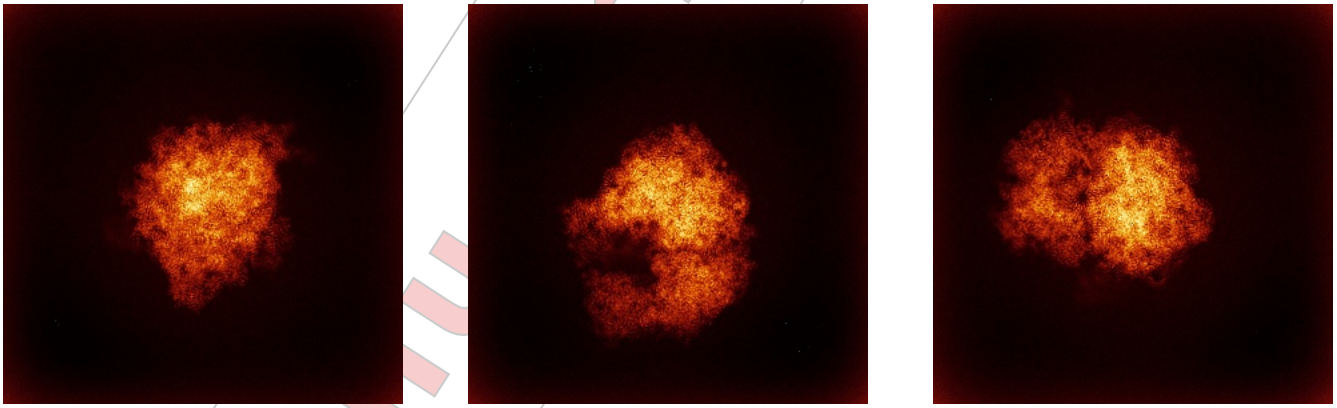
6.4 Orthogonal standard-deviation projections (False-color)

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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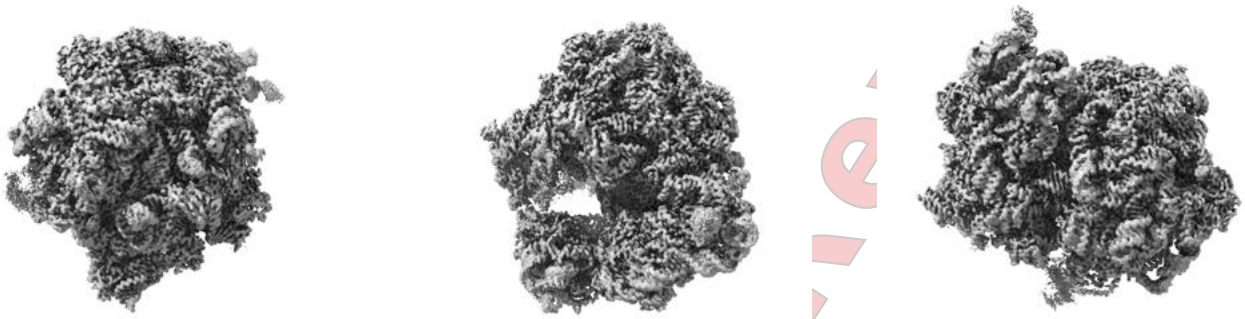
6.5 Orthogonal surface views (i)

