Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 01:07 PM JST

PDB ID	:	44IK / pdb_000044ik
EMDB ID	:	EMD-82634
Title	:	Structural basis of ribosomal RNA modification of P-tRNA bound 70S
Deposited on	:	2026-07-30
Resolution	:	2.42 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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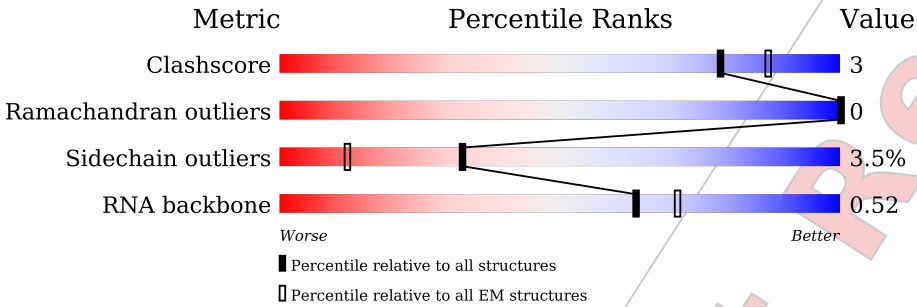
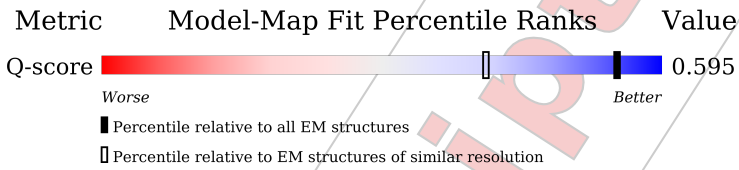
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.42 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	5729 (1.92 - 2.92)

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	77% 18% • 5%
2	1	120	84% 16%

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Mol	Chain	Length	Quality of chain
3	2	1542	73% 23%
4	3	3	100%
5	4	77	8% 71% 22% 6%
6	A	273	88% 11%
7	B	209	89% 10%
8	C	201	94% 6%
9	D	179	76% 21%
10	E	177	86% 11%
11	F	149	66% 90% 9%
12	G	142	91% 9%
13	H	123	90% 10%
14	I	144	90% 8%
15	J	136	90% 10%
16	K	127	83% 9% 7%
17	L	117	93% 5%
18	M	115	83% 17%
19	N	118	96%
20	O	103	93% 7%
21	P	110	95% 5%
22	Q	100	79% 13% 7%
23	R	104	88% 10%
24	S	94	82% 17%
25	T	85	85% 12%
26	U	78	97%
27	V	63	86% 8% 5%

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Mol	Chain	Length	Quality of chain
28	W	59	92% 5%
29	X	70	16% 77% 9% 14%
30	a	57	93%
31	b	55	85% 7% 7%
32	c	46	91% 9%
33	d	65	94%
34	e	38	95% 5%
35	f	241	7% 76% 17% 7%
36	g	233	75% 13% 12%
37	h	206	88% 11%
38	i	167	89% 7%
39	j	131	73% 8% 19%
40	k	179	10% 68% 17% 16%
41	l	130	84% 14%
42	m	130	75% 20%
43	n	103	17% 78% 17%
44	o	129	78% 11% 9%
45	p	124	89% 10%
46	q	118	81% 15%
47	r	101	7% 87% 12%
48	s	89	90% 9%
49	t	82	94% 6%
50	u	84	85% 10% 5%
51	v	75	73% 15% 12%
52	w	92	7% 74% 12% 14%

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Mol	Chain	Length	Quality of chain
53	x	87	90% 8%
54	y	71	23% 89% 10%

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2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 140881 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	0	2758	59219	26417	10911	19134	2757	0	0

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

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

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

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

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	3	3	65	29	12	21	3	0	0

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

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL2.

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

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- Molecule 7 is a protein called 50S ribosomal protein L3.

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

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L5.

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

- Molecule 10 is a protein called 50S ribosomal protein L6.

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

- Molecule 11 is a protein called 50S ribosomal protein L9.

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

- Molecule 12 is a protein called 50S ribosomal protein L13.

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

- Molecule 13 is a protein called 50S ribosomal protein L14.

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

- Molecule 14 is a protein called 50S ribosomal protein L15.

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

- Molecule 15 is a protein called 50S ribosomal protein L16.

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

- Molecule 16 is a protein called 50S ribosomal protein L17.

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

- Molecule 17 is a protein called 50S ribosomal protein L18.

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

- Molecule 18 is a protein called 50S ribosomal protein L19.

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

- Molecule 19 is a protein called 50S ribosomal protein L20.

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

- Molecule 20 is a protein called 50S ribosomal protein L21.

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

- Molecule 21 is a protein called 50S ribosomal protein L22.

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

- Molecule 22 is a protein called 50S ribosomal protein L23.

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

- Molecule 23 is a protein called 50S ribosomal protein L24.

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

- Molecule 24 is a protein called 50S ribosomal protein L25.

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

- Molecule 25 is a protein called 50S ribosomal protein L27.

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

- Molecule 26 is a protein called 50S ribosomal protein L28.

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

- Molecule 27 is a protein called 50S ribosomal protein L29.

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

- Molecule 28 is a protein called 50S ribosomal protein L30.

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

- Molecule 29 is a protein called 50S ribosomal protein L31.

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

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called 50S ribosomal protein L33.

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

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a protein called 30S ribosomal protein S2.

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

- Molecule 36 is a protein called 30S ribosomal protein S3.

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

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

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

- Molecule 39 is a protein called Small ribosomal subunit protein bS6, non-modified isoform.

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

- Molecule 40 is a protein called 30S ribosomal protein S7.

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

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

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

- Molecule 44 is a protein called 30S ribosomal protein S11.

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

- Molecule 45 is a protein called 30S ribosomal protein S12.

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

- Molecule 46 is a protein called 30S ribosomal protein S13.

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

- Molecule 47 is a protein called 30S ribosomal protein S14.

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

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

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

- Molecule 52 is a protein called 30S ribosomal protein S19.

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

- Molecule 53 is a protein called 30S ribosomal protein S20.

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

- Molecule 54 is a protein called 30S ribosomal protein S21.

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

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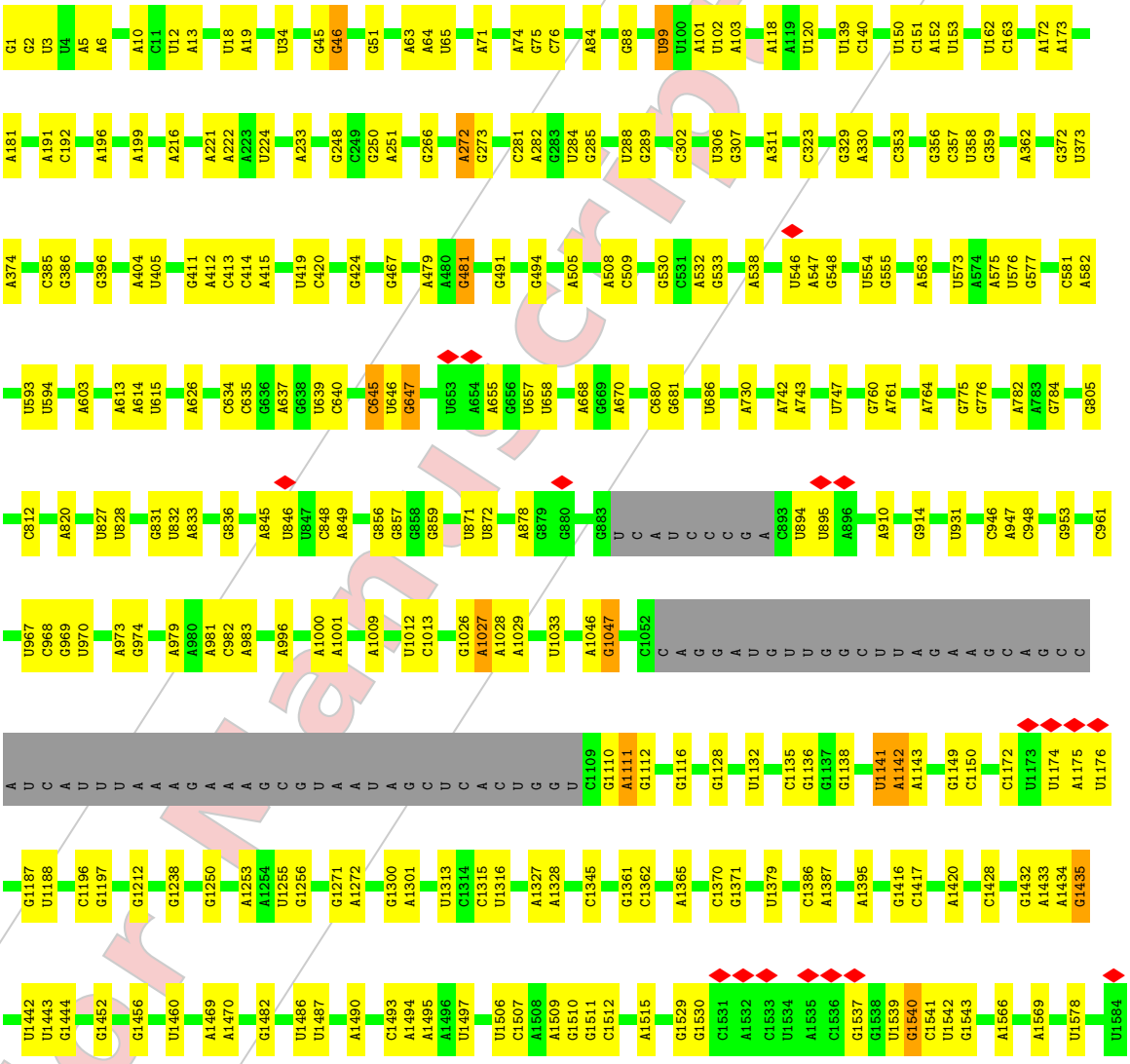
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S rRNA

Chain 0:





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• Molecule 2: 5S rRNA

Chain 1:

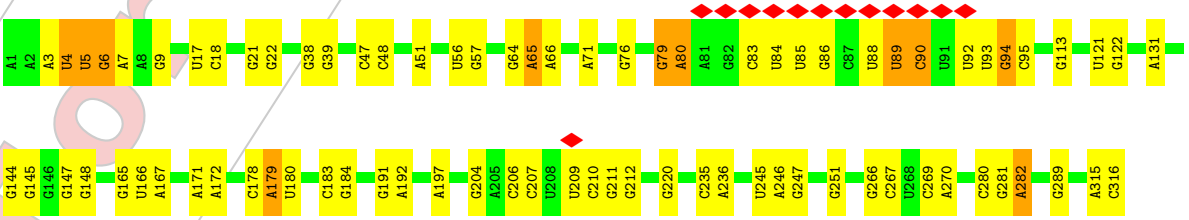




• Molecule 3: 16S rRNA

Chain 2:





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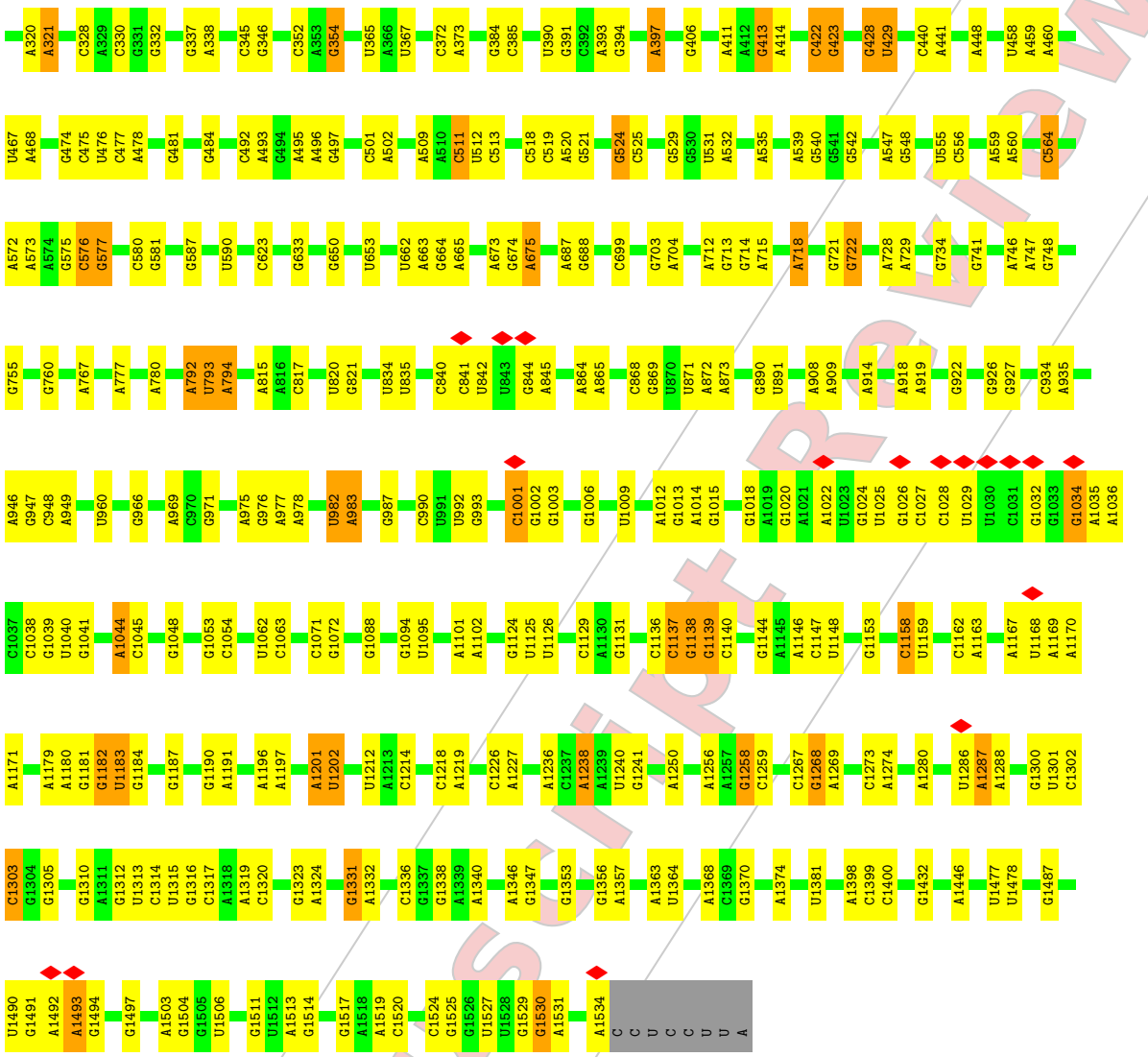
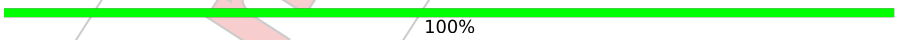


• Molecule 4: mRNA

Chain 3:

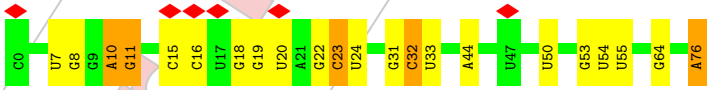


There are no outlier residues recorded for this chain.

• Molecule 5: P-site tRNA

Chain 4:





• Molecule 6: Large ribosomal subunit protein uL2

Chain A:



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• Molecule 7: 50S ribosomal protein L3

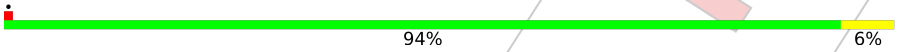
Chain B:

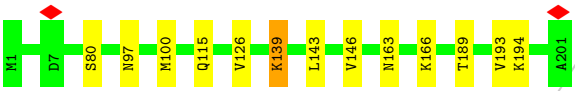




• Molecule 8: 50S ribosomal protein L4

Chain C:

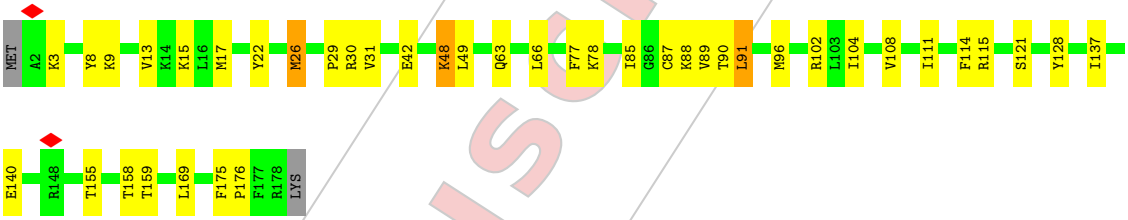




• Molecule 9: 50S ribosomal protein L5

Chain D:

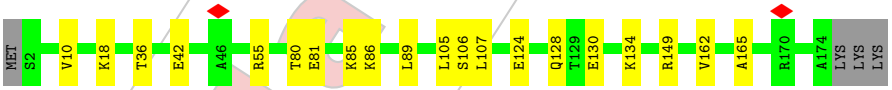




• Molecule 10: 50S ribosomal protein L6

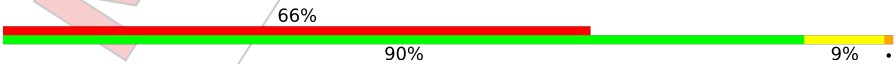
Chain E:

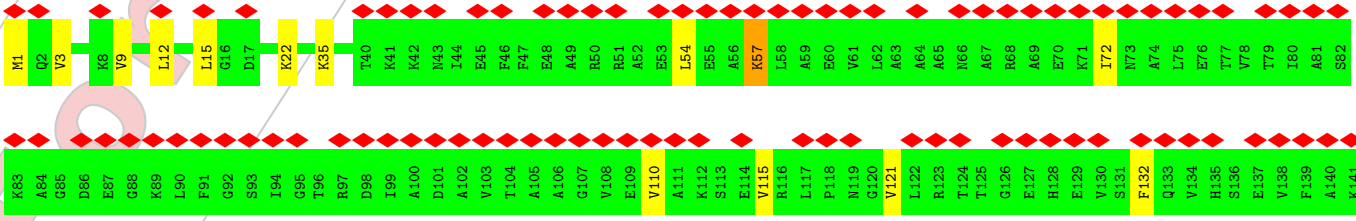




• Molecule 11: 50S ribosomal protein L9

Chain F:





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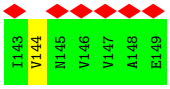
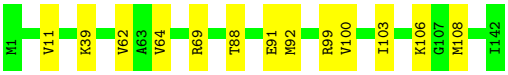


• Molecule 12: 50S ribosomal protein L13

Chain G:





• Molecule 13: 50S ribosomal protein L14

Chain H:

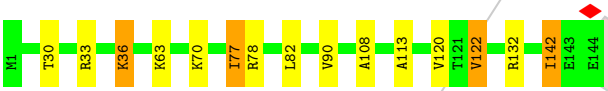




• Molecule 14: 50S ribosomal protein L15

Chain I:

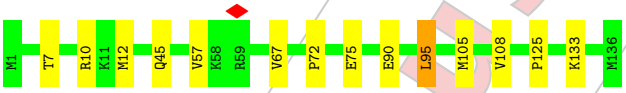




• Molecule 15: 50S ribosomal protein L16

Chain J:





• Molecule 16: 50S ribosomal protein L17

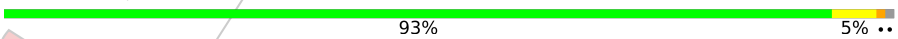
Chain K:





