



Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 11:46 pm BST

PDB ID : 28NT / pdb_000028nt
EMDB ID : EMD-56659
Title : Cryo-EM structure of the 70S ribosome from Francisella tularensis
Authors : Silhan, J.; Klima, M.; Boura, E.
Deposited on : 2026-02-10
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

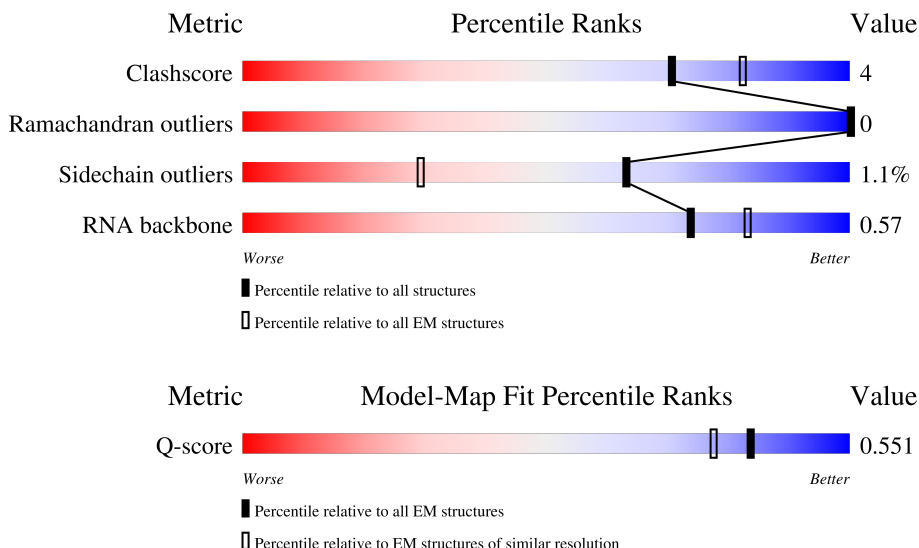
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.95 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.



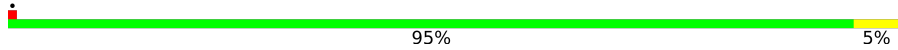
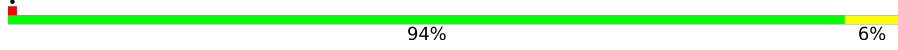
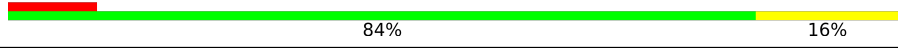
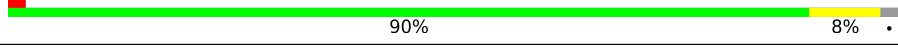
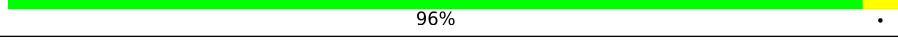
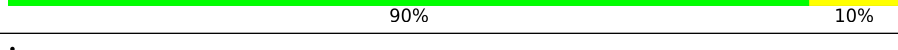
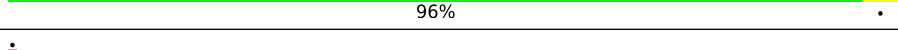
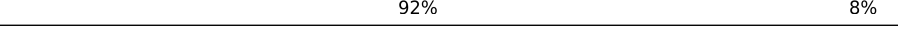
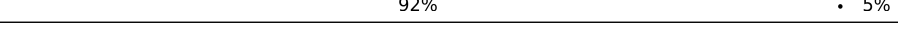
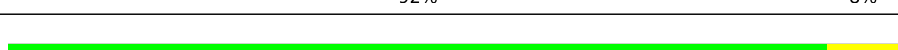
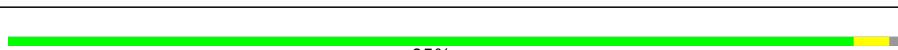
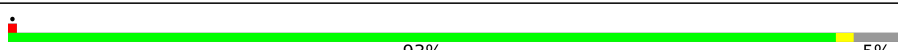