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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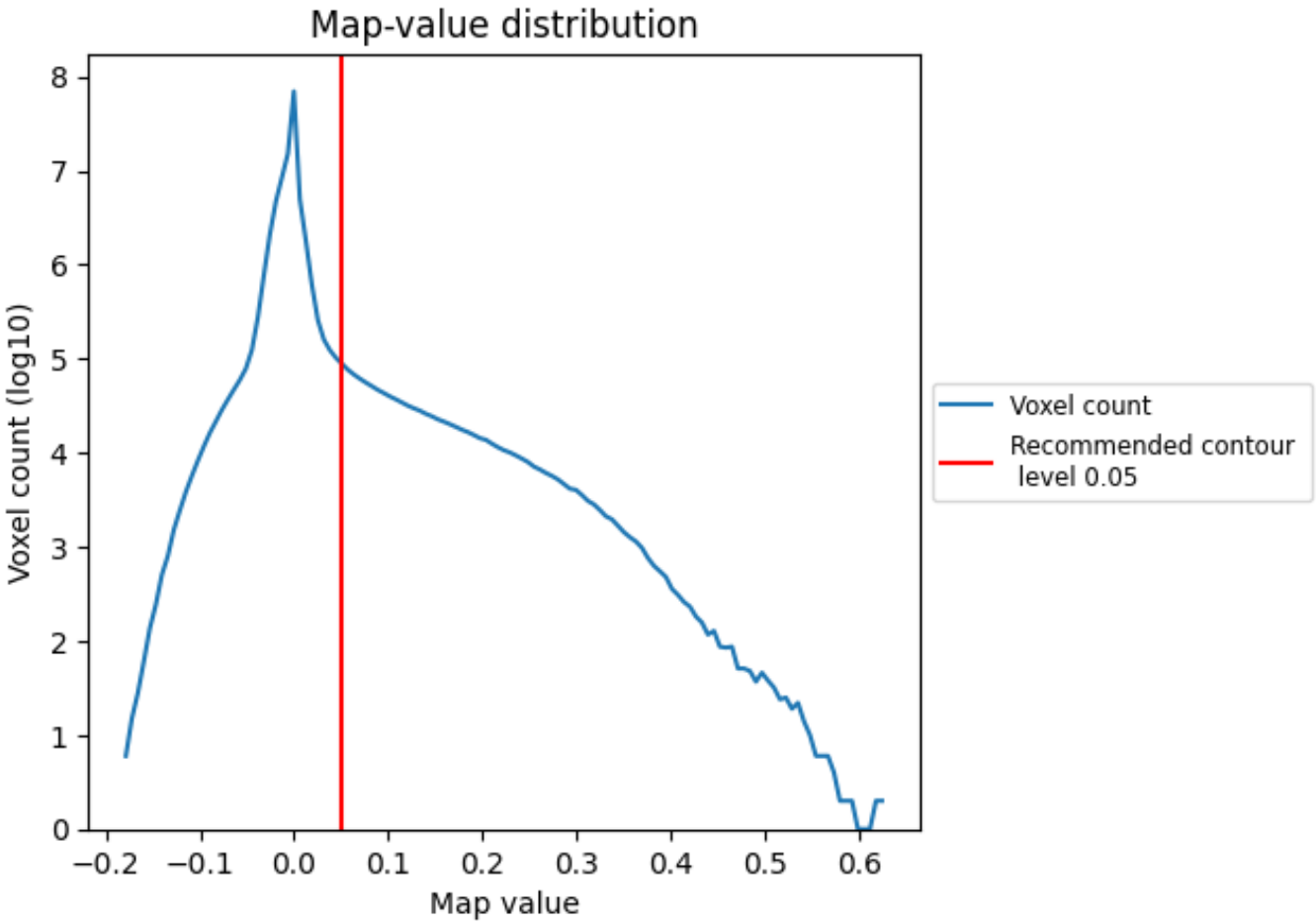
7 Map analysis