• Molecule 17: 50S ribosomal protein L18

Chain L:





• Molecule 18: 50S ribosomal protein L19

Chain M:



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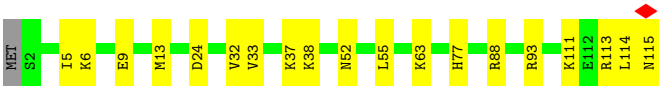
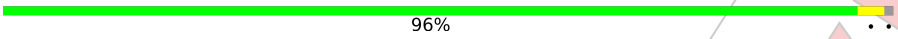
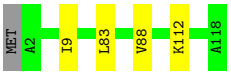


• Molecule 19: 50S ribosomal protein L20

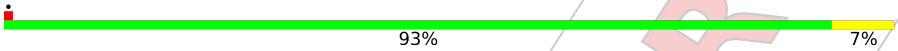
Chain N:

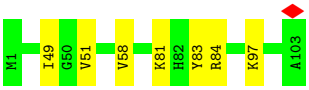




• Molecule 20: 50S ribosomal protein L21

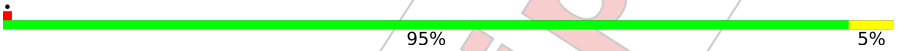
Chain O:

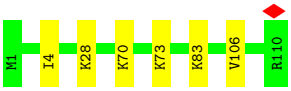




• Molecule 21: 50S ribosomal protein L22

Chain P:

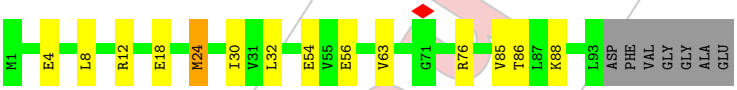




• Molecule 22: 50S ribosomal protein L23

Chain Q:





• Molecule 23: 50S ribosomal protein L24

Chain R:

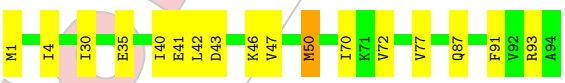




• Molecule 24: 50S ribosomal protein L25

Chain S:





• Molecule 25: 50S ribosomal protein L27

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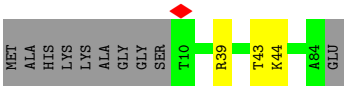
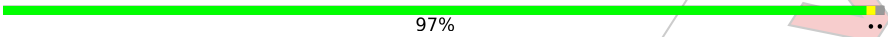
Chain T:

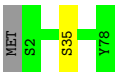




- Molecule 26: 50S ribosomal protein L28

Chain U:





- Molecule 27: 50S ribosomal protein L29

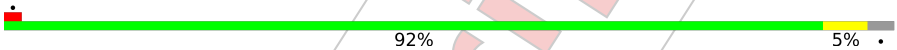
Chain V:

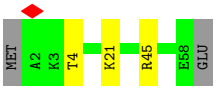




- Molecule 28: 50S ribosomal protein L30

Chain W:

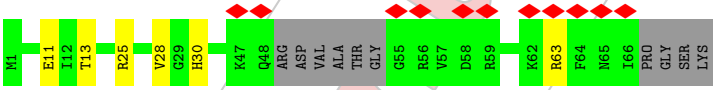




- Molecule 29: 50S ribosomal protein L31

Chain X:

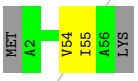




- Molecule 30: 50S ribosomal protein L32

Chain a:





- Molecule 31: 50S ribosomal protein L33

Chain b:





- Molecule 32: 50S ribosomal protein L34

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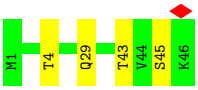
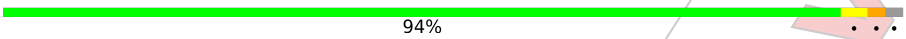
Chain c:





• Molecule 33: 50S ribosomal protein L35

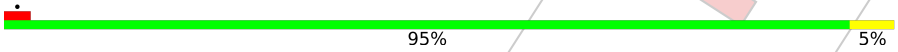
Chain d:

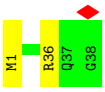




• Molecule 34: 50S ribosomal protein L36

Chain e:

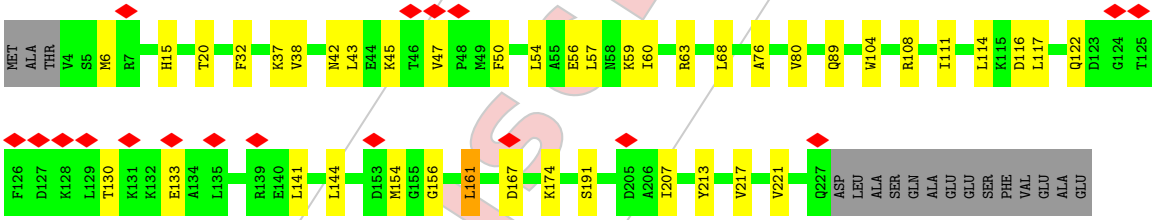




• Molecule 35: 30S ribosomal protein S2

Chain f:

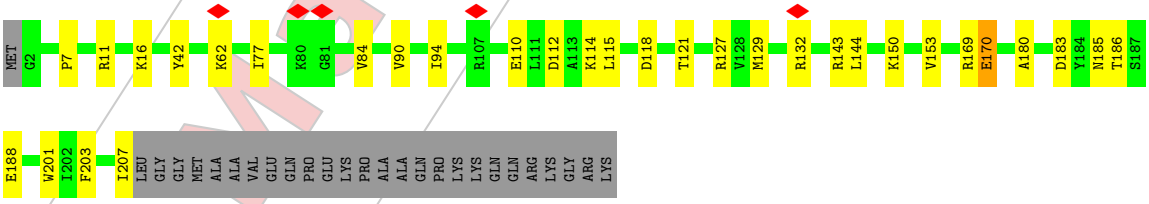




• Molecule 36: 30S ribosomal protein S3

Chain g:





• Molecule 37: 30S ribosomal protein S4

Chain h:





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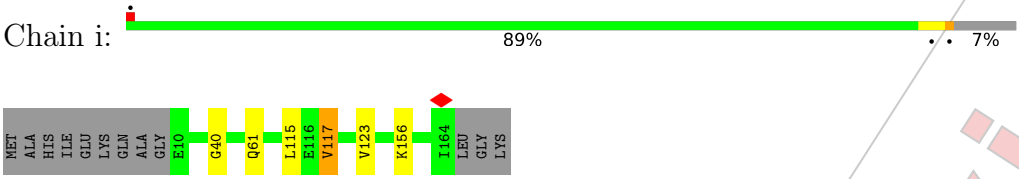
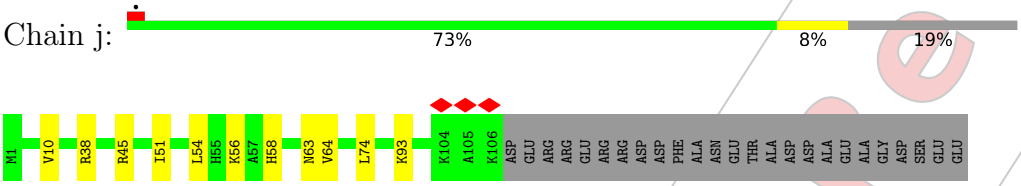
• Molecule 38: 30S ribosomal protein S5

Chain i:



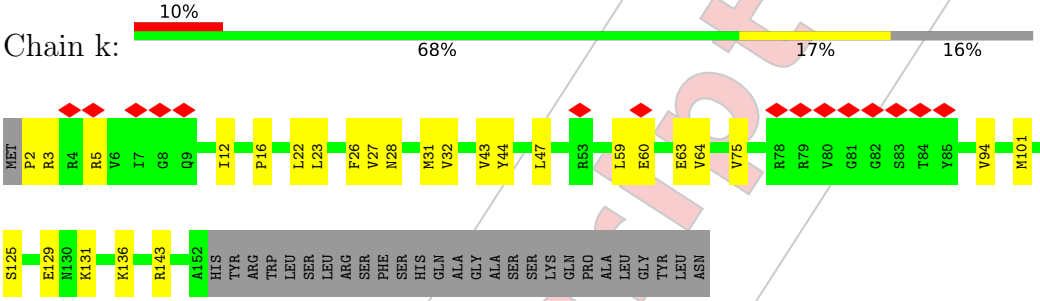
• Molecule 39: Small ribosomal subunit protein bS6, non-modified isoform

Chain j:



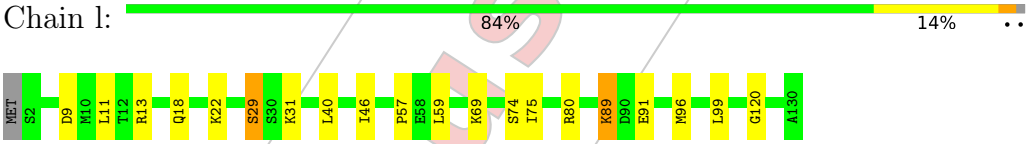
• Molecule 40: 30S ribosomal protein S7

Chain k:



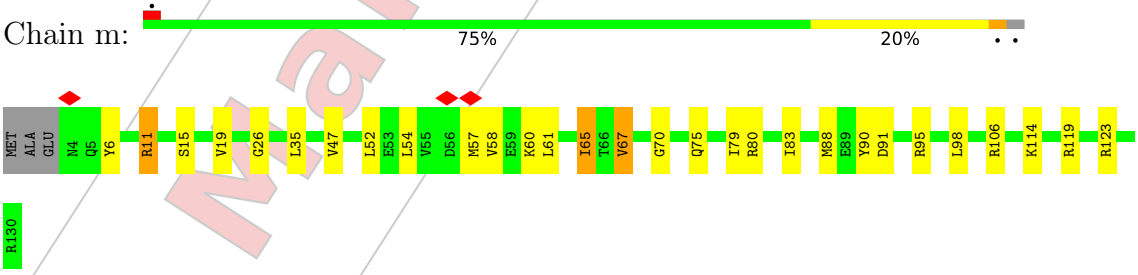
• Molecule 41: 30S ribosomal protein S8

Chain l:



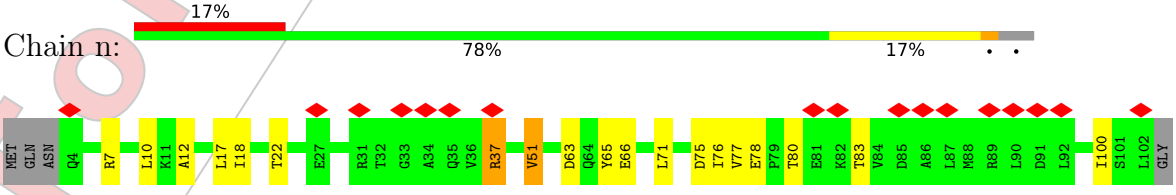
• Molecule 42: 30S ribosomal protein S9

Chain m:



• Molecule 43: 30S ribosomal protein S10

Chain n:



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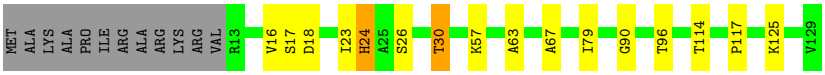
• Molecule 44: 30S ribosomal protein S11

Chain o:

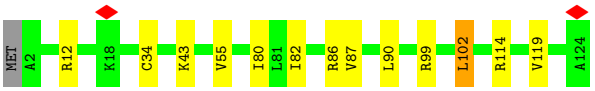




• Molecule 45: 30S ribosomal protein S12

Chain p:





• Molecule 46: 30S ribosomal protein S13

Chain q:

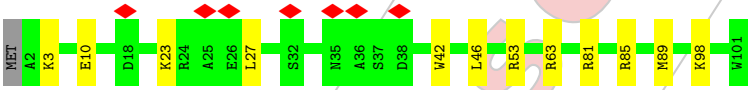




• Molecule 47: 30S ribosomal protein S14

Chain r:

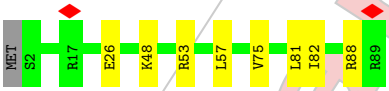




• Molecule 48: 30S ribosomal protein S15

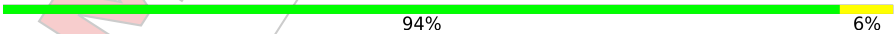
Chain s:





• Molecule 49: 30S ribosomal protein S16

Chain t:





• Molecule 50: 30S ribosomal protein S17

Chain u:



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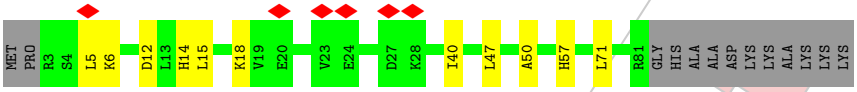
• Molecule 51: 30S ribosomal protein S18



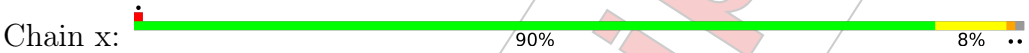


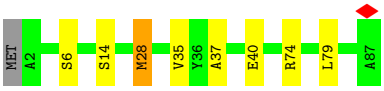
• Molecule 52: 30S ribosomal protein S19



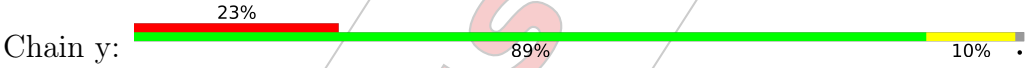


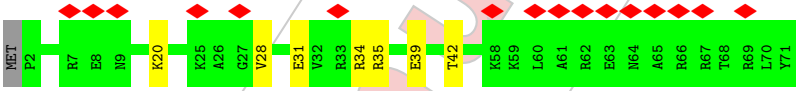
• Molecule 53: 30S ribosomal protein S20





• Molecule 54: 30S ribosomal protein S21





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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	28621	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	0.557	Depositor
Minimum map value	-0.192	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)

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

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	0.18	0/66326	0.31	0/103471
2	1	0.18	0/2869	0.28	0/4474
3	2	0.19	0/36859	0.34	0/57501
4	3	0.15	0/72	0.22	0/110
5	4	0.18	0/1766	0.28	0/2753
6	A	0.17	0/2121	0.34	0/2852
7	B	0.16	0/1580	0.34	0/2127
8	C	0.14	0/1571	0.28	0/2113
9	D	0.17	0/1434	0.34	0/1926
10	E	0.14	0/1315	0.29	0/1783
11	F	0.10	0/1122	0.31	0/1515
12	G	0.16	0/1152	0.32	0/1551
13	H	0.15	0/956	0.32	0/1279
14	I	0.16	0/1062	0.35	0/1413
15	J	0.18	0/1093	0.36	0/1460
16	K	0.15	0/958	0.30	0/1281
17	L	0.16	0/902	0.32	0/1209
18	M	0.15	0/929	0.28	0/1242
19	N	0.15	0/960	0.28	0/1278
20	O	0.16	0/829	0.33	0/1107
21	P	0.14	0/864	0.25	0/1156
22	Q	0.15	0/744	0.31	0/994
23	R	0.15	0/787	0.29	0/1051
24	S	0.16	0/766	0.31	0/1025
25	T	0.18	0/579	0.33	0/767
26	U	0.15	0/635	0.29	0/848
27	V	0.13	0/492	0.33	0/655
28	W	0.14	0/443	0.24	0/593
29	X	0.13	0/488	0.32	0/649
30	a	0.14	0/440	0.28	0/588
31	b	0.15	0/424	0.31	0/565
32	c	0.16	0/380	0.34	0/498

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Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	d	0.16	0/513	0.33	0/676
34	e	0.18	0/303	0.29	0/397
35	f	0.14	0/1784	0.38	0/2403
36	g	0.17	0/1651	0.31	0/2225
37	h	0.16	0/1665	0.32	0/2227
38	i	0.16	0/1157	0.31	0/1557
39	j	0.14	0/881	0.29	0/1189
40	k	0.15	0/1195	0.36	0/1602
41	l	0.17	0/989	0.32	0/1326
42	m	0.18	0/1034	0.42	0/1375
43	n	0.17	0/805	0.38	0/1089
44	o	0.14	0/893	0.27	0/1205
45	p	0.14	0/969	0.31	0/1300
46	q	0.18	0/892	0.42	0/1193
47	r	0.17	0/817	0.27	0/1088
48	s	0.14	0/722	0.27	0/964
49	t	0.16	0/659	0.31	0/884
50	u	0.16	0/657	0.36	0/881
51	v	0.14	0/553	0.29	0/742
52	w	0.19	0/652	0.41	0/877
53	x	0.14	0/676	0.28	0/895
54	y	0.09	0/598	0.20	0/792
All	All	0.18	0/152983	0.32	0/228721

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59219	0	29790	170	0
2	1	2566	0	1302	7	0
3	2	32917	0	16564	155	0

Continued on next page...