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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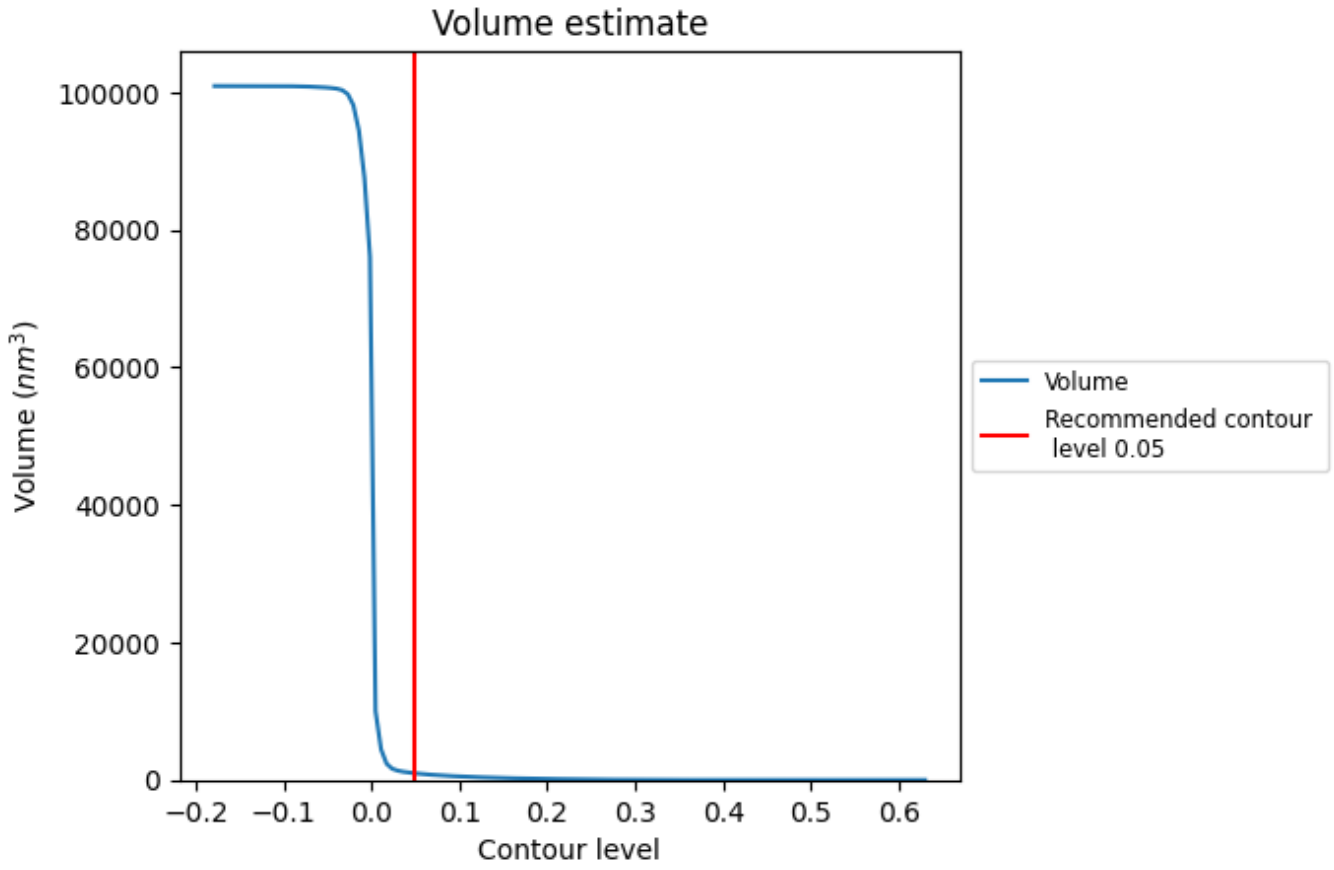
7.2 Volume estimate (i)

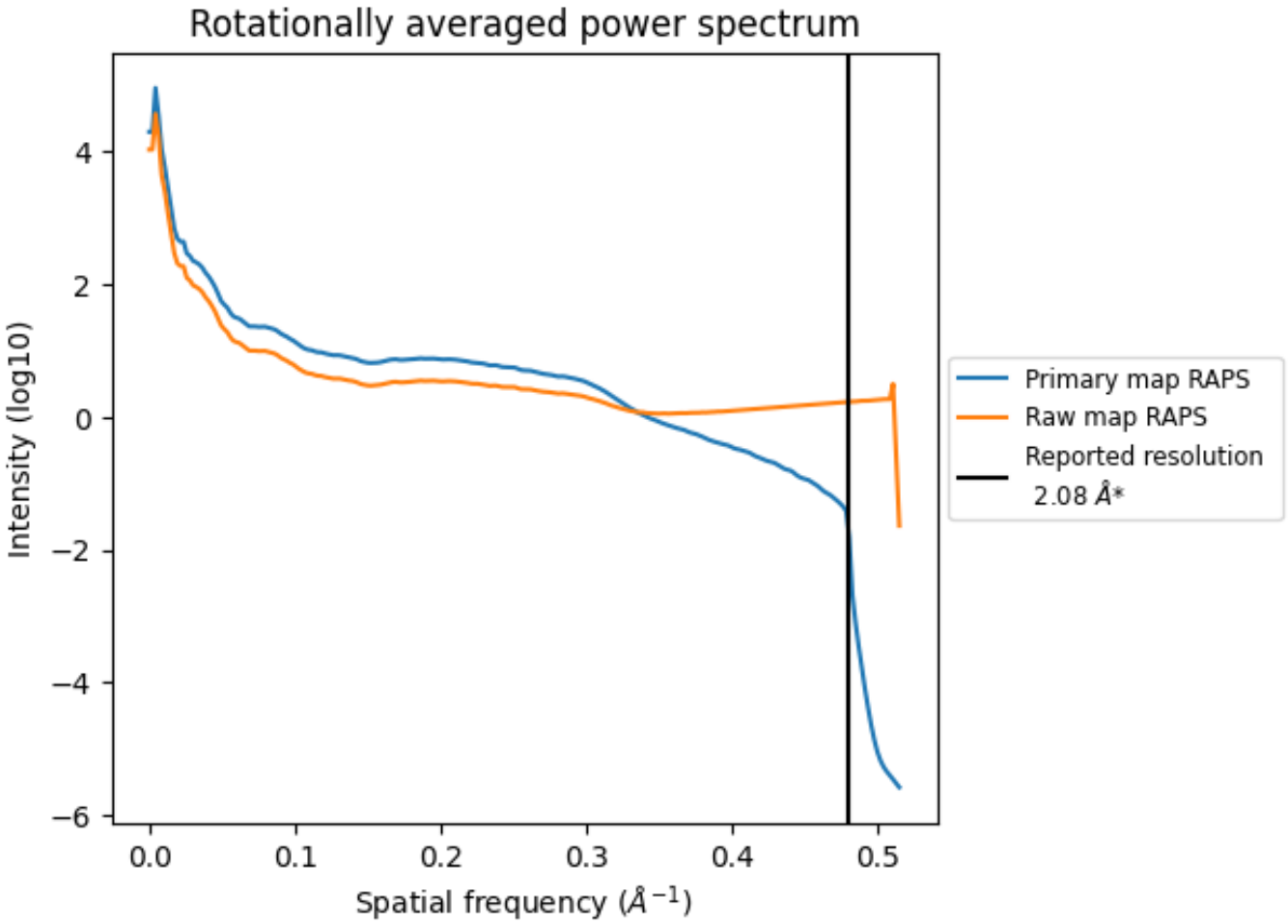


The volume at the recommended contour level is 963 nm^3; this corresponds to an approximate mass of 870 kDa.

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)



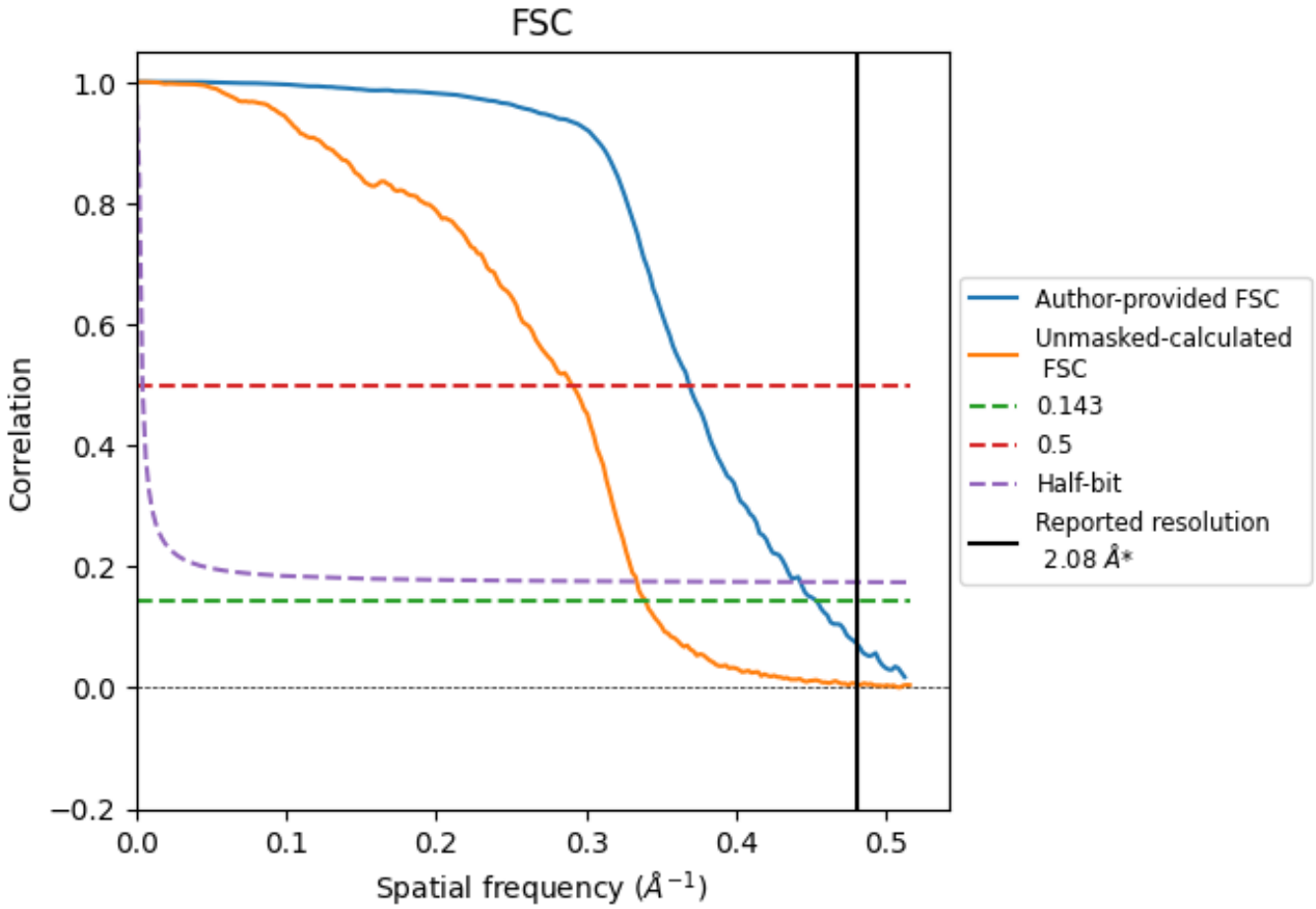
*Reported resolution corresponds to spatial frequency of 0.481 Å^{-1}