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3	65	0	33	0	0
5	4	1642	0	841	7	0
6	A	2082	0	2154	17	0
7	B	1559	0	1611	11	0
8	C	1552	0	1619	6	0
9	D	1410	0	1444	26	0
10	E	1295	0	1332	11	0
11	F	1111	0	1148	7	0
12	G	1129	0	1162	7	0
13	H	947	0	1023	8	0
14	I	1053	0	1129	10	0
15	J	1074	0	1157	10	0
16	K	945	0	989	5	0
17	L	892	0	923	6	0
18	M	917	0	962	12	0
19	N	947	0	1019	2	0
20	O	816	0	839	4	0
21	P	857	0	922	3	0
22	Q	738	0	807	9	0
23	R	779	0	831	4	0
24	S	753	0	780	7	0
25	T	572	0	593	3	0
26	U	625	0	652	0	0
27	V	491	0	523	4	0
28	W	439	0	482	0	0
29	X	480	0	482	4	0
30	a	434	0	445	1	0
31	b	417	0	451	2	0
32	c	377	0	418	1	0
33	d	504	0	572	2	0
34	e	302	0	343	1	0
35	f	1753	0	1780	28	0
36	g	1624	0	1696	17	0
37	h	1643	0	1707	10	0
38	i	1144	0	1185	2	0
39	j	862	0	864	5	0
40	k	1181	0	1238	14	0
41	l	979	0	1031	10	0
42	m	1022	0	1070	17	0
43	n	795	0	836	8	0
44	o	877	0	887	11	0
45	p	955	0	1016	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	q	883	0	941	12	0
47	r	805	0	844	9	0
48	s	714	0	734	5	0
49	t	649	0	666	2	0
50	u	648	0	691	4	0
51	v	544	0	565	6	0
52	w	637	0	665	7	0
53	x	670	0	719	3	0
54	y	590	0	629	7	0
All	All	140881	0	95106	666	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 (666) 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)
1:0:1047:G:H21	1:0:1111:A:N6	1.70	0.89
2:1:48:U:H4'	17:L:100:HIS:HE1	1.39	0.84
3:2:1009:U:H3	3:2:1018:G:H22	1.25	0.82
40:k:113:ASP:HB2	40:k:119:ARG:HG2	1.61	0.82
42:m:88:MET:HE1	42:m:95:ARG:HA	1.67	0.76
1:0:1047:G:N2	1:0:1111:A:N6	2.33	0.76
3:2:76:G:H1	3:2:93:U:H3	1.33	0.75
1:0:2796:U:H3	1:0:2799:A:H61	1.32	0.74
24:S:40:ILE:HD12	24:S:42:LEU:HD21	1.69	0.73
11:F:9:VAL:HG21	11:F:12:LEU:HG	1.68	0.73
3:2:673:A:H2'	3:2:674:G:C8	2.24	0.73
9:D:111:ILE:HD11	9:D:114:PHE:HD2	1.54	0.73
7:B:133:THR:HG22	7:B:134:HIS:H	1.55	0.71
3:2:1003:G:C5	3:2:1034:G:N2	2.60	0.70
15:J:105:MET:HE2	15:J:108:VAL:HG21	1.72	0.70
1:0:981:A:H8	1:0:2027:G:H21	1.38	0.70
1:0:1138:G:H21	12:G:108:MET:HE2	1.57	0.69
42:m:88:MET:HE3	42:m:98:LEU:HD12	1.75	0.69
9:D:63:GLN:HE21	9:D:89:VAL:HG22	1.58	0.69
1:0:2324:U:H3'	1:0:2325:G:H5"	1.74	0.68
35:f:60:ILE:HA	35:f:63:ARG:HH12	1.59	0.68
48:s:82:ILE:HD11	48:s:88:ARG:HE	1.58	0.68
3:2:949:A:H2	46:q:105:ASN:HD21	1.41	0.68
35:f:6:MET:HE1	35:f:43:LEU:HD13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2502:G:H5'	1:0:2503:A:H5"	1.75	0.67
3:2:1003:G:N7	3:2:1034:G:N2	2.42	0.67
7:B:105:LYS:HE3	7:B:105:LYS:HA	1.76	0.67
18:M:9:GLU:HB3	18:M:55:LEU:HD22	1.77	0.67
19:N:112:LYS:HD2	20:O:49:ILE:HD11	1.75	0.67
46:q:97:VAL:HG23	46:q:98:ARG:HG3	1.77	0.66
3:2:714:G:H2'	3:2:715:A:C8	2.31	0.66
45:p:55:VAL:HG11	45:p:80:ILE:HD11	1.77	0.65
3:2:1013:G:H21	3:2:1219:A:H1'	1.62	0.65
9:D:30:ARG:H	9:D:159:THR:HG22	1.61	0.65
1:0:856:G:H2'	1:0:857:G:C8	2.31	0.64
3:2:147:G:H2'	3:2:148:G:C8	2.32	0.64
3:2:688:G:H1	3:2:699:C:H5	1.43	0.64
49:t:48:GLU:HG3	49:t:51:ARG:HH12	1.62	0.64
3:2:1218:C:H2'	3:2:1219:A:C8	2.33	0.64
3:2:1305:G:H22	3:2:1331:G:H2'	1.63	0.64
3:2:458:U:H2'	3:2:459:A:H8	1.62	0.63
14:I:132:ARG:HG3	14:I:142:ILE:HD11	1.80	0.63
9:D:111:ILE:HD11	9:D:114:PHE:CD2	2.32	0.63
3:2:1038:C:H2'	3:2:1039:G:H8	1.63	0.63
10:E:42:GLU:HB3	10:E:55:ARG:HE	1.64	0.63
1:0:848:C:H2'	1:0:849:A:H8	1.64	0.62
35:f:130:THR:HB	35:f:133:GLU:HB2	1.79	0.62
42:m:47:VAL:HG22	42:m:80:ARG:HD3	1.81	0.62
2:1:48:U:H4'	17:L:100:HIS:CE1	2.28	0.62
14:I:30:THR:HG22	14:I:33:ARG:H	1.65	0.62
9:D:17:MET:HE1	9:D:22:TYR:HB2	1.81	0.62
10:E:89:LEU:HD22	10:E:162:VAL:HG22	1.82	0.62
1:0:1047:G:N2	1:0:1111:A:H62	1.97	0.61
6:A:118:SER:HB2	6:A:129:THR:HB	1.82	0.61
3:2:492:C:H2'	3:2:493:A:C8	2.35	0.61
40:k:26:PHE:HB2	40:k:101:MET:HE2	1.81	0.61
31:b:11:LEU:HD21	31:b:34:LEU:HD23	1.81	0.61
3:2:1356:G:H2'	3:2:1357:A:C8	2.36	0.61
1:0:626:A:H2'	14:I:78:ARG:NH2	2.16	0.61
3:2:1312:G:H5"	29:X:63:ARG:HH21	1.66	0.61
35:f:6:MET:HE3	35:f:6:MET:O	2.01	0.60
5:4:10:A:H2'	5:4:11:G:C8	2.37	0.60
52:w:12:ASP:OD1	52:w:15:LEU:HB3	2.02	0.60
9:D:111:ILE:HG22	9:D:137:ILE:HG21	1.84	0.60
52:w:40:ILE:HD11	52:w:71:LEU:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:K:32:GLU:HG2	16:K:115:LEU:HD12	1.83	0.59
24:S:47:VAL:HA	24:S:50:MET:HE2	1.83	0.59
35:f:56:GLU:HA	35:f:59:LYS:HD2	1.84	0.59
51:v:30:LYS:HD2	51:v:33:ILE:HD11	1.84	0.59
1:0:1141:U:H4'	1:0:1142:A:O4'	2.01	0.59
3:2:477:C:H2'	3:2:478:A:C8	2.38	0.59
12:G:99:ARG:O	12:G:103:ILE:HG13	2.02	0.59
1:0:1138:G:N2	12:G:108:MET:HE2	2.18	0.59
36:g:7:PRO:O	36:g:11:ARG:HG3	2.03	0.58
41:l:89:LYS:HD3	41:l:120:GLY:HA2	1.85	0.58
3:2:1182:G:H4'	3:2:1183:U:H5'	1.84	0.58
35:f:104:TRP:O	35:f:108:ARG:HG3	2.04	0.58
35:f:32:PHE:HB2	35:f:42:ASN:HA	1.85	0.58
35:f:207:ILE:HD12	35:f:207:ILE:H	1.68	0.58
3:2:337:G:H2'	3:2:338:A:C8	2.37	0.58
3:2:1226:C:N4	46:q:103:LYS:HD2	2.19	0.58
33:d:32:ILE:HG22	33:d:35:LYS:HD2	1.85	0.58
22:Q:54:GLU:HB3	22:Q:88:LYS:HG3	1.86	0.57
1:0:1869:G:H21	1:0:1872:A:H2	1.50	0.57
3:2:1038:C:H2'	3:2:1039:G:C8	2.39	0.57
15:J:45:GLN:NE2	15:J:125:PRO:HD3	2.19	0.57
22:Q:30:ILE:HG13	22:Q:85:VAL:HB	1.85	0.57
1:0:272:A:H2'	1:0:273:G:H8	1.69	0.57
3:2:673:A:H2'	3:2:674:G:H8	1.69	0.57
3:2:1158:C:H5	3:2:1181:G:H1	1.53	0.57
22:Q:56:GLU:HB3	22:Q:86:THR:HG23	1.86	0.57
42:m:57:MET:HE2	42:m:57:MET:O	2.03	0.57
8:C:97:ASN:HB2	8:C:100:MET:HG3	1.87	0.57
9:D:31:VAL:HA	9:D:158:THR:HG22	1.87	0.57
3:2:411:A:C4	3:2:413:G:H1'	2.40	0.57
3:2:718:A:H2	51:v:38:LYS:HE3	1.70	0.56
1:0:1808:A:H3'	1:0:1809:A:C8	2.41	0.56
1:0:2329:U:H2'	1:0:2330:G:C8	2.40	0.56
2:1:116:G:H4'	17:L:54:VAL:HG12	1.87	0.56
3:2:662:U:H2'	3:2:663:A:C8	2.41	0.56
3:2:17:U:H2'	3:2:18:C:C6	2.41	0.56
3:2:511:C:H4'	37:h:44:ARG:HH22	1.71	0.56
3:2:746:A:H2'	3:2:747:A:C8	2.41	0.56
6:A:175:ARG:HB2	6:A:181:MET:HE1	1.86	0.56
9:D:66:LEU:HD23	9:D:88:LYS:HD3	1.87	0.56
35:f:114:LEU:HD13	35:f:144:LEU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1268:G:H2'	3:2:1269:A:C8	2.39	0.56
9:D:140:GLU:HA	29:X:28:VAL:HG12	1.88	0.55
1:0:2898:U:H2'	1:0:2899:A:H8	1.71	0.55
3:2:1014:A:H2'	3:2:1015:G:C8	2.42	0.55
3:2:458:U:H2'	3:2:459:A:C8	2.42	0.55
6:A:71:LYS:HE2	6:A:74:ILE:HD12	1.89	0.55
1:0:1539:U:H2'	1:0:1540:G:H8	1.71	0.55
1:0:1847:A:O2'	1:0:1848:A:H8	1.90	0.55
3:2:946:A:H2'	3:2:947:G:C8	2.42	0.55
37:h:70:ARG:HH11	37:h:73:ARG:NH2	2.05	0.55
40:k:28:ASN:HA	40:k:31:MET:HE2	1.88	0.55
48:s:53:ARG:O	48:s:57:LEU:HD22	2.06	0.55
1:0:2246:G:H2'	1:0:2247:A:H8	1.71	0.54
14:I:122:VAL:HG13	14:I:142:ILE:HG22	1.89	0.54
21:P:4:ILE:HG13	21:P:106:VAL:HG22	1.88	0.54
13:H:108:ARG:HA	13:H:113:MET:HE1	1.90	0.54
3:2:1305:G:H1'	3:2:1332:A:N6	2.22	0.54
7:B:55:LYS:HD3	7:B:60:VAL:HG22	1.90	0.54
7:B:56:LYS:HD2	7:B:59:ARG:HG3	1.90	0.54
10:E:86:LYS:HB3	10:E:165:ALA:HB2	1.89	0.54
42:m:60:LYS:O	42:m:61:LEU:HD23	2.07	0.54
1:0:2193:G:H2'	1:0:2194:U:C6	2.43	0.54
3:2:337:G:H2'	3:2:338:A:H8	1.72	0.54
3:2:1009:U:H3	3:2:1018:G:N2	2.02	0.54
15:J:45:GLN:HE22	15:J:125:PRO:HD3	1.71	0.54
1:0:1802:A:H2'	1:0:1803:A:C8	2.43	0.54
3:2:178:C:H2'	3:2:179:A:H5"	1.90	0.54
36:g:110:GLU:HG3	36:g:144:LEU:HD12	1.90	0.54
1:0:668:A:H2'	1:0:670:A:H62	1.73	0.54
18:M:13:MET:HE3	18:M:77:HIS:NE2	2.23	0.53
38:i:115:LEU:HD13	38:i:123:VAL:HG11	1.91	0.53
42:m:65:ILE:HG21	42:m:79:ILE:HD12	1.90	0.53
34:e:1:MET:HE3	34:e:36:ARG:HB2	1.90	0.53
40:k:2:PRO:HG2	40:k:5:ARG:HB2	1.90	0.53
3:2:1048:G:H5"	47:r:3:LYS:HG2	1.90	0.53
3:2:94:G:H4'	3:2:95:C:H5'	1.91	0.53
44:o:17:SER:HA	44:o:79:ILE:HA	1.91	0.53
1:0:1047:G:N2	1:0:1111:A:C6	2.75	0.53
1:0:1746:A:H2'	1:0:1747:U:C6	2.44	0.53
24:S:70:ILE:HG22	24:S:72:VAL:HG13	1.90	0.53
1:0:2788:C:H2'	1:0:2789:C:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:f:117:LEU:HG	35:f:141:LEU:HD12	1.91	0.53
30:a:54:VAL:HG23	30:a:55:ILE:HG12	1.90	0.52
1:0:742:A:H2'	1:0:743:A:C8	2.43	0.52
1:0:848:C:H2'	1:0:849:A:C8	2.44	0.52
1:0:2328:A:H2'	1:0:2329:U:C6	2.45	0.52
3:2:235:C:H2'	3:2:236:A:H8	1.73	0.52
6:A:240:PHE:O	6:A:242:LYS:HG2	2.09	0.52
9:D:91:LEU:HD13	9:D:96:MET:HA	1.90	0.52
47:r:10:GLU:HG3	47:r:63:ARG:HD2	1.90	0.52
35:f:213:TYR:O	35:f:217:VAL:HG23	2.10	0.52
18:M:5:ILE:O	18:M:9:GLU:HG3	2.10	0.52
7:B:133:THR:HG22	7:B:134:HIS:N	2.21	0.52
9:D:104:ILE:HD11	9:D:175:PHE:HA	1.92	0.52
15:J:57:VAL:HG11	15:J:105:MET:HE1	1.92	0.52
38:i:40:GLY:HA3	38:i:117:VAL:HG13	1.92	0.52
46:q:19:LEU:O	46:q:22:ILE:HG12	2.10	0.52
1:0:581:C:H2'	1:0:582:A:H8	1.74	0.52
36:g:143:ARG:NH1	36:g:144:LEU:HD21	2.25	0.52
1:0:2812:G:H2'	1:0:2813:A:C8	2.45	0.52
3:2:144:G:H2'	3:2:145:G:C8	2.44	0.52
37:h:145:ILE:HD13	37:h:178:MET:HB2	1.91	0.52
3:2:171:A:H2'	3:2:172:A:C8	2.44	0.51
3:2:390:U:H2'	3:2:391:G:C8	2.44	0.51
1:0:1386:C:H2'	1:0:1387:A:C8	2.45	0.51
22:Q:24:MET:HE1	22:Q:30:ILE:HG22	1.92	0.51
1:0:832:U:H2'	1:0:833:A:H8	1.75	0.51
1:0:2394:C:H5"	14:I:63:LYS:HE2	1.93	0.51
10:E:124:GLU:HG2	10:E:134:LYS:HZ1	1.76	0.51
3:2:539:A:H2'	3:2:540:G:C8	2.45	0.51
3:2:1314:C:H2'	3:2:1315:U:C6	2.44	0.51
35:f:114:LEU:HD13	35:f:144:LEU:HD22	1.92	0.51
42:m:75:GLN:O	42:m:79:ILE:HG12	2.09	0.51
1:0:593:U:H2'	1:0:594:U:C6	2.46	0.51
3:2:269:C:H2'	3:2:270:A:H8	1.74	0.51
3:2:1356:G:H2'	3:2:1357:A:H8	1.75	0.51
1:0:76:C:O2'	27:V:55:THR:HG21	2.10	0.51
3:2:946:A:H2'	3:2:947:G:H8	1.74	0.51
42:m:26:GLY:HA2	42:m:61:LEU:O	2.11	0.51
3:2:5:U:H4'	3:2:6:G:O5'	2.10	0.51
43:n:7:ARG:HG2	43:n:75:ASP:HB3	1.92	0.51
51:v:36:SER:HA	51:v:72:ASP:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1323:G:H2'	3:2:1324:A:C8	2.46	0.51
44:o:67:ALA:HB2	44:o:96:THR:HG23	1.92	0.51
1:0:191:A:H2'	1:0:192:C:H6	1.76	0.51
15:J:75:GLU:HB2	15:J:90:GLU:HG3	1.92	0.50
22:Q:76:ARG:HG2	22:Q:76:ARG:HH11	1.75	0.50
49:t:5:ARG:HH12	49:t:24:SER:HA	1.76	0.50
11:F:1:MET:HB3	11:F:3:VAL:HG13	1.92	0.50
1:0:2329:U:H2'	1:0:2330:G:H8	1.76	0.50
6:A:29:PRO:HG2	6:A:34:LEU:HD11	1.93	0.50
35:f:15:HIS:HB3	35:f:43:LEU:HD11	1.94	0.50
1:0:272:A:H2'	1:0:273:G:C8	2.46	0.50
1:0:1028:A:H2'	1:0:1029:A:C8	2.47	0.50
1:0:1869:G:H2'	1:0:1871:A:OP2	2.12	0.50
1:0:2071:A:H2'	1:0:2072:C:C6	2.47	0.50
3:2:4:U:H2'	3:2:5:U:H2'	1.94	0.50
3:2:864:A:H2'	3:2:865:A:C8	2.46	0.50
44:o:16:VAL:HG12	44:o:18:ASP:H	1.75	0.50
1:0:2192:U:H2'	1:0:2193:G:H8	1.76	0.50
47:r:42:TRP:O	47:r:46:LEU:HD12	2.11	0.50
1:0:45:G:H5'	1:0:46:G:OP1	2.12	0.50
3:2:780:A:H5"	44:o:125:LYS:HD3	1.94	0.50
3:2:1477:U:H2'	3:2:1478:U:C6	2.47	0.50
10:E:149:ARG:HG2	10:E:149:ARG:HH11	1.77	0.50
42:m:52:LEU:HB3	42:m:58:VAL:HG23	1.93	0.50
53:x:35:VAL:HG11	53:x:79:LEU:HD13	1.93	0.50
1:0:2273:A:H2'	1:0:2274:A:C8	2.46	0.49
3:2:728:A:H2'	3:2:729:A:C8	2.47	0.49
36:g:42:TYR:OH	36:g:90:VAL:HG11	2.13	0.49
23:R:28:VAL:HG22	23:R:34:VAL:HG12	1.95	0.49
10:E:105:LEU:HB3	10:E:107:LEU:HD21	1.95	0.49
46:q:49:SER:HB3	46:q:52:GLN:HG3	1.94	0.49
1:0:742:A:H2'	1:0:743:A:H8	1.77	0.49
3:2:475:C:H2'	3:2:476:U:H6	1.78	0.49
8:C:194:LYS:HB2	8:C:194:LYS:HE3	1.54	0.49
41:l:29:SER:OG	41:l:59:LEU:HB3	2.12	0.49
50:u:12:VAL:HG12	50:u:23:VAL:HG22	1.93	0.49
36:g:77:ILE:HD13	36:g:84:VAL:HG21	1.95	0.49
1:0:2030:A:C2	1:0:2499:C:H5"	2.48	0.49
3:2:1490:U:H2'	3:2:1491:G:C8	2.48	0.49
1:0:820:A:H4'	1:0:836:G:H22	1.76	0.49
3:2:235:C:H2'	3:2:236:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1238:A:N7	3:2:1303:C:H1'	2.28	0.49
43:n:65:TYR:OH	47:r:85:ARG:HG3	2.13	0.49
1:0:581:C:H2'	1:0:582:A:C8	2.47	0.48
1:0:1794:A:H2'	1:0:1795:C:C6	2.48	0.48
3:2:1340:A:O2'	5:4:32:OMC:H5"	2.13	0.48
6:A:258:ARG:HH22	6:A:263:THR:HG22	1.78	0.48
35:f:45:LYS:HG2	35:f:50:PHE:HB2	1.94	0.48
3:2:1071:C:H2'	3:2:1072:G:H8	1.78	0.48
17:L:25:ARG:HB2	17:L:93:ASP:OD1	2.13	0.48
1:0:1590:A:H2'	1:0:1591:A:C8	2.48	0.48
3:2:390:U:H2'	3:2:391:G:H8	1.79	0.48
35:f:68:LEU:HB3	35:f:161:LEU:HD12	1.95	0.48
54:y:34:ARG:HG2	54:y:34:ARG:HH11	1.78	0.48
1:0:2243:U:H2'	1:0:2244:U:C6	2.48	0.48
3:2:1490:U:H2'	3:2:1491:G:H8	1.79	0.48
13:H:65:THR:HG22	13:H:67:LYS:H	1.79	0.48
24:S:35:GLU:HB2	24:S:93:ARG:HH21	1.78	0.48
29:X:28:VAL:HG23	29:X:30:HIS:H	1.78	0.48
51:v:70:TYR:HB2	51:v:74:HIS:NE2	2.27	0.48
3:2:1137:C:H1'	3:2:1138:G:C2	2.49	0.48
36:g:127:ARG:HB2	36:g:127:ARG:CZ	2.43	0.48
40:k:115:SER:O	40:k:119:ARG:HG3	2.13	0.48
1:0:1432:G:H2'	1:0:1433:A:C8	2.49	0.48
1:0:1:G:H2'	1:0:2:G:H8	1.79	0.48
1:0:64:A:H2'	1:0:65:U:C6	2.49	0.48
1:0:1434:A:HO2'	1:0:1435:G:H8	1.62	0.48
3:2:1162:C:H2'	3:2:1163:A:C8	2.49	0.48
1:0:358:U:H2'	1:0:359:G:H8	1.77	0.48
10:E:80:THR:HG22	10:E:81:GLU:HG2	1.96	0.48
13:H:66:LYS:HB3	13:H:66:LYS:HE2	1.56	0.48
16:K:103:ARG:HB2	16:K:110:MET:HE3	1.96	0.48
50:u:13:VAL:HG22	50:u:22:VAL:HG23	1.96	0.48
17:L:13:ARG:HG2	17:L:13:ARG:HH11	1.78	0.47
1:0:1469:A:H2'	1:0:1470:A:C8	2.49	0.47
1:0:2192:U:H2'	1:0:2193:G:C8	2.49	0.47
1:0:2307:G:H4'	1:0:2308:G:O5'	2.14	0.47
8:C:139:LYS:HE3	8:C:139:LYS:HB2	1.67	0.47
15:J:57:VAL:HG11	15:J:105:MET:CE	2.44	0.47
41:l:96:MET:HE2	41:l:99:LEU:HB2	1.96	0.47
42:m:11:ARG:HB3	42:m:106:ARG:NH1	2.29	0.47
44:o:114:THR:HG21	54:y:28:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:p:102:LEU:HD23	45:p:102:LEU:H	1.78	0.47
1:0:284:U:H3	1:0:356:G:H1	1.61	0.47
1:0:357:C:H2'	1:0:358:U:C6	2.49	0.47
1:0:1746:A:H2'	1:0:1747:U:H6	1.79	0.47
1:0:2324:U:H3'	1:0:2325:G:C5'	2.44	0.47
43:n:10:LEU:HD12	43:n:22:THR:HG23	1.97	0.47
25:T:44:LYS:NZ	25:T:44:LYS:HB3	2.30	0.47
3:2:792:A:H4'	3:2:793:U:O5'	2.14	0.47
48:s:26:GLU:HG3	48:s:81:LEU:HD22	1.96	0.47
1:0:639:U:H2'	1:0:640:C:H6	1.80	0.47
1:0:2246:G:H2'	1:0:2247:A:C8	2.48	0.47
1:0:2554:U:H2'	1:0:2555:U:O2	2.15	0.47
3:2:948:C:H3'	46:q:105:ASN:HD22	1.80	0.47
3:2:1313:U:H2'	3:2:1314:C:C6	2.50	0.47
5:4:32:OMC:HM22	5:4:33:U:H5'	1.95	0.47
7:B:133:THR:CG2	7:B:134:HIS:H	2.25	0.47
1:0:2740:A:H2'	1:0:2741:A:C8	2.50	0.47
6:A:8:PRO:HB3	6:A:14:ARG:HG3	1.96	0.47
1:0:64:A:H2'	1:0:65:U:H6	1.80	0.47
1:0:973:A:H5"	20:O:81:LYS:HD2	1.96	0.47
1:0:1809:A:H2'	1:0:1810:A:C8	2.50	0.47
3:2:113:G:H1'	3:2:354:G:H5'	1.95	0.47
39:j:93:LYS:HB3	39:j:93:LYS:HE2	1.64	0.47
1:0:1:G:H2'	1:0:2:G:C8	2.50	0.47
1:0:191:A:H2'	1:0:192:C:C6	2.50	0.47
1:0:832:U:H2'	1:0:833:A:C8	2.50	0.47
1:0:2350:C:H2'	1:0:2351:G:O4'	2.15	0.47
1:0:1889:A:H2'	1:0:1890:A:C8	2.49	0.46
1:0:2591:C:H2'	1:0:2592:G:H8	1.80	0.46
3:2:56:U:H2'	3:2:57:G:H8	1.80	0.46
3:2:539:A:H2'	3:2:540:G:H8	1.80	0.46
3:2:1219:A:H5"	47:r:53:ARG:NH1	2.29	0.46
9:D:96:MET:HE2	9:D:96:MET:HB3	1.75	0.46
31:b:11:LEU:HB3	31:b:49:TYR:HB3	1.97	0.46
1:0:639:U:H2'	1:0:640:C:C6	2.50	0.46
1:0:2193:G:H2'	1:0:2194:U:H6	1.78	0.46
3:2:21:G:H2'	3:2:22:G:C8	2.50	0.46
3:2:269:C:H2'	3:2:270:A:C8	2.49	0.46
17:L:13:ARG:HG2	17:L:13:ARG:NH1	2.30	0.46
54:y:20:LYS:HB3	54:y:20:LYS:HE3	1.73	0.46
1:0:2636:C:H2'	1:0:2637:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:w:47:LEU:HD12	52:w:47:LEU:HA	1.82	0.46
1:0:2799:A:O2'	1:0:2800:A:H5"	2.15	0.46
3:2:820:U:H5	3:2:873:A:N7	2.13	0.46
1:0:645:C:H2'	1:0:647:G:N7	2.30	0.46
36:g:11:ARG:HB2	36:g:16:LYS:HG3	1.96	0.46
1:0:2025:C:H2'	1:0:2026:U:C6	2.49	0.46
3:2:555:U:H2'	3:2:556:C:C6	2.51	0.46
3:2:1201:A:H4'	3:2:1202:U:H5'	1.96	0.46
9:D:85:ILE:HD13	9:D:85:ILE:HA	1.83	0.46
10:E:149:ARG:HG2	10:E:149:ARG:NH1	2.31	0.46
45:p:114:ARG:HB3	45:p:119:VAL:HB	1.98	0.46
3:2:1162:C:H2'	3:2:1163:A:H8	1.80	0.46
14:I:82:LEU:HD22	14:I:90:VAL:HG21	1.98	0.46
35:f:60:ILE:HA	35:f:63:ARG:NH1	2.29	0.46
1:0:12:U:H2'	1:0:12:U:O2	2.16	0.46
1:0:306:U:H2'	1:0:307:G:O4'	2.16	0.46
1:0:356:G:H2'	1:0:357:C:C6	2.51	0.45
1:0:554:U:H2'	1:0:555:G:O4'	2.16	0.45
3:2:1273:C:H2'	3:2:1274:A:O4'	2.16	0.45
7:B:1:MET:HB2	7:B:2:ILE:H	1.67	0.45
9:D:29:PRO:HB2	9:D:169:LEU:HD12	1.98	0.45
35:f:154:MET:HE3	35:f:156:GLY:O	2.17	0.45
1:0:1386:C:H2'	1:0:1387:A:H8	1.81	0.45
1:0:1540:G:H2'	1:0:1541:C:O4'	2.16	0.45
3:2:384:G:H2'	3:2:385:C:C6	2.51	0.45
3:2:1287:A:H2'	3:2:1288:A:C8	2.51	0.45
14:I:36:LYS:H	14:I:36:LYS:HG3	1.57	0.45
1:0:1196:C:H2'	1:0:1197:G:C8	2.51	0.45
52:w:18:LYS:HE2	52:w:18:LYS:HA	1.98	0.45
3:2:590:U:OP1	41:l:31:LYS:HG3	2.17	0.45
11:F:9:VAL:HG12	11:F:35:LYS:HD3	1.98	0.45
41:l:29:SER:HB2	41:l:57:PRO:HB2	1.99	0.45
42:m:67:VAL:HG11	42:m:75:GLN:HB3	1.97	0.45
1:0:634:C:H2'	1:0:635:C:C6	2.51	0.45
1:0:947:A:H2'	1:0:948:C:C6	2.52	0.45
6:A:182:ARG:HG3	6:A:183:LYS:N	2.31	0.45
1:0:2591:C:H2'	1:0:2592:G:C8	2.51	0.45
3:2:1250:A:H4'	42:m:70:GLY:H	1.82	0.45
3:2:1530:G:H2'	3:2:1531:A:C8	2.52	0.45
39:j:38:ARG:HH21	39:j:63:ASN:ND2	2.15	0.45