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 0.481 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	2.08	-	-
Author-provided FSC curve	2.21	2.71	2.26
Unmasked-calculated*	2.94	3.44	3.00

*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 2.94 differs from the reported value 2.08 by more than 10 %

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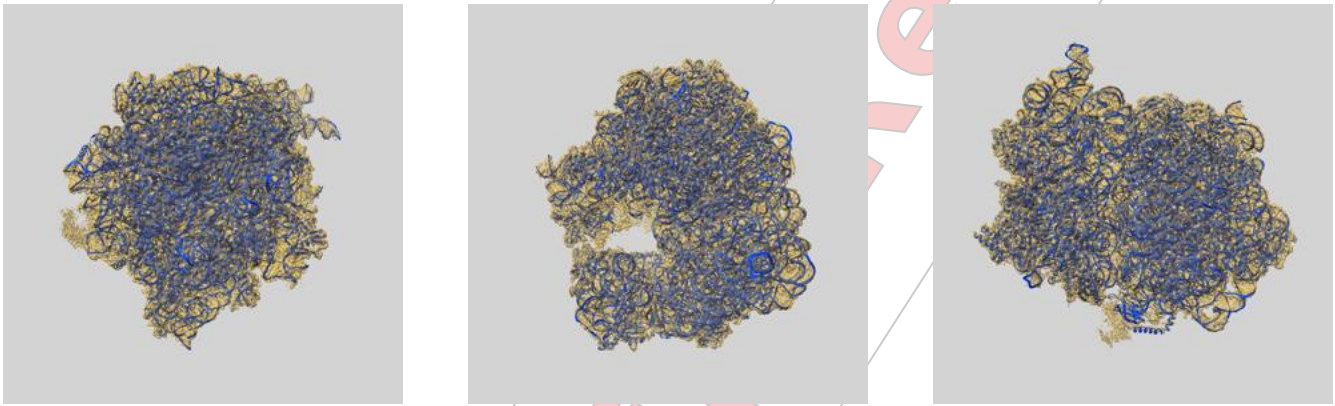
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-82633 and PDB model 44IJ. Per-residue inclusion information can be found in section 3 on page 13.