46:q:71:ARG:O	46:q:75:MET:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:r:23:LYS:O	47:r:27:LEU:HB2	2.17	0.45
6:A:63:ARG:HD3	6:A:84:ASP:OD1	2.16	0.45
23:R:26:LYS:HG3	23:R:37:GLU:HG2	1.99	0.45
3:2:56:U:H2'	3:2:57:G:C8	2.51	0.45
36:g:112:ASP:OD1	36:g:115:LEU:HD12	2.17	0.45
3:2:1003:G:C6	3:2:1034:G:N2	2.84	0.45
12:G:92:MET:HE3	12:G:100:VAL:HG22	1.98	0.45
36:g:180:ALA:HB1	36:g:203:PHE:HE1	1.82	0.45
3:2:1131:G:H2'	3:2:1131:G:N3	2.32	0.44
6:A:117:GLN:HG3	6:A:118:SER:N	2.32	0.44
9:D:42:GLU:OE1	9:D:49:LEU:HD22	2.17	0.44
22:Q:76:ARG:HG2	22:Q:76:ARG:NH1	2.32	0.44
1:0:2451:A:H1'	5:4:76:A:H2'	1.99	0.44
1:0:2898:U:H2'	1:0:2899:A:C8	2.51	0.44
3:2:1218:C:H2'	3:2:1219:A:H8	1.77	0.44
32:c:43:THR:HG22	32:c:45:SER:H	1.82	0.44
3:2:79:G:H2'	3:2:80:A:C2	2.52	0.44
7:B:108:ASP:OD1	7:B:173:GLN:HA	2.17	0.44
13:H:1:MET:HB2	13:H:67:LYS:HG3	1.99	0.44
43:n:12:ALA:HB3	43:n:18:ILE:HG23	1.99	0.44
10:E:18:LYS:HB3	10:E:18:LYS:HE2	1.70	0.44
18:M:24:ASP:HB2	18:M:88:ARG:O	2.17	0.44
22:Q:8:LEU:HD13	27:V:22:LEU:HB3	2.00	0.44
37:h:99:ASP:OD2	37:h:133:ALA:HB1	2.18	0.44
54:y:34:ARG:HG2	54:y:34:ARG:NH1	2.31	0.44
43:n:37:ARG:NH2	43:n:77:VAL:HG22	2.31	0.44
3:2:576:C:H3'	3:2:577:G:H5"	1.99	0.44
10:E:85:LYS:HE2	10:E:85:LYS:HB3	1.86	0.44
29:X:11:GLU:HA	29:X:25:ARG:HG2	1.99	0.44
3:2:413:G:H2'	3:2:428:G:H22	1.81	0.44
3:2:664:G:H22	3:2:741:G:H1	1.64	0.44
3:2:722:G:H2'	3:2:722:G:N3	2.33	0.44
3:2:1513:A:H2'	3:2:1514:G:C8	2.53	0.44
35:f:47:VAL:HB	35:f:50:PHE:HE1	1.83	0.44
35:f:89:GLN:HE21	35:f:221:VAL:HG11	1.83	0.44
3:2:1492:A:H2'	3:2:1493:A:O4'	2.18	0.44
37:h:129:VAL:HG22	37:h:146:ARG:HD2	2.00	0.44
1:0:871:U:H2'	1:0:872:U:C6	2.53	0.44
1:0:1443:U:H2'	1:0:1444:G:H8	1.82	0.44
3:2:767:A:H8	3:2:1511:G:H21	1.64	0.44
5:4:50:U:H3	5:4:64:G:H1	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:54:LEU:HD12	11:F:57:LYS:HE2	1.99	0.44
11:F:110:VAL:HG11	11:F:132:PHE:HE2	1.83	0.44
23:R:91:LYS:HE2	23:R:91:LYS:HB3	1.77	0.44
40:k:60:GLU:O	40:k:64:VAL:HG12	2.18	0.44
1:0:969:G:H2'	1:0:970:U:C6	2.53	0.43
1:0:1000:A:H2'	1:0:1001:A:C8	2.53	0.43
1:0:1853:A:H2'	1:0:1854:A:C8	2.53	0.43
5:4:53:G:H3'	5:4:54:5MU:H73	1.99	0.43
6:A:107:PRO:HD2	6:A:110:LEU:HD22	2.00	0.43
46:q:65:VAL:HG23	46:q:66:GLU:H	1.83	0.43
1:0:760:G:H2'	1:0:761:A:O4'	2.17	0.43
1:0:1442:U:H2'	1:0:1443:U:C6	2.53	0.43
1:0:1486:U:H2'	1:0:1487:U:H6	1.83	0.43
11:F:110:VAL:HG11	11:F:132:PHE:CE2	2.53	0.43
53:x:28:MET:HE3	53:x:28:MET:HB3	1.86	0.43
1:0:414:C:H2'	1:0:415:A:C8	2.53	0.43
1:0:479:A:N3	1:0:481:G:H5"	2.33	0.43
1:0:2521:C:O2'	1:0:2564:A:H8	2.01	0.43
1:0:2897:U:H2'	1:0:2898:U:C6	2.53	0.43
3:2:1003:G:N7	3:2:1034:G:C2	2.86	0.43
3:2:1314:C:H2'	3:2:1315:U:H6	1.82	0.43
37:h:185:LYS:HD2	37:h:185:LYS:C	2.44	0.43
1:0:2051:A:H8	1:0:2051:A:OP2	2.02	0.43
3:2:89:U:H4'	3:2:90:C:O5'	2.18	0.43
3:2:459:A:H2'	3:2:460:A:H8	1.84	0.43
3:2:978:A:C4	3:2:1319:A:C2	3.06	0.43
40:k:22:LEU:O	40:k:101:MET:HE1	2.18	0.43
1:0:2074:U:H2'	1:0:2075:U:C6	2.53	0.43
3:2:440:C:C2	3:2:441:A:C8	3.06	0.43
3:2:524:G:H2'	3:2:525:C:C6	2.54	0.43
3:2:834:U:H2'	3:2:835:U:C6	2.53	0.43
3:2:1013:G:H4'	52:w:14:HIS:CE1	2.54	0.43
9:D:15:LYS:HB2	9:D:15:LYS:NZ	2.33	0.43
12:G:88:THR:OG1	12:G:91:GLU:HG3	2.18	0.43
45:p:87:VAL:HG11	45:p:90:LEU:HD12	2.01	0.43
1:0:1511:G:H2'	1:0:1512:C:H6	1.84	0.43
1:0:1597:A:H5"	1:0:1598:A:H5'	2.00	0.43
3:2:147:G:H2'	3:2:148:G:H8	1.79	0.43
3:2:320:A:H2'	3:2:321:A:O4'	2.19	0.43
25:T:43:THR:O	25:T:43:THR:HG23	2.18	0.43
53:x:37:ALA:O	53:x:40:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:657:U:H2'	1:0:658:U:C6	2.52	0.43
1:0:1506:U:H2'	1:0:1507:C:C6	2.54	0.43
1:0:1542:U:H2'	1:0:1543:G:O4'	2.18	0.43
3:2:475:C:H2'	3:2:476:U:C6	2.54	0.43
8:C:189:THR:O	8:C:193:VAL:HG23	2.18	0.43
25:T:39:ARG:HE	25:T:39:ARG:HB3	1.64	0.43
33:d:3:LYS:H	33:d:3:LYS:HG3	1.64	0.43
35:f:117:LEU:HD12	35:f:117:LEU:O	2.19	0.43
39:j:10:VAL:HB	39:j:58:HIS:HB3	2.01	0.43
54:y:31:GLU:O	54:y:35:ARG:HG3	2.19	0.43
1:0:5:A:H2'	1:0:6:A:C8	2.54	0.43
1:0:1187:G:H5'	20:O:83:TYR:CE1	2.54	0.43
35:f:57:LEU:HD23	35:f:57:LEU:HA	1.83	0.43
39:j:45:ARG:O	39:j:56:LYS:HA	2.18	0.43
42:m:19:VAL:HG21	42:m:83:ILE:HG12	2.00	0.43
3:2:1138:G:H3'	3:2:1138:G:N3	2.34	0.43
6:A:154:LEU:HD22	6:A:176:LEU:HD22	2.01	0.43
18:M:113:ARG:HE	18:M:115:ASN:HD21	1.67	0.43
45:p:34:CYS:HA	45:p:55:VAL:HG12	2.00	0.43
1:0:1027:A:C2	1:0:2488:G:H5'	2.53	0.43
1:0:1486:U:H2'	1:0:1487:U:C6	2.54	0.43
3:2:576:C:H3'	3:2:577:G:C5'	2.49	0.43
9:D:115:ARG:HD2	46:q:71:ARG:HH22	1.84	0.43
52:w:5:LEU:C	52:w:6:LYS:HG3	2.43	0.43
8:C:97:ASN:HB2	8:C:100:MET:CG	2.49	0.42
37:h:9:LEU:HD23	37:h:32:CYS:HB3	2.00	0.42
40:k:129:GLU:OE2	40:k:131:LYS:HB3	2.19	0.42
42:m:6:TYR:HE2	42:m:90:TYR:HD1	1.67	0.42
1:0:1327:A:H2'	1:0:1328:A:O4'	2.19	0.42
3:2:918:A:H2'	3:2:919:A:C8	2.54	0.42
3:2:1527:U:OP2	54:y:42:THR:HG23	2.19	0.42
10:E:130:GLU:OE1	10:E:130:GLU:HA	2.19	0.42
48:s:88:ARG:HA	48:s:88:ARG:CZ	2.50	0.42
1:0:973:A:H5'	1:0:1188:U:H1'	2.01	0.42
1:0:1433:A:O2'	1:0:1434:A:H5'	2.18	0.42
3:2:1305:G:H1'	3:2:1332:A:H61	1.84	0.42
13:H:7:MET:SD	13:H:20:MET:HG3	2.60	0.42
1:0:1805:A:H1'	6:A:50:THR:HG23	2.01	0.42
1:0:2291:U:H2'	1:0:2292:U:C6	2.54	0.42
3:2:712:A:H2'	3:2:713:G:C8	2.55	0.42
3:2:908:A:H2'	3:2:909:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:143:LEU:HD13	8:C:146:VAL:HG11	2.02	0.42
36:g:129:MET:HB2	36:g:132:ARG:HG3	2.02	0.42
1:0:2:G:H2'	1:0:3:U:C6	2.54	0.42
2:1:1:U:H2'	2:1:2:G:H8	1.85	0.42
3:2:393:A:C2	3:2:394:G:C8	3.07	0.42
3:2:675:A:H4'	51:v:73:ARG:HH12	1.85	0.42
3:2:792:A:H4'	3:2:793:U:C5'	2.50	0.42
3:2:1001:C:H2'	3:2:1002:G:C8	2.54	0.42
3:2:1368:A:OP2	42:m:114:LYS:HG2	2.19	0.42
9:D:108:VAL:HG11	9:D:176:PRO:HG3	2.01	0.42
16:K:20:MET:HE2	16:K:20:MET:HB3	1.85	0.42
22:Q:24:MET:HE1	22:Q:30:ILE:CG2	2.50	0.42
35:f:167:ASP:HB2	35:f:191:SER:OG	2.19	0.42
44:o:24:HIS:HD1	44:o:24:HIS:C	2.28	0.42
1:0:634:C:H2'	1:0:635:C:H6	1.84	0.42
1:0:1196:C:H2'	1:0:1197:G:H8	1.84	0.42
3:2:713:G:H2'	3:2:714:G:C8	2.54	0.42
12:G:106:LYS:HE3	12:G:106:LYS:HB2	1.87	0.42
15:J:45:GLN:HE22	15:J:125:PRO:CD	2.33	0.42
40:k:2:PRO:HB2	40:k:3:ARG:H	1.65	0.42
42:m:90:TYR:CD2	42:m:91:ASP:HB2	2.54	0.42
1:0:150:U:H2'	1:0:151:C:C6	2.55	0.42
1:0:2557:G:H2'	1:0:2558:C:C6	2.55	0.42
3:2:501:C:H2'	3:2:502:A:C8	2.55	0.42
3:2:1044:A:N7	3:2:1045:C:H1'	2.35	0.42
6:A:97:LYS:HE2	6:A:97:LYS:HB3	1.70	0.42
14:I:77:ILE:HD12	14:I:108:ALA:HB1	2.02	0.42
18:M:111:LYS:HB3	18:M:111:LYS:HE3	1.75	0.42
19:N:83:LEU:HD22	19:N:88:VAL:HG21	2.02	0.42
20:O:51:VAL:HG23	20:O:51:VAL:O	2.19	0.42
24:S:43:ASP:OD2	24:S:46:LYS:HG3	2.20	0.42
35:f:20:THR:HG23	35:f:37:LYS:O	2.20	0.42
41:l:11:LEU:HD22	41:l:75:ILE:HD11	2.02	0.42
46:q:33:ILE:HG23	46:q:59:GLU:HG2	2.02	0.42
48:s:88:ARG:HA	48:s:88:ARG:NE	2.34	0.42
1:0:1682:G:H2'	1:0:1683:U:C6	2.54	0.42
1:0:1915:U:H2'	1:0:1916:A:O4'	2.20	0.42
1:0:2795:C:H2'	1:0:2796:U:C6	2.55	0.42
9:D:26:MET:HE3	9:D:26:MET:HB3	1.82	0.42
18:M:9:GLU:O	18:M:13:MET:HG3	2.20	0.42
36:g:62:LYS:HD3	36:g:62:LYS:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:k:59:LEU:O	40:k:63:GLU:HG2	2.19	0.42
1:0:288:U:H2'	1:0:289:G:H8	1.85	0.42
1:0:2194:U:H2'	1:0:2195:U:H6	1.84	0.42
3:2:191:G:H2'	3:2:192:A:C8	2.55	0.42
3:2:982:U:H4'	3:2:983:A:O5'	2.20	0.42
42:m:54:LEU:HD23	42:m:98:LEU:HD23	2.01	0.42
50:u:9:GLN:NE2	50:u:79:VAL:HG11	2.34	0.42
52:w:50:ALA:HB1	52:w:57:HIS:HB3	2.00	0.42
1:0:172:A:H2'	1:0:173:A:C8	2.55	0.42
1:0:979:A:H2'	1:0:982:C:H42	1.84	0.42
1:0:1902:C:H4'	6:A:242:LYS:O	2.19	0.42
3:2:792:A:H1'	3:2:794:A:N7	2.34	0.42
43:n:51:VAL:HG22	47:r:81:ARG:HB2	2.02	0.42
1:0:576:U:H2'	1:0:577:G:C8	2.55	0.41
1:0:2086:U:H2'	1:0:2087:G:C8	2.55	0.41
3:2:3:A:H5"	3:2:4:U:O4'	2.20	0.41
3:2:191:G:H2'	3:2:192:A:H8	1.85	0.41
7:B:183:GLU:HG3	7:B:184:ARG:HG2	2.02	0.41
36:g:114:LYS:HD3	36:g:185:ASN:OD1	2.20	0.41
36:g:129:MET:HE3	36:g:129:MET:HB3	1.89	0.41
36:g:169:ARG:HG2	36:g:170:GLU:N	2.35	0.41
37:h:159:LEU:HA	37:h:159:LEU:HD12	1.81	0.41
44:o:24:HIS:C	44:o:24:HIS:ND1	2.78	0.41
44:o:117:PRO:HG2	54:y:35:ARG:HE	1.85	0.41
1:0:373:U:H2'	1:0:374:A:H8	1.85	0.41
2:1:66:A:H61	2:1:107:G:H2'	1.85	0.41
9:D:48:LYS:HD2	9:D:48:LYS:HA	1.67	0.41
15:J:95:LEU:HD23	15:J:95:LEU:HA	1.87	0.41
35:f:108:ARG:O	35:f:111:ILE:HG13	2.20	0.41
36:g:114:LYS:O	36:g:118:ASP:HB2	2.20	0.41
41:l:40:LEU:HB3	41:l:46:ILE:HG12	2.01	0.41
44:o:26:SER:O	44:o:90:GLY:HA3	2.20	0.41
3:2:564:C:OP1	45:p:12:ARG:HD2	2.20	0.41
3:2:1144:G:N2	3:2:1146:A:H62	2.19	0.41
9:D:8:TYR:O	9:D:13:VAL:HG23	2.20	0.41
18:M:63:LYS:HB2	18:M:63:LYS:HE2	1.76	0.41
22:Q:4:GLU:OE1	27:V:19:LEU:HD21	2.20	0.41
41:l:69:LYS:HB3	41:l:69:LYS:HE2	1.73	0.41
46:q:33:ILE:HD13	46:q:60:VAL:HG22	2.02	0.41
1:0:1315:C:H2'	1:0:1316:U:C6	2.56	0.41
1:0:1716:U:H2'	1:0:1717:A:H8	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2661:G:H2'	1:0:2662:A:C8	2.55	0.41
3:2:21:G:H2'	3:2:22:G:H8	1.85	0.41
3:2:64:G:H4'	3:2:65:A:H5"	2.00	0.41
3:2:246:A:C2	3:2:282:A:C5	3.08	0.41
3:2:422:C:H4'	3:2:423:G:O5'	2.20	0.41
24:S:41:GLU:C	24:S:42:LEU:HD23	2.45	0.41
43:n:80:THR:OG1	43:n:83:THR:HG23	2.21	0.41
51:v:14:THR:HG21	51:v:48:ARG:HD3	2.01	0.41
1:0:1047:G:N2	1:0:1111:A:C5	2.88	0.41
1:0:2037:A:H2'	1:0:2038:G:C8	2.56	0.41
2:1:106:G:H2'	2:1:107:G:O4'	2.19	0.41
3:2:1530:G:H2'	3:2:1531:A:H8	1.85	0.41
6:A:132:MET:HE3	6:A:190:ALA:HB2	2.03	0.41
9:D:3:LYS:HD2	9:D:3:LYS:C	2.46	0.41
21:P:70:LYS:HB2	21:P:70:LYS:HE2	1.83	0.41
44:o:30:THR:HG21	44:o:63:ALA:HB2	2.02	0.41
1:0:84:A:N6	1:0:99:U:H5'	2.35	0.41
1:0:250:G:H2'	1:0:251:A:C8	2.56	0.41
1:0:419:U:H2'	1:0:420:C:C6	2.56	0.41
1:0:1443:U:H2'	1:0:1444:G:C8	2.56	0.41
1:0:2809:A:H2'	1:0:2810:A:C8	2.56	0.41
3:2:206:C:H2'	3:2:207:C:C6	2.55	0.41
3:2:580:C:H2'	3:2:581:G:O4'	2.21	0.41
3:2:868:C:H2'	3:2:869:G:O4'	2.20	0.41
3:2:1147:C:H2'	3:2:1148:U:C6	2.56	0.41
5:4:23:C:H2'	5:4:24:U:C6	2.56	0.41
12:G:39:LYS:HE2	12:G:39:LYS:HB3	1.90	0.41
18:M:114:LEU:HD23	18:M:114:LEU:HA	1.90	0.41
35:f:42:ASN:O	35:f:43:LEU:HB2	2.20	0.41
47:r:89:MET:HE1	47:r:98:LYS:HD3	2.02	0.41
50:u:17:MET:HB2	50:u:20:SER:HB2	2.03	0.41
1:0:152:A:H2'	1:0:153:U:C6	2.55	0.41
1:0:1149:G:H2'	1:0:1150:C:C6	2.55	0.41
23:R:26:LYS:HE3	23:R:26:LYS:HB3	1.88	0.41
37:h:88:GLU:HG2	37:h:188:ARG:HB2	2.03	0.41
37:h:188:ARG:HA	37:h:191:LEU:HD12	2.03	0.41
41:l:9:ASP:O	41:l:13:ARG:HG3	2.20	0.41
1:0:2728:U:O2'	1:0:2729:G:H8	2.03	0.41
3:2:1129:C:H2'	3:2:1139:G:N7	2.36	0.41
9:D:9:LYS:HE2	9:D:9:LYS:HB3	1.95	0.41
13:H:51:LYS:NZ	13:H:96:GLY:HA2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:K:109:PRO:O	16:K:110:MET:HE2	2.21	0.41
36:g:16:LYS:HE3	36:g:16:LYS:HB3	1.82	0.41
40:k:143:ARG:HD2	40:k:143:ARG:HA	1.81	0.41
1:0:12:U:O2	1:0:2626:C:H4'	2.21	0.41
1:0:172:A:H2'	1:0:173:A:H8	1.84	0.41
1:0:967:U:H2'	1:0:968:C:C6	2.56	0.41
1:0:1511:G:H2'	1:0:1512:C:C6	2.55	0.41
1:0:1808:A:H3'	1:0:1809:A:H8	1.85	0.41
1:0:2637:U:H2'	1:0:2638:G:O4'	2.21	0.41
3:2:38:G:H22	3:2:397:A:H5'	1.86	0.41
3:2:166:U:H2'	3:2:167:A:H8	1.85	0.41
7:B:5:VAL:H	7:B:32:ASN:HD21	1.68	0.41
9:D:88:LYS:HG2	9:D:89:VAL:N	2.36	0.41
13:H:1:MET:HE3	13:H:32:TYR:CZ	2.56	0.41
13:H:65:THR:HG22	13:H:67:LYS:N	2.35	0.41
18:M:13:MET:HE2	18:M:13:MET:HB3	1.86	0.41
40:k:27:VAL:HG22	40:k:43:VAL:HG11	2.03	0.41
3:2:987:G:H21	3:2:1013:G:H22	1.68	0.41
6:A:245:VAL:HG12	6:A:251:GLN:HA	2.02	0.41
9:D:77:PHE:C	9:D:78:LYS:HG2	2.46	0.41
18:M:33:VAL:HG22	18:M:38:LYS:HG2	2.02	0.41
21:P:28:LYS:HE3	21:P:28:LYS:HB3	1.82	0.41
27:V:51:ALA:O	27:V:55:THR:HG22	2.21	0.41
43:n:17:LEU:HD23	43:n:17:LEU:HA	1.86	0.41
1:0:18:U:H2'	1:0:19:A:C8	2.55	0.40
1:0:1370:C:H2'	1:0:1371:G:O4'	2.21	0.40
3:2:519:C:H2'	3:2:520:A:O4'	2.20	0.40
3:2:1062:U:H2'	3:2:1063:C:C6	2.56	0.40
3:2:1313:U:H2'	3:2:1314:C:H6	1.86	0.40
3:2:1524:C:H2'	3:2:1525:G:C8	2.56	0.40
14:I:78:ARG:HG2	14:I:113:ALA:HB3	2.02	0.40
24:S:30:ILE:HG12	24:S:91:PHE:HB2	2.03	0.40
39:j:51:ILE:O	39:j:54:LEU:HB2	2.20	0.40
1:0:1494:A:H2'	1:0:1495:A:C8	2.55	0.40
1:0:1596:A:H2'	1:0:1597:A:C8	2.55	0.40
1:0:2845:U:H5"	18:M:52:ASN:O	2.21	0.40
2:1:1:U:H2'	2:1:2:G:C8	2.56	0.40
3:2:512:U:H2'	3:2:513:C:C6	2.57	0.40
3:2:1169:A:H2'	3:2:1170:A:C8	2.56	0.40
3:2:1258:G:H2'	3:2:1259:C:C6	2.57	0.40
3:2:1493:A:O2'	3:2:1494:G:H8	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:129:THR:HG22	7:B:130:GLN:O	2.22	0.40
35:f:76:ALA:O	35:f:80:VAL:HG13	2.21	0.40
35:f:114:LEU:HB2	35:f:144:LEU:HD22	2.02	0.40
40:k:16:PRO:HD2	40:k:44:TYR:OH	2.22	0.40
44:o:23:ILE:HG12	44:o:96:THR:HG21	2.03	0.40
1:0:414:C:H2'	1:0:415:A:H8	1.86	0.40
1:0:680:C:H2'	1:0:681:G:C8	2.56	0.40
1:0:1361:G:H2'	1:0:1362:C:C6	2.56	0.40
1:0:2292:U:H2'	1:0:2293:G:H8	1.86	0.40
1:0:2485:G:O3'	15:J:125:PRO:HB3	2.21	0.40
3:2:165:G:H2'	3:2:166:U:C6	2.56	0.40
15:J:12:MET:HG2	15:J:72:PRO:HD2	2.03	0.40
35:f:54:LEU:HA	35:f:57:LEU:HB2	2.03	0.40
36:g:150:LYS:HG2	36:g:201:TRP:CE3	2.56	0.40
40:k:47:LEU:HD23	40:k:47:LEU:HA	1.80	0.40
41:l:29:SER:HA	41:l:59:LEU:HD22	2.04	0.40
46:q:69:LEU:O	46:q:73:ILE:HD12	2.21	0.40
1:0:2241:A:H2'	1:0:2242:G:C8	2.56	0.40
3:2:1088:G:H21	3:2:1167:A:H62	1.69	0.40
14:I:70:LYS:HE3	14:I:70:LYS:HB2	1.78	0.40
45:p:99:ARG:HE	45:p:99:ARG:HB3	1.71	0.40
3:2:428:G:H1'	3:2:429:U:OP2	2.21	0.40
9:D:121:SER:HB3	9:D:128:TYR:CE1	2.57	0.40
11:F:54:LEU:O	11:F:57:LYS:HG2	2.21	0.40
16:K:8:ARG:HD2	16:K:43:GLU:HG2	2.03	0.40
45:p:86:ARG:HD2	45:p:87:VAL:O	2.22	0.40
47:r:42:TRP:NE1	47:r:46:LEU:HD11	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	A	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
7	B	206/209 (99%)	201 (98%)	5 (2%)	0	100	100
8	C	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
9	D	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
10	E	171/177 (97%)	165 (96%)	6 (4%)	0	100	100
11	F	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
12	G	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
13	H	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
14	I	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
15	J	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
16	K	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
17	L	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
18	M	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
19	N	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
20	O	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
21	P	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
22	Q	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
23	R	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
24	S	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
25	T	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
26	U	75/78 (96%)	75 (100%)	0	0	100	100
27	V	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
28	W	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
29	X	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
30	a	53/57 (93%)	53 (100%)	0	0	100	100
31	b	49/55 (89%)	49 (100%)	0	0	100	100
32	c	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
33	d	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
34	e	36/38 (95%)	36 (100%)	0	0	100	100
35	f	222/241 (92%)	206 (93%)	16 (7%)	0	100	100
36	g	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
37	h	203/206 (98%)	201 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	i	153/167 (92%)	148 (97%)	5 (3%)	0	100	100
39	j	104/131 (79%)	103 (99%)	1 (1%)	0	100	100
40	k	149/179 (83%)	144 (97%)	5 (3%)	0	100	100
41	l	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
42	m	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
43	n	97/103 (94%)	93 (96%)	4 (4%)	0	100	100
44	o	115/129 (89%)	110 (96%)	5 (4%)	0	100	100
45	p	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
46	q	112/118 (95%)	99 (88%)	13 (12%)	0	100	100
47	r	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
48	s	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
49	t	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
50	u	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
51	v	64/75 (85%)	64 (100%)	0	0	100	100
52	w	77/92 (84%)	70 (91%)	7 (9%)	0	100	100
53	x	84/87 (97%)	84 (100%)	0	0	100	100
54	y	68/71 (96%)	68 (100%)	0	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.