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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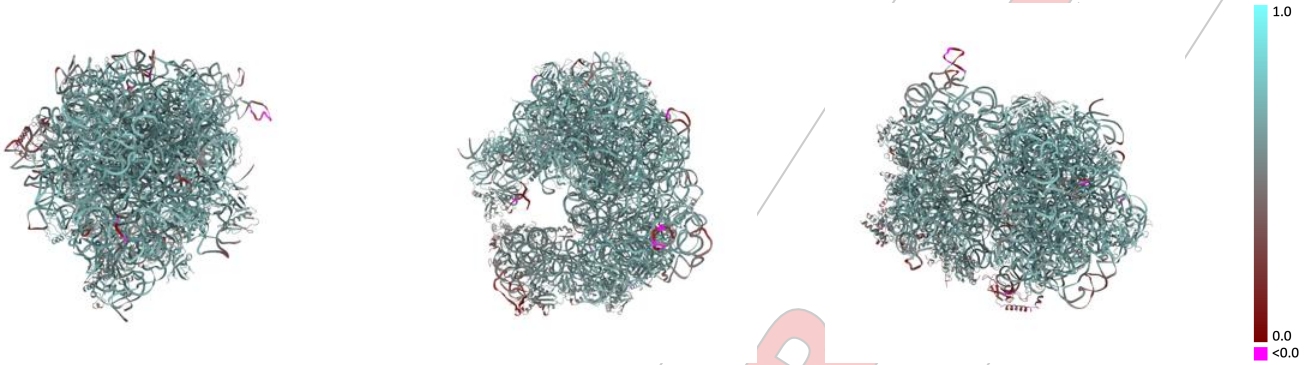
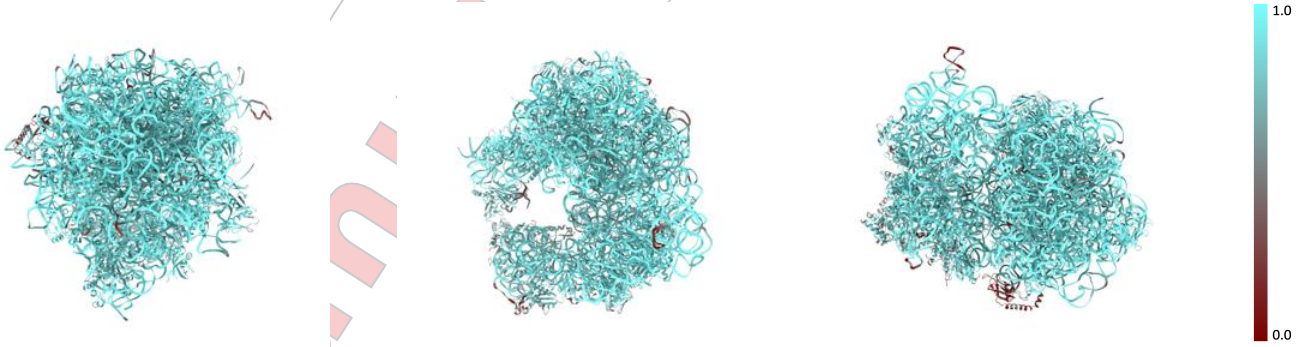
9.2 Q-score mapped to coordinate model