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	
6	A	216/218 (99%)	214 (99%)	2 (1%)	70	84
7	B	164/164 (100%)	160 (98%)	4 (2%)	43	63
8	C	165/165 (100%)	159 (96%)	6 (4%)	31	50
9	D	148/150 (99%)	141 (95%)	7 (5%)	23	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	E	134/138 (97%)	130 (97%)	4 (3%)	36	56
11	F	114/114 (100%)	107 (94%)	7 (6%)	17	28
12	G	116/116 (100%)	112 (97%)	4 (3%)	32	52
13	H	104/104 (100%)	103 (99%)	1 (1%)	68	82
14	I	103/103 (100%)	98 (95%)	5 (5%)	22	37
15	J	109/109 (100%)	104 (95%)	5 (5%)	24	39
16	K	98/103 (95%)	94 (96%)	4 (4%)	27	44
17	L	86/87 (99%)	83 (96%)	3 (4%)	32	51
18	M	99/100 (99%)	95 (96%)	4 (4%)	28	45
19	N	89/90 (99%)	88 (99%)	1 (1%)	65	81
20	O	84/84 (100%)	81 (96%)	3 (4%)	31	50
21	P	93/93 (100%)	91 (98%)	2 (2%)	45	66
22	Q	80/84 (95%)	75 (94%)	5 (6%)	16	27
23	R	83/85 (98%)	78 (94%)	5 (6%)	17	29
24	S	78/78 (100%)	73 (94%)	5 (6%)	16	26
25	T	57/63 (90%)	57 (100%)	0	100	100
26	U	67/68 (98%)	66 (98%)	1 (2%)	57	75
27	V	54/55 (98%)	51 (94%)	3 (6%)	19	31
28	W	47/49 (96%)	44 (94%)	3 (6%)	16	26
29	X	55/62 (89%)	54 (98%)	1 (2%)	51	71
30	a	46/48 (96%)	46 (100%)	0	100	100
31	b	46/49 (94%)	45 (98%)	1 (2%)	45	66
32	c	38/38 (100%)	36 (95%)	2 (5%)	20	34
33	d	51/52 (98%)	50 (98%)	1 (2%)	48	68
34	e	34/34 (100%)	34 (100%)	0	100	100
35	f	186/199 (94%)	181 (97%)	5 (3%)	39	60
36	g	170/190 (90%)	162 (95%)	8 (5%)	23	39
37	h	172/173 (99%)	163 (95%)	9 (5%)	21	34
38	i	118/126 (94%)	115 (98%)	3 (2%)	42	62
39	j	92/112 (82%)	90 (98%)	2 (2%)	45	66
40	k	124/147 (84%)	117 (94%)	7 (6%)	19	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	l	104/105 (99%)	97 (93%)	7 (7%)	15	24
42	m	105/107 (98%)	98 (93%)	7 (7%)	15	24
43	n	87/90 (97%)	79 (91%)	8 (9%)	8	13
44	o	90/99 (91%)	87 (97%)	3 (3%)	33	53
45	p	103/104 (99%)	100 (97%)	3 (3%)	37	57
46	q	92/96 (96%)	89 (97%)	3 (3%)	33	53
47	r	83/84 (99%)	83 (100%)	0	100	100
48	s	76/77 (99%)	74 (97%)	2 (3%)	40	61
49	t	65/65 (100%)	64 (98%)	1 (2%)	57	75
50	u	74/78 (95%)	72 (97%)	2 (3%)	39	60
51	v	57/65 (88%)	56 (98%)	1 (2%)	51	71
52	w	70/79 (89%)	70 (100%)	0	100	100
53	x	65/66 (98%)	61 (94%)	4 (6%)	16	27
54	y	60/61 (98%)	59 (98%)	1 (2%)	53	73
All	All	4651/4826 (96%)	4486 (96%)	165 (4%)	32	51

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	A	97	LYS
6	A	219	THR
7	B	40	LEU
7	B	84	LEU
7	B	107	VAL
7	B	168	GLU
8	C	80	SER
8	C	115	GLN
8	C	126	VAL
8	C	139	LYS
8	C	163	ASN
8	C	166	LYS
9	D	26	MET
9	D	48	LYS
9	D	87	CYS
9	D	90	THR
9	D	91	LEU
9	D	102	ARG

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Mol	Chain	Res	Type
9	D	155	THR
10	E	10	VAL
10	E	36	THR
10	E	106	SER
10	E	128	GLN
11	F	15	LEU
11	F	22	LYS
11	F	57	LYS
11	F	72	ILE
11	F	115	VAL
11	F	121	VAL
11	F	144	VAL
12	G	11	VAL
12	G	62	VAL
12	G	64	VAL
12	G	69	ARG
13	H	76	VAL
14	I	36	LYS
14	I	77	ILE
14	I	120	VAL
14	I	122	VAL
14	I	142	ILE
15	J	7	THR
15	J	10	ARG
15	J	67	VAL
15	J	95	LEU
15	J	133	LYS
16	K	15	SER
16	K	30	ARG
16	K	33	ILE
16	K	95	THR
17	L	12	THR
17	L	49	VAL
17	L	100	HIS
18	M	6	LYS
18	M	32	VAL
18	M	37	LYS
18	M	93	ARG
19	N	9	ILE
20	O	58	VAL
20	O	84	ARG
20	O	97	LYS

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Mol	Chain	Res	Type
21	P	73	LYS
21	P	83	LYS
22	Q	12	ARG
22	Q	18	GLU
22	Q	24	MET
22	Q	32	LEU
22	Q	63	VAL
23	R	12	ILE
23	R	43	LYS
23	R	46	GLN
23	R	66	GLN
23	R	68	SER
24	S	1	MET
24	S	4	ILE
24	S	50	MET
24	S	77	VAL
24	S	87	GLN
26	U	35	SER
27	V	6	LEU
27	V	22	LEU
27	V	56	LEU
28	W	4	THR
28	W	21	LYS
28	W	45	ARG
29	X	13	THR
31	b	46	HIS
32	c	4	THR
32	c	29	GLN
33	d	3	LYS
35	f	38	VAL
35	f	116	ASP
35	f	122	GLN
35	f	161	LEU
35	f	174	LYS
36	g	94	ILE
36	g	121	THR
36	g	153	VAL
36	g	170	GLU
36	g	183	ASP
36	g	186	THR
36	g	188	GLU
36	g	207	ILE

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Mol	Chain	Res	Type
37	h	28	ILE
37	h	81	ARG
37	h	88	GLU
37	h	124	MET
37	h	134	SER
37	h	138	SER
37	h	181	THR
37	h	183	LYS
37	h	192	SER
38	i	61	GLN
38	i	117	VAL
38	i	156	LYS
39	j	64	VAL
39	j	74	LEU
40	k	12	ILE
40	k	23	LEU
40	k	32	VAL
40	k	75	VAL
40	k	94	VAL
40	k	125	SER
40	k	136	LYS
41	l	18	GLN
41	l	22	LYS
41	l	29	SER
41	l	74	SER
41	l	80	ARG
41	l	89	LYS
41	l	91	GLU
42	m	11	ARG
42	m	15	SER
42	m	35	LEU
42	m	65	ILE
42	m	67	VAL
42	m	119	ARG
42	m	123	ARG
43	n	37	ARG
43	n	51	VAL
43	n	63	ASP
43	n	66	GLU
43	n	71	LEU
43	n	76	ILE
43	n	78	GLU

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Mol	Chain	Res	Type
43	n	100	ILE
44	o	24	HIS
44	o	30	THR
44	o	57	LYS
45	p	43	LYS
45	p	82	ILE
45	p	102	LEU
46	q	13	LYS
46	q	25	VAL
46	q	52	GLN
48	s	48	LYS
48	s	75	VAL
49	t	1	MET
50	u	12	VAL
50	u	60	GLU
51	v	47	THR
53	x	6	SER
53	x	14	SER
53	x	28	MET
53	x	74	ARG
54	y	39	GLU

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

Mol	Chain	Res	Type
6	A	143	ASN
7	B	130	GLN
7	B	150	GLN
8	C	41	GLN
9	D	27	GLN
9	D	63	GLN
11	F	18	GLN
11	F	43	ASN
12	G	86	GLN
13	H	5	GLN
15	J	45	GLN
15	J	97	GLN
17	L	100	HIS
18	M	41	GLN
20	O	6	GLN
22	Q	48	GLN
22	Q	91	GLN

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Mol	Chain	Res	Type
24	S	44	HIS
27	V	25	GLN
29	X	61	ASN
34	e	33	HIS
35	f	94	HIS
36	g	3	GLN
36	g	6	HIS
37	h	54	GLN
37	h	164	GLN
37	h	196	ASN
44	o	22	HIS
45	p	73	ASN
46	q	105	ASN
51	v	54	GLN
52	w	57	HIS
53	x	3	ASN
53	x	52	ASN
53	x	55	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2754/2904 (94%)	313 (11%)	5 (0%)
2	1	119/120 (99%)	12 (10%)	0
3	2	1533/1542 (99%)	228 (14%)	28 (1%)
4	3	2/3 (66%)	0	0
5	4	76/77 (98%)	13 (17%)	1 (1%)
All	All	4484/4646 (96%)	566 (12%)	34 (0%)

All (566) 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	51	G
1	0	63	A
1	0	71	A
1	0	74	A
1	0	75	G

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Mol	Chain	Res	Type
1	0	88	G
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	162	U
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	224	U
1	0	233	A
1	0	248	G
1	0	266	G
1	0	272	A
1	0	281	C
1	0	282	A
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	353	C
1	0	362	A
1	0	372	G
1	0	385	C
1	0	386	G
1	0	396	G
1	0	404	A
1	0	405	U
1	0	411	G
1	0	412	A
1	0	413	C
1	0	424	G

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Mol	Chain	Res	Type
1	0	467	G
1	0	481	G
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	533	G
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	603	A
1	0	613	A
1	0	614	A
1	0	615	U
1	0	637	A
1	0	645	C
1	0	646	U
1	0	647	G
1	0	655	A
1	0	686	U
1	0	730	A
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	805	G
1	0	812	C
1	0	827	U
1	0	828	U
1	0	831	G
1	0	845	A
1	0	846	U
1	0	859	G
1	0	878	A

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Mol	Chain	Res	Type
1	0	894	U
1	0	895	U
1	0	910	A
1	0	914	G
1	0	931	U
1	0	946	C
1	0	953	G
1	0	961	C
1	0	974	G
1	0	983	A
1	0	996	A
1	0	1009	A
1	0	1012	U
1	0	1013	C
1	0	1026	G
1	0	1027	A
1	0	1033	U
1	0	1046	A
1	0	1047	G
1	0	1110	G
1	0	1111	A
1	0	1112	G
1	0	1116	G
1	0	1128	G
1	0	1132	U
1	0	1135	C
1	0	1136	G
1	0	1141	U
1	0	1142	A
1	0	1143	A
1	0	1172	C
1	0	1174	U
1	0	1175	A
1	0	1176	U
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

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Mol	Chain	Res	Type
1	0	1300	G
1	0	1301	A
1	0	1313	U
1	0	1345	C
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	1428	C
1	0	1435	G
1	0	1452	G
1	0	1456	G
1	0	1460	U
1	0	1482	G
1	0	1490	A
1	0	1493	C
1	0	1497	U
1	0	1509	A
1	0	1510	G
1	0	1515	A
1	0	1529	G
1	0	1530	G
1	0	1537	G
1	0	1540	G
1	0	1566	A
1	0	1569	A
1	0	1578	U
1	0	1585	C
1	0	1608	A
1	0	1616	A
1	0	1618	A
1	0	1622	G
1	0	1634	A
1	0	1647	U
1	0	1648	U
1	0	1674	G
1	0	1715	G
1	0	1729	U
1	0	1730	C
1	0	1733	G

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Mol	Chain	Res	Type
1	0	1738	G
1	0	1740	G
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	1829	A
1	0	1871	A
1	0	1872	A
1	0	1873	G
1	0	1882	U
1	0	1906	G
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	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	2036	C
1	0	2043	C
1	0	2055	C
1	0	2056	G

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Mol	Chain	Res	Type
1	0	2060	A
1	0	2061	G
1	0	2069	G
1	0	2194	U
1	0	2198	A
1	0	2204	G
1	0	2225	A
1	0	2234	G
1	0	2238	G
1	0	2239	G
1	0	2251	G
1	0	2273	A
1	0	2283	C
1	0	2287	A
1	0	2288	A
1	0	2294	G
1	0	2297	A
1	0	2308	G
1	0	2311	A
1	0	2312	U
1	0	2322	A
1	0	2325	G
1	0	2333	A
1	0	2345	G
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	2426	A
1	0	2429	G
1	0	2430	A
1	0	2441	U
1	0	2448	A
1	0	2465	C
1	0	2470	G
1	0	2475	C
1	0	2476	A

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Mol	Chain	Res	Type
1	0	2491	U
1	0	2492	U
1	0	2494	G
1	0	2498	C
1	0	2502	G
1	0	2503	A
1	0	2504	U
1	0	2505	G
1	0	2507	C
1	0	2518	A
1	0	2520	C
1	0	2529	G
1	0	2535	G
1	0	2547	A
1	0	2566	A
1	0	2567	G
1	0	2572	A
1	0	2578	G
1	0	2582	G
1	0	2602	A
1	0	2603	G
1	0	2609	U
1	0	2613	U
1	0	2615	U
1	0	2629	U
1	0	2646	C
1	0	2659	G
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	2765	A
1	0	2778	A
1	0	2820	A
1	0	2821	A
1	0	2832	U
1	0	2835	A

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Mol	Chain	Res	Type
1	0	2849	U
1	0	2867	G
1	0	2869	G
1	0	2873	A
1	0	2877	G
1	0	2880	C
1	0	2884	U
1	0	2886	A
1	0	2894	G
1	0	2903	U
2	1	13	G
2	1	35	C
2	1	41	G
2	1	44	G
2	1	45	A
2	1	56	G
2	1	67	G
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	39	G
3	2	47	C
3	2	48	C
3	2	51	A
3	2	65	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

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Mol	Chain	Res	Type
3	2	121	U
3	2	122	G
3	2	131	A
3	2	179	A
3	2	180	U
3	2	183	C
3	2	184	G
3	2	197	A
3	2	204	G
3	2	209	U
3	2	210	C
3	2	211	G
3	2	212	G
3	2	220	G
3	2	245	U
3	2	247	G
3	2	251	G
3	2	266	G
3	2	267	C
3	2	280	C
3	2	281	G
3	2	282	A
3	2	289	G
3	2	316	C
3	2	321	A
3	2	328	C
3	2	330	C
3	2	332	G
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	373	A
3	2	397	A
3	2	406	G
3	2	413	G
3	2	414	A
3	2	422	C
3	2	423	G
3	2	429	U

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Mol	Chain	Res	Type
3	2	448	A
3	2	468	A
3	2	474	G
3	2	481	G
3	2	484	G
3	2	495	A
3	2	496	A
3	2	497	G
3	2	509	A
3	2	511	C
3	2	518	C
3	2	521	G
3	2	524	G
3	2	529	G
3	2	531	U
3	2	532	A
3	2	535	A
3	2	542	G
3	2	547	A
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	587	G
3	2	623	C
3	2	633	G
3	2	650	G
3	2	653	U
3	2	665	A
3	2	675	A
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	734	G
3	2	748	G

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Mol	Chain	Res	Type
3	2	755	G
3	2	760	G
3	2	777	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	871	U
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	990	C
3	2	992	U
3	2	993	G
3	2	1001	C
3	2	1006	G
3	2	1012	A
3	2	1020	G
3	2	1022	A
3	2	1025	U
3	2	1026	G
3	2	1027	C

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Mol	Chain	Res	Type
3	2	1028	C
3	2	1029	U
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
3	2	1095	U
3	2	1101	A
3	2	1102	A
3	2	1124	G
3	2	1125	U
3	2	1126	U
3	2	1136	C
3	2	1138	G
3	2	1139	G
3	2	1140	C
3	2	1153	G
3	2	1158	C
3	2	1159	U
3	2	1168	U
3	2	1171	A
3	2	1180	A
3	2	1183	U
3	2	1184	G
3	2	1187	G
3	2	1191	A
3	2	1196	A
3	2	1197	A
3	2	1202	U
3	2	1212	U
3	2	1214	C
3	2	1227	A
3	2	1236	A
3	2	1238	A
3	2	1240	U
3	2	1241	G
3	2	1256	A

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Mol	Chain	Res	Type
3	2	1258	G
3	2	1268	G
3	2	1280	A
3	2	1286	U
3	2	1287	A
3	2	1300	G
3	2	1301	U
3	2	1302	C
3	2	1303	C
3	2	1310	G
3	2	1316	G
3	2	1317	C
3	2	1320	C
3	2	1331	G
3	2	1336	C
3	2	1338	G
3	2	1346	A
3	2	1347	G
3	2	1353	G
3	2	1363	A
3	2	1364	U
3	2	1370	G
3	2	1374	A
3	2	1381	U
3	2	1398	A
3	2	1400	C
3	2	1432	G
3	2	1446	A
3	2	1487	G
3	2	1493	A
3	2	1497	G
3	2	1503	A
3	2	1504	G
3	2	1506	U
3	2	1517	G
3	2	1519	A
3	2	1520	C
3	2	1529	G
3	2	1530	G
3	2	1534	A
5	4	8	G
5	4	11	G

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Mol	Chain	Res	Type
5	4	15	C
5	4	16	C
5	4	18	G
5	4	19	G
5	4	20	U
5	4	22	G
5	4	23	C
5	4	31	G
5	4	44	A
5	4	55	U
5	4	76	A

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	546	U
1	0	1026	G
1	0	1111	A
1	0	2193	G
1	0	2307	G
3	2	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	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	1137	C

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Mol	Chain	Res	Type
3	2	1179	A
3	2	1182	G
3	2	1190	G
3	2	1201	A
3	2	1267	C
3	2	1399	C
5	4	10	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	5MU	4	54	5	19,22,23	0.42	0	28,32,35	0.57	0
5	OMC	4	32	5	19,22,23	0.60	0	26,31,34	0.86	1 (3%)
5	4SU	4	7	5	18,21,22	3.73	8 (44%)	26,30,33	2.20	4 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	5MU	4	54	5	-	0/7/25/26	0/2/2/2
5	OMC	4	32	5	-	1/9/27/28	0/2/2/2
5	4SU	4	7	5	-	0/7/25/26	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	7	4SU	C4-N3	7.73	1.45	1.37
5	4	7	4SU	C2-N3	7.11	1.50	1.38
5	4	7	4SU	C4-S4	-6.79	1.55	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	7	4SU	C6-C5	5.05	1.46	1.35
5	4	7	4SU	C2-N1	4.77	1.46	1.38
5	4	7	4SU	C5-C4	4.10	1.47	1.42
5	4	7	4SU	C6-N1	3.98	1.47	1.38
5	4	7	4SU	O2-C2	-3.47	1.16	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	4	7	4SU	C4-N3-C2	-7.67	119.89	127.34
5	4	7	4SU	C5-C4-N3	5.34	119.65	114.69
5	4	7	4SU	N3-C2-N1	3.91	120.08	114.89
5	4	7	4SU	C5-C4-S4	-3.43	120.04	124.47
5	4	32	OMC	C1'-N1-C2	2.46	123.91	118.42

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	4	32	OMC	C2'-C1'-N1-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	4	54	5MU	1	0
5	4	32	OMC	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

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5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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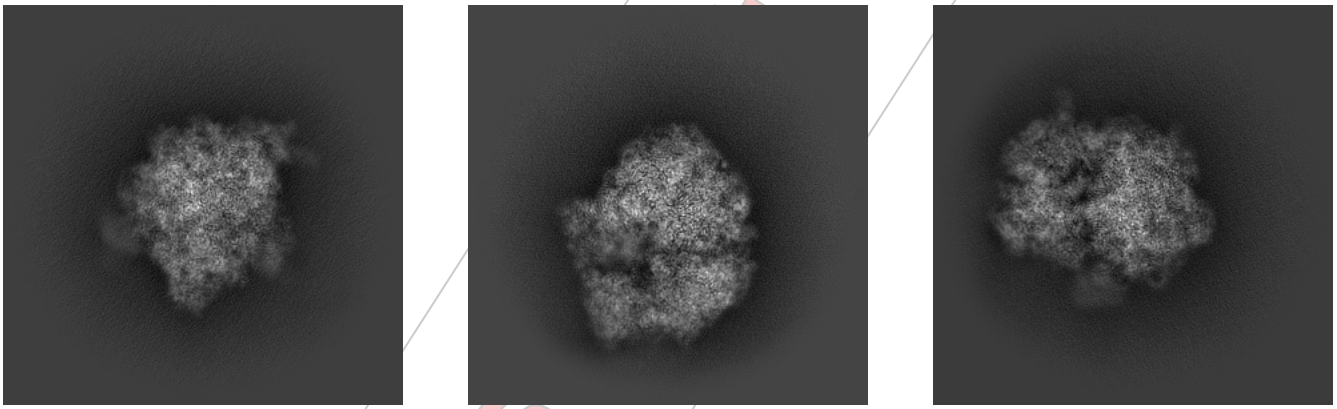
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-82634. 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.