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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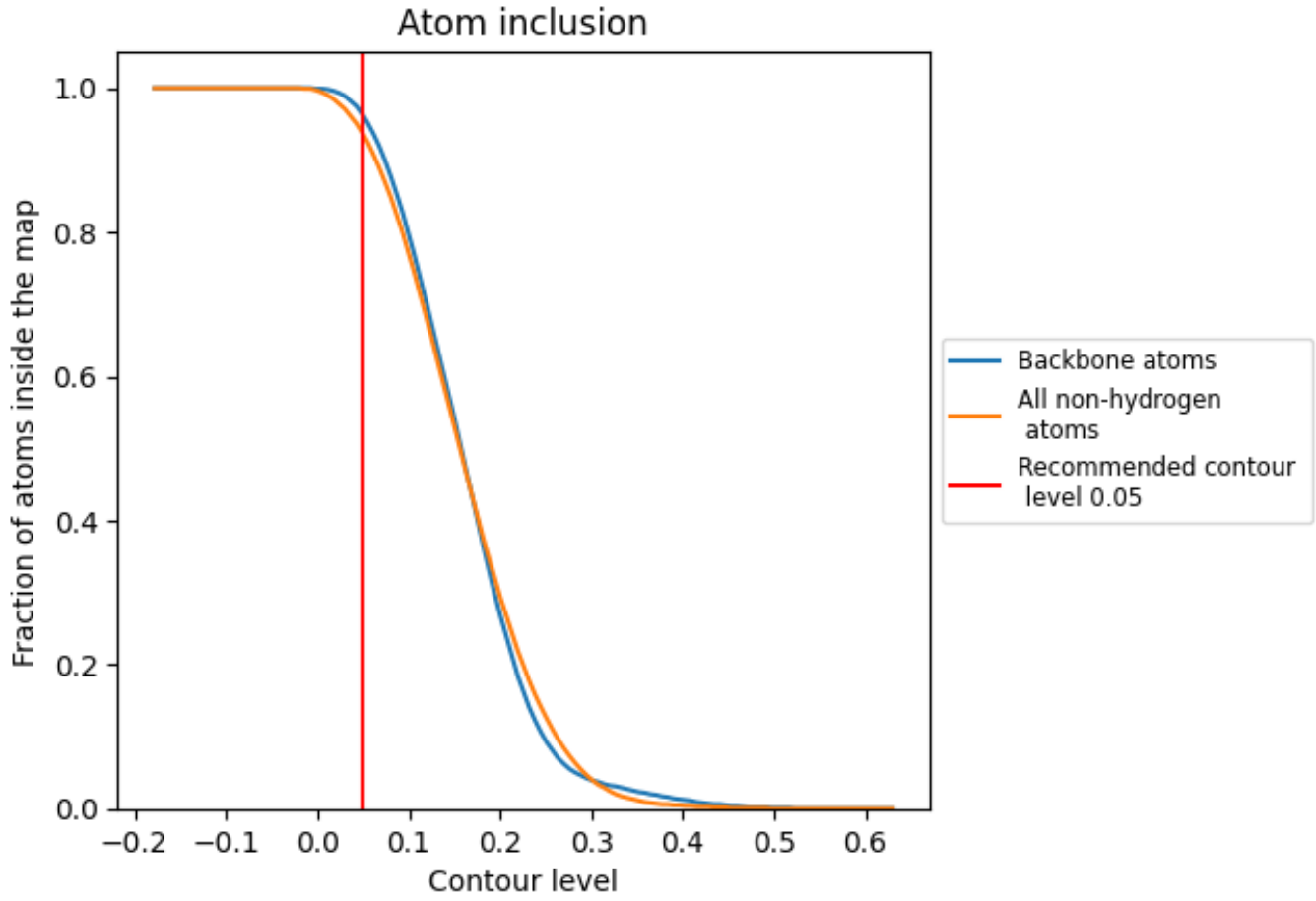
9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 94% 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	0.9360	0.6160
0	0.9770	0.6450
1	0.9790	0.6230
2	0.9590	0.6030
A	0.9620	0.6700
B	0.9540	0.6610
C	0.8990	0.6200
D	0.8120	0.5260
E	0.8650	0.5620
F	0.3680	0.3180
G	0.9490	0.6560
H	0.9440	0.6580
I	0.9460	0.6520
J	0.9390	0.6440
K	0.9710	0.6780
L	0.9030	0.5900
M	0.9200	0.6480
N	0.9700	0.6730
O	0.9260	0.6330
P	0.9370	0.6490
Q	0.8920	0.6090
R	0.8970	0.5980
S	0.8920	0.6160
T	0.9390	0.6480
U	0.9370	0.6480
V	0.8790	0.5900
W	0.9320	0.6560
X	0.6480	0.4220
a	0.9550	0.6640
b	0.9070	0.6240
c	0.9660	0.6750
d	0.9720	0.6790
e	0.9450	0.6430
f	0.7250	0.5070
g	0.8490	0.5700



Continued on next page...

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Chain	Atom inclusion	Q-score
h	0.8690	0.5790
i	0.9220	0.6250
j	0.8250	0.5420
k	0.6250	0.4610
l	0.9280	0.6320
m	0.7420	0.4900
n	0.6920	0.4670
o	0.8720	0.5780
p	0.9030	0.6100
q	0.7360	0.4970
r	0.8420	0.5450
s	0.8880	0.5970
t	0.9150	0.5880
u	0.8730	0.5870
v	0.8410	0.5630
w	0.7130	0.4740
x	0.9010	0.5920
y	0.5110	0.4460

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