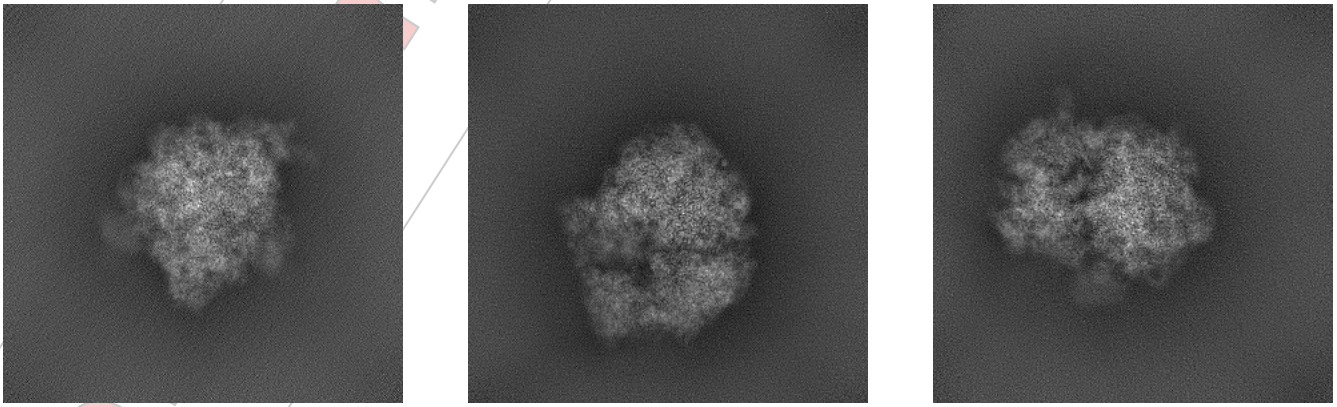
6.1 Orthogonal projections

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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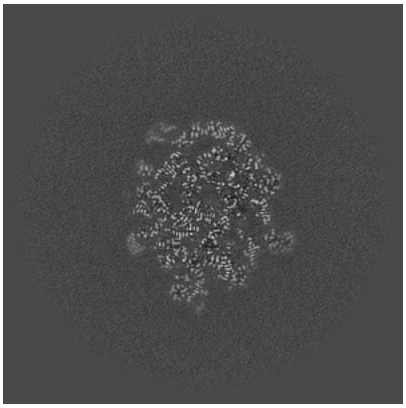
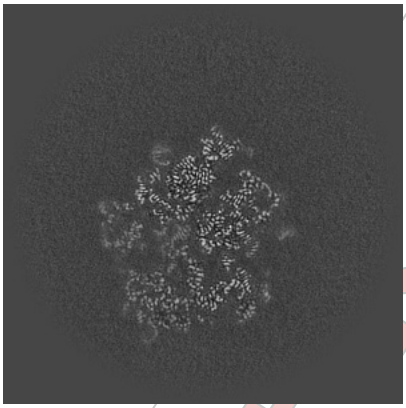
6.2 Central slices (i)

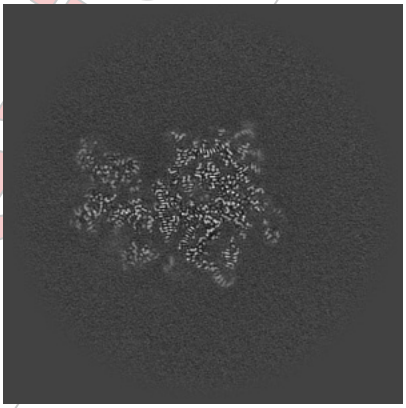
6.2.1 Primary map



X Index: 240

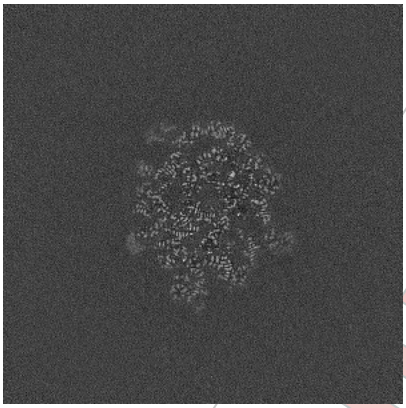


Y Index: 240

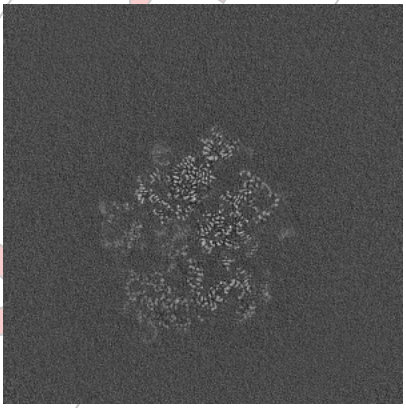


Z Index: 240

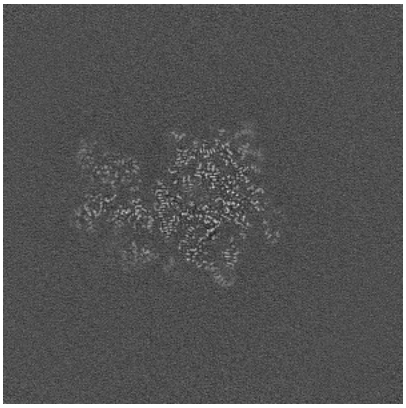
6.2.2 Raw map



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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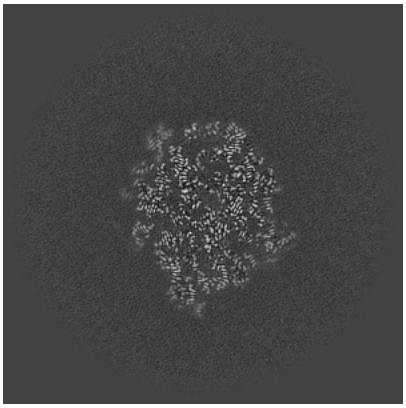
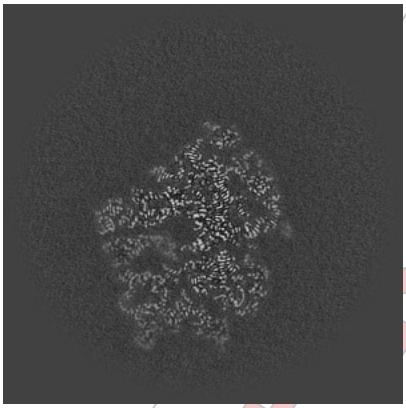
6.3 Largest variance slices (i)

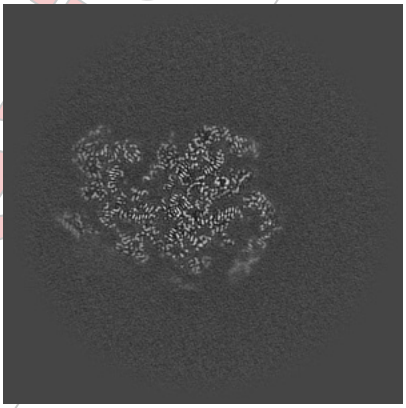
6.3.1 Primary map



X Index: 234

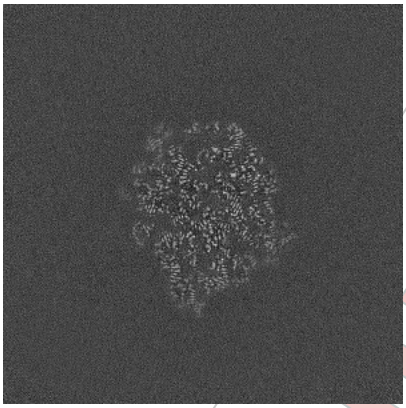


Y Index: 225

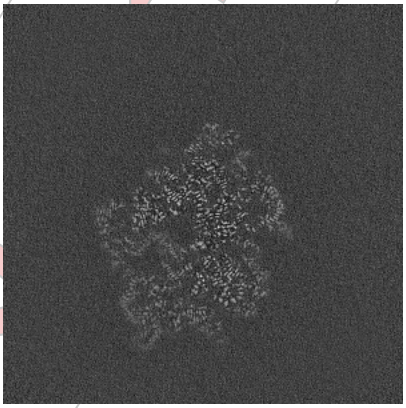


Z Index: 263

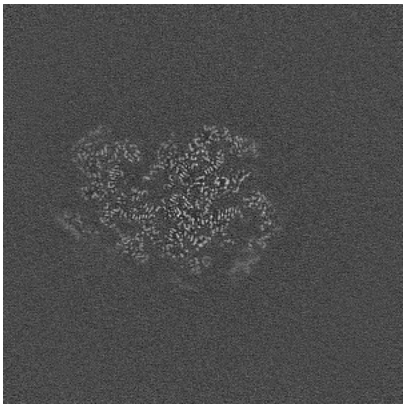
6.3.2 Raw map



X Index: 233



Y Index: 229



Z Index: 263

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

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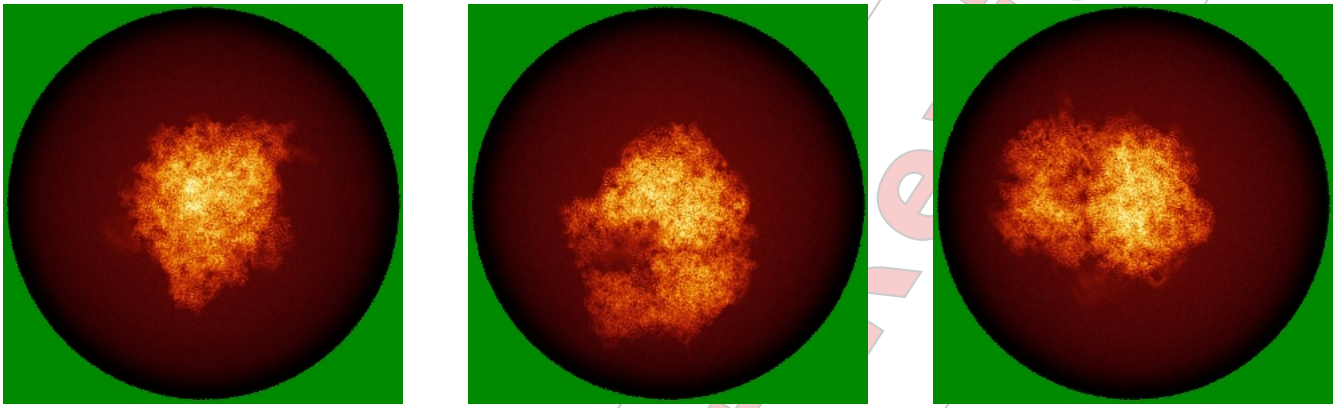
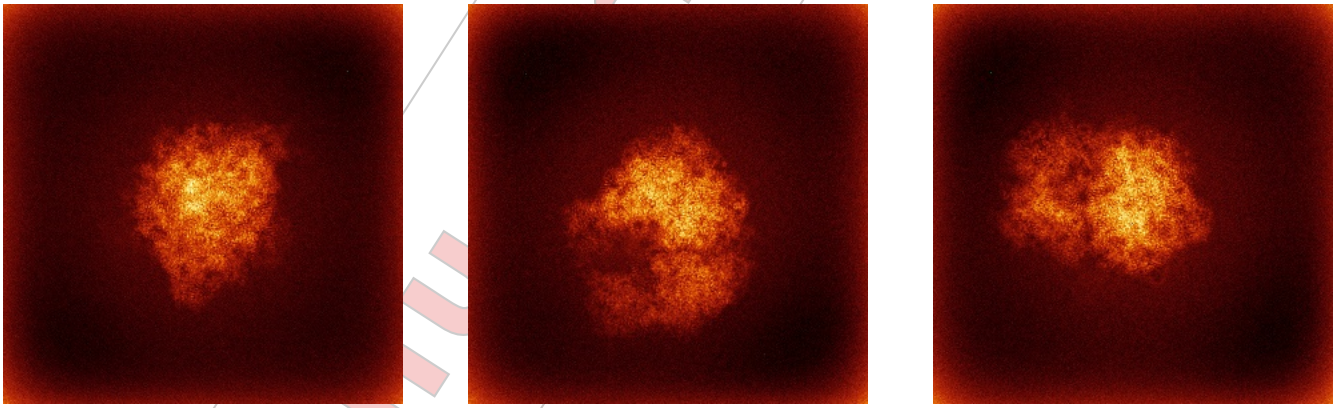
6.4 Orthogonal standard-deviation projections (False-color)

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

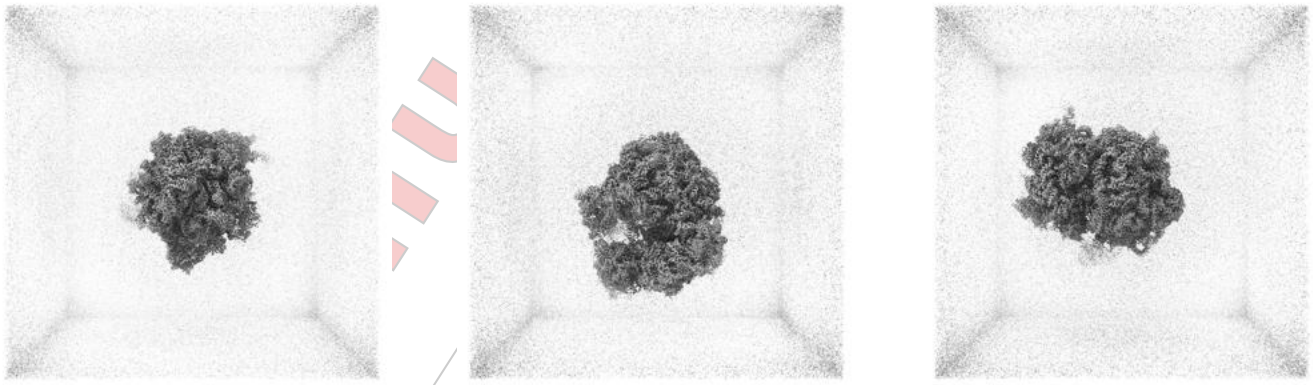
6.5.1 Primary map



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

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

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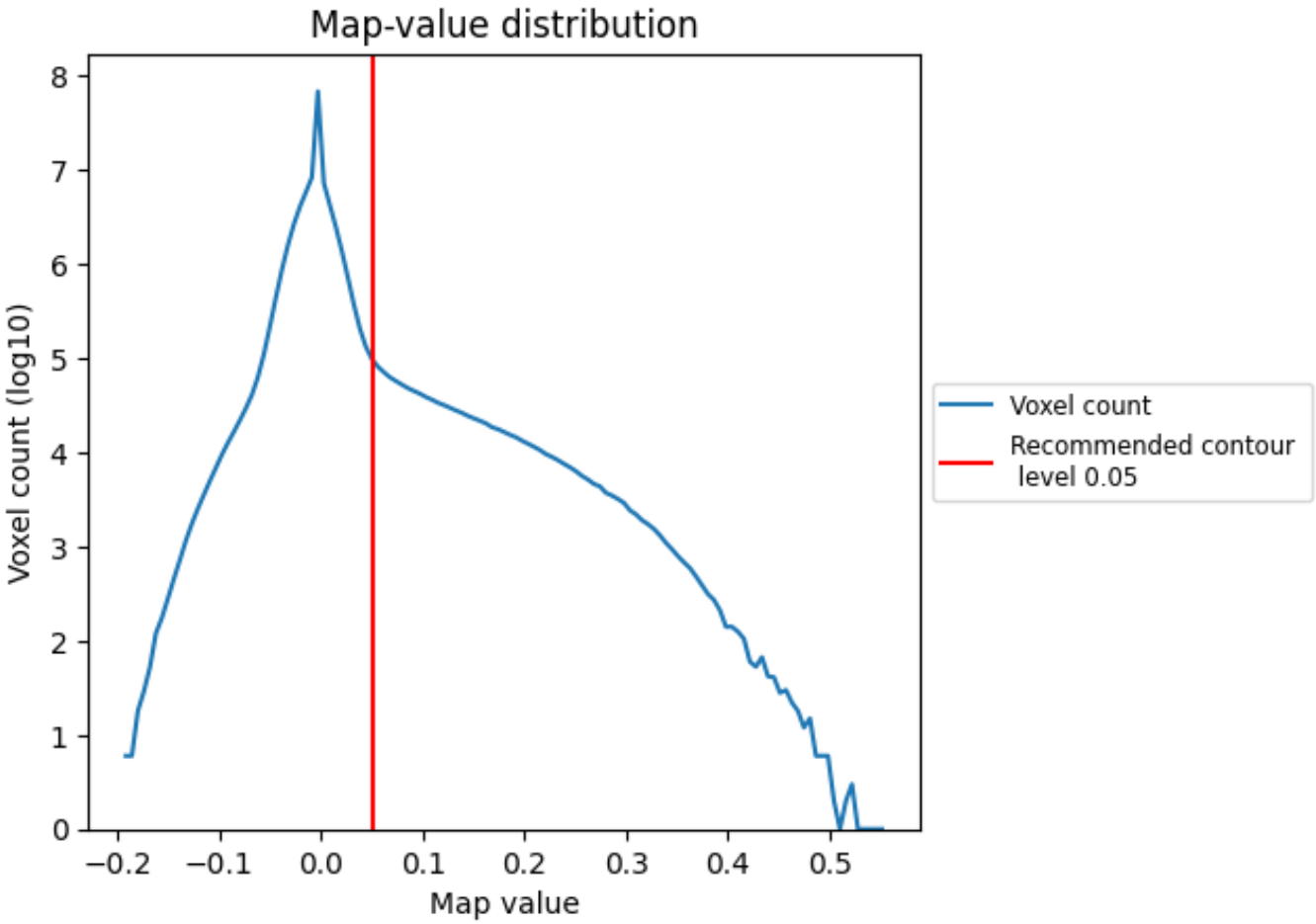
7 Map analysis

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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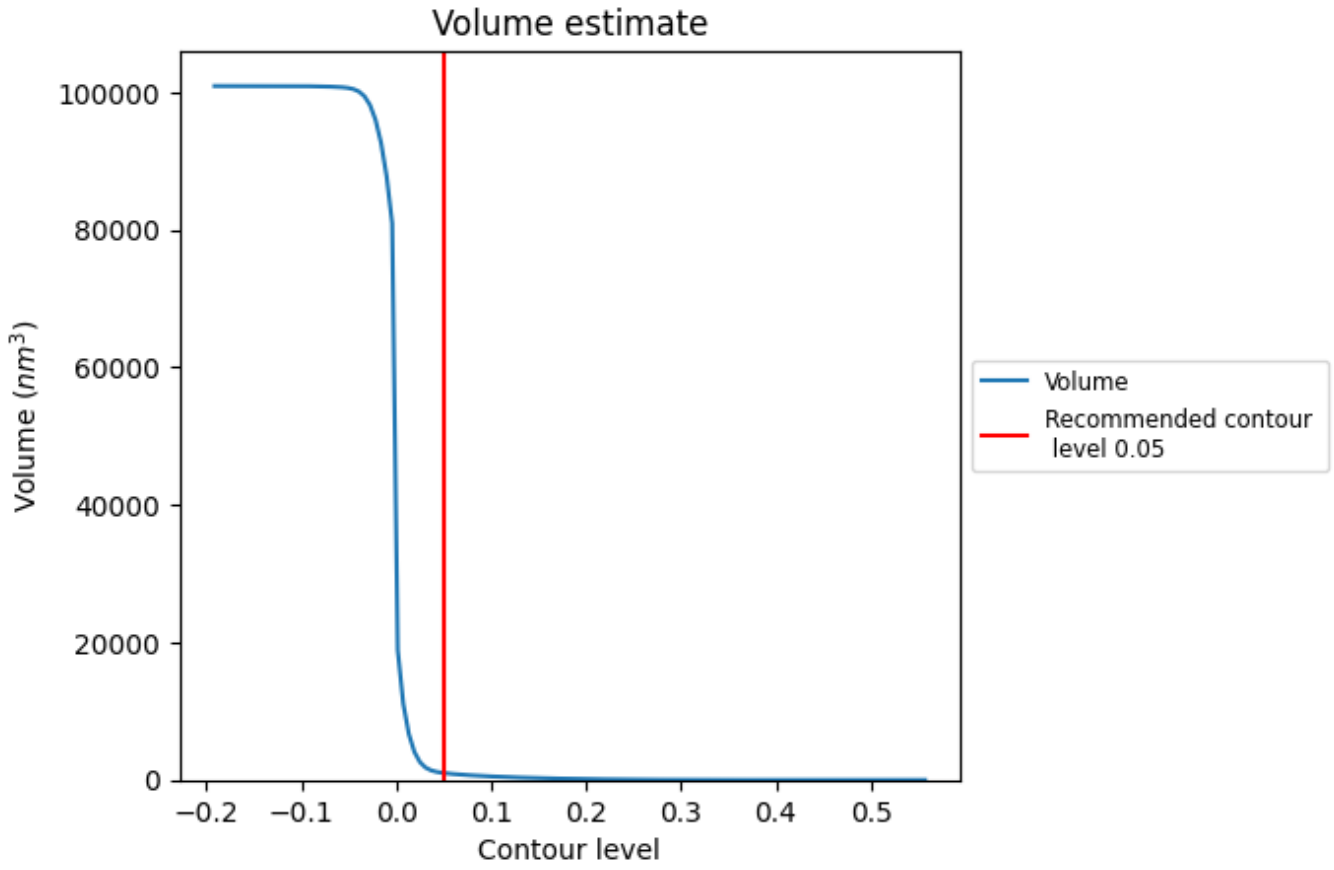
7.2 Volume estimate (i)

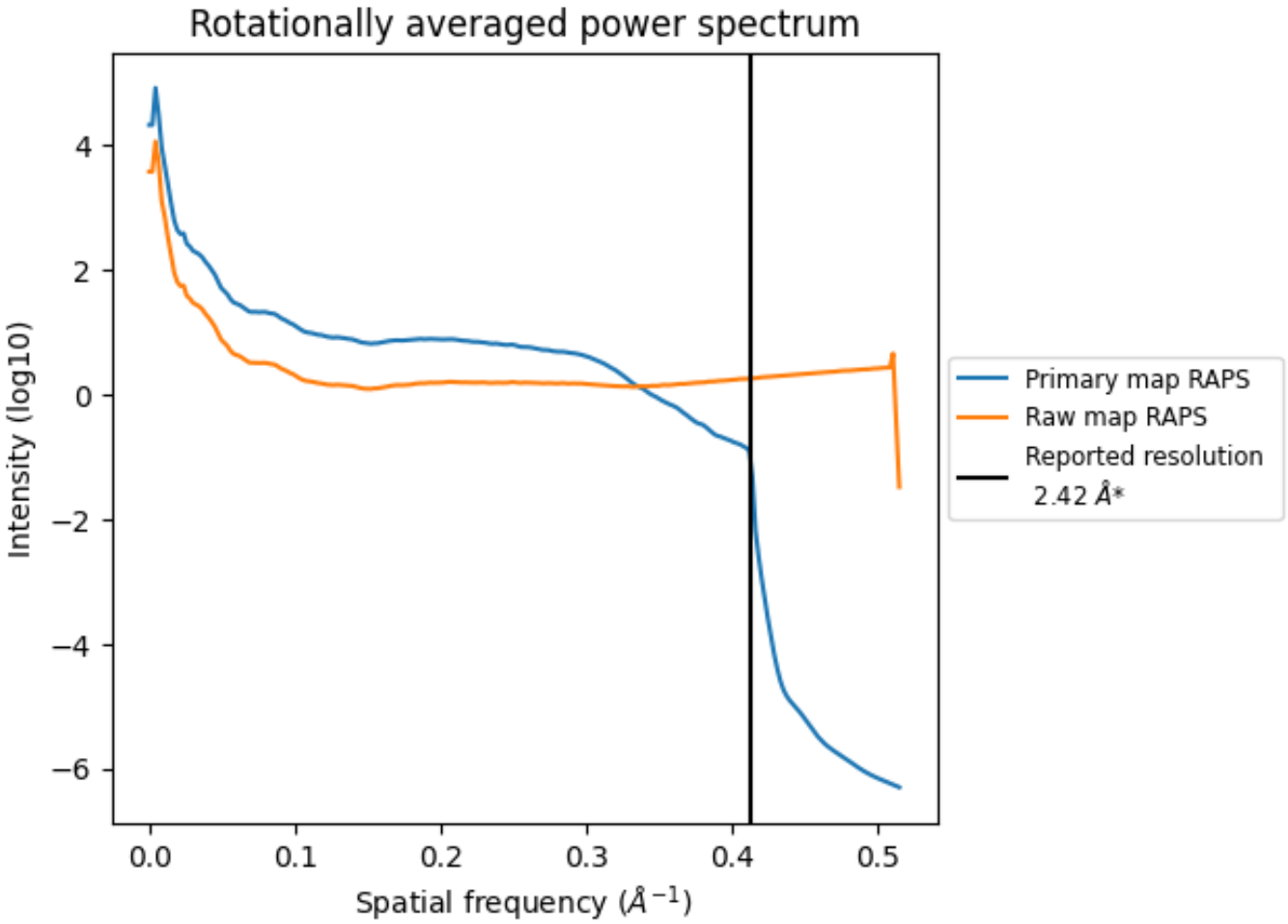


The volume at the recommended contour level is 1011 nm^3; this corresponds to an approximate mass of 914 kDa.

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)



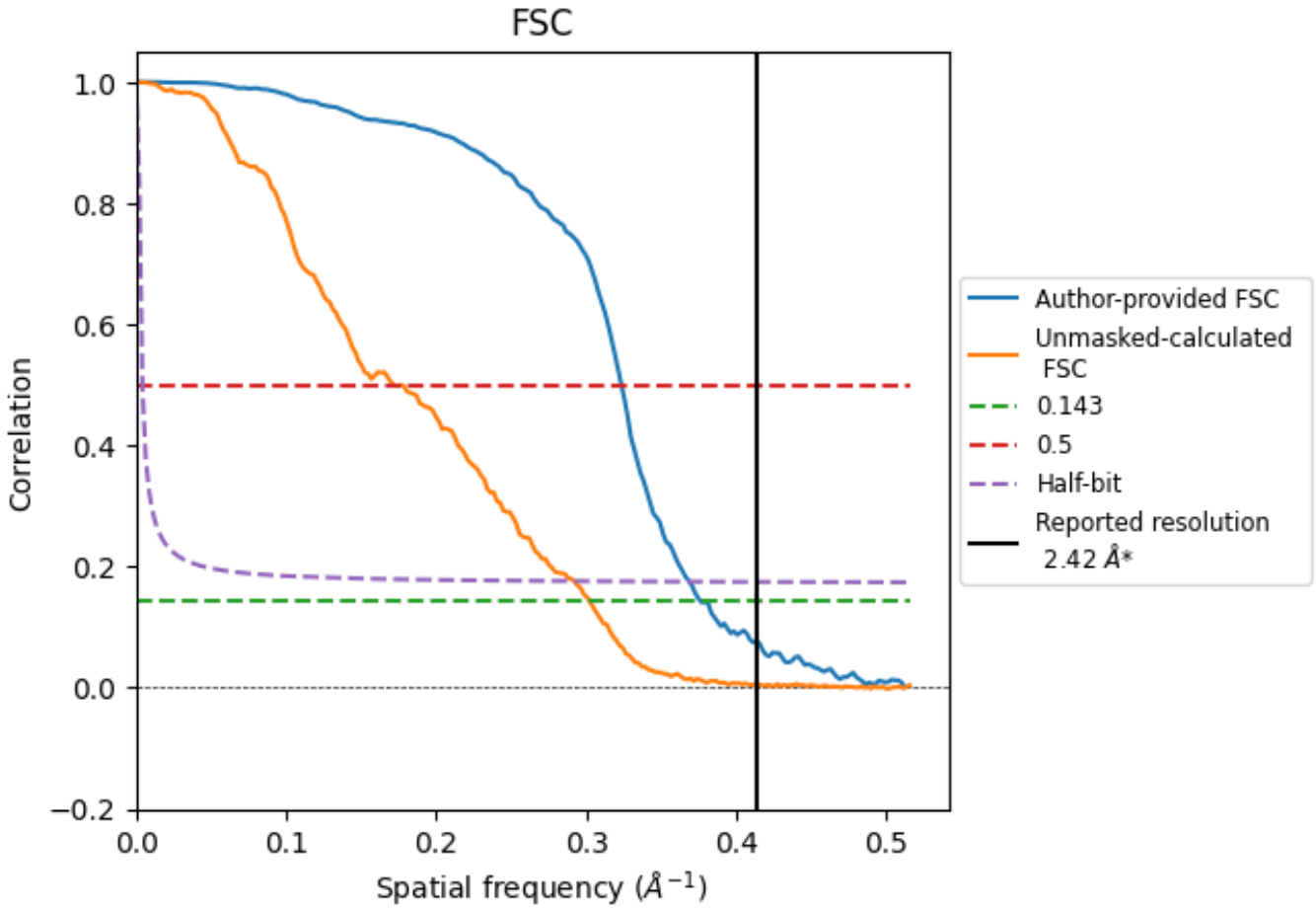
*Reported resolution corresponds to spatial frequency of 0.413 Å^{-1}

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 0.413 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	2.42	-	-
Author-provided FSC curve	2.66	3.09	2.71
Unmasked-calculated*	3.31	5.82	3.43

*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 3.31 differs from the reported value 2.42 by more than 10 %

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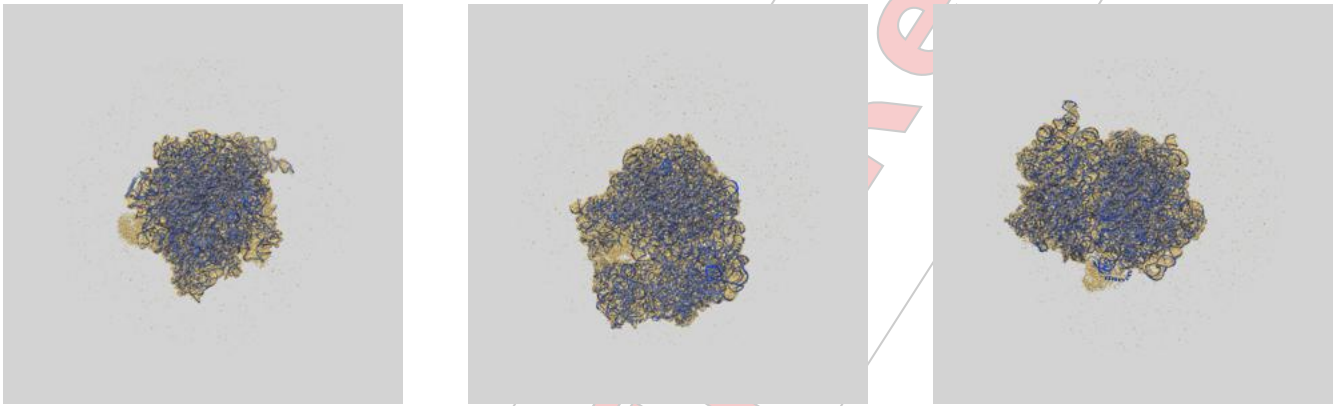
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-82634 and PDB model 44IK. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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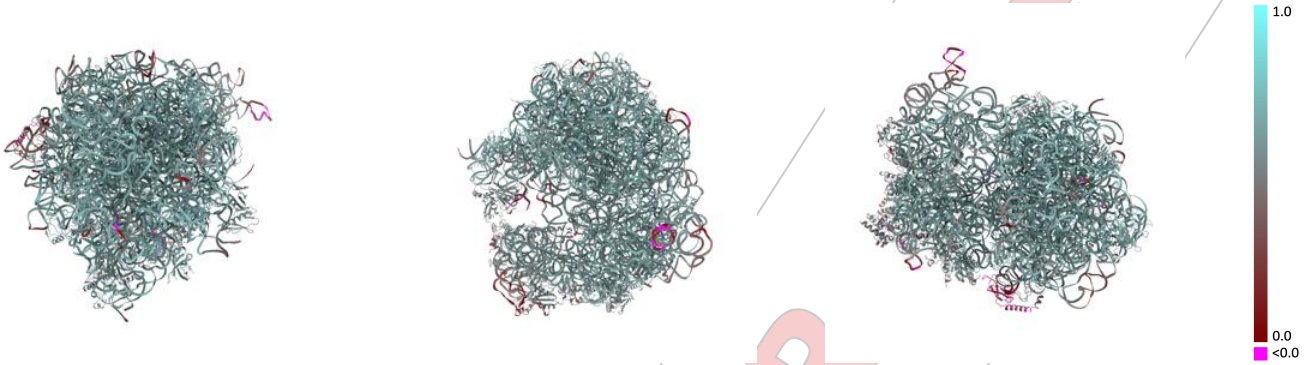
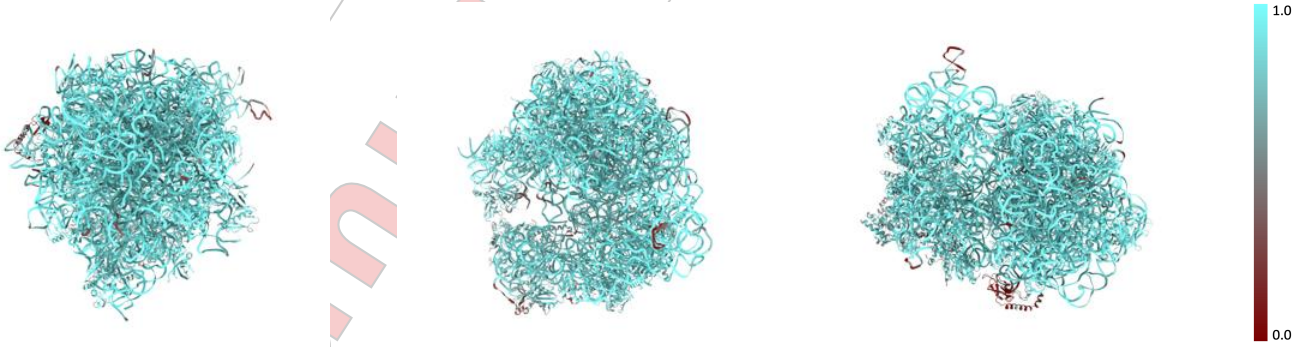
9.2 Q-score mapped to coordinate model



X Y Z

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

9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

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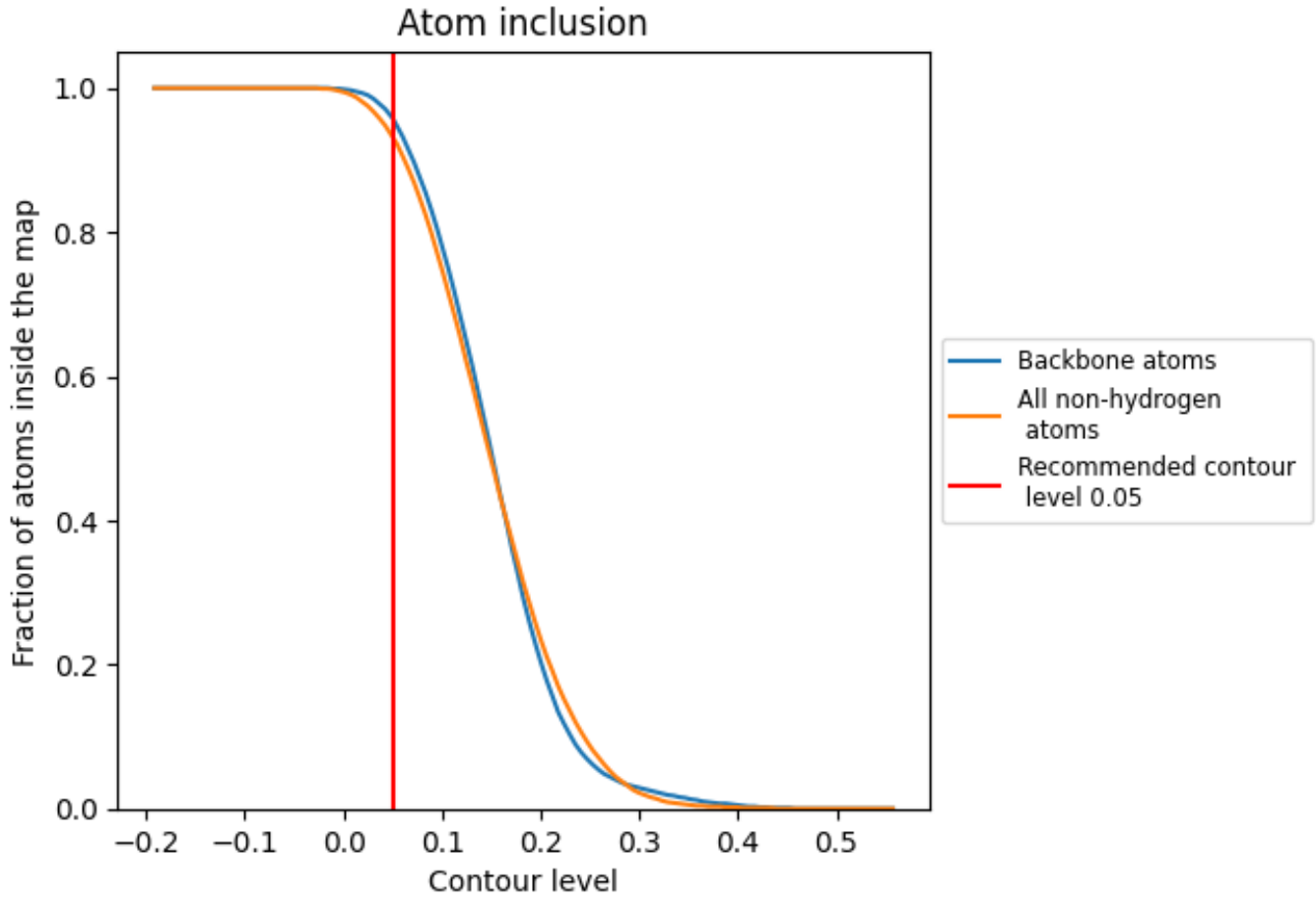
9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 93% 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	0.9320	0.5950
0	0.9750	0.6200
1	0.9750	0.6060
2	0.9530	0.5860
3	0.9850	0.6370
4	0.8490	0.5160
A	0.9510	0.6390
B	0.9480	0.6370
C	0.8980	0.5990
D	0.8300	0.5320
E	0.8420	0.5440
F	0.3140	0.2700
G	0.9440	0.6260
H	0.9360	0.6310
I	0.9350	0.6230
J	0.9220	0.6110
K	0.9670	0.6480
L	0.9130	0.5880
M	0.9190	0.6190
N	0.9650	0.6480
O	0.9200	0.6200
P	0.9270	0.6230
Q	0.8840	0.5870
R	0.8870	0.5840
S	0.8930	0.5980
T	0.9390	0.6280
U	0.9400	0.6190
V	0.8730	0.5640
W	0.9370	0.6350
X	0.7070	0.4330
a	0.9430	0.6310
b	0.9020	0.6020
c	0.9440	0.6470
d	0.9610	0.6540
e	0.9310	0.6180



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Chain	Atom inclusion	Q-score
f	0.7420	0.4830
g	0.8450	0.5530
h	0.8710	0.5640
i	0.9170	0.5990
j	0.8220	0.5320
k	0.6660	0.4670
l	0.9120	0.6030
m	0.7790	0.5080
n	0.6820	0.4590
o	0.8710	0.5670
p	0.8860	0.5910
q	0.8080	0.5310
r	0.8410	0.5490
s	0.8800	0.5710
t	0.8990	0.5750
u	0.8540	0.5620
v	0.8390	0.5480
w	0.7750	0.5080
x	0.8950	0.5800
y	0.6020	0.4290

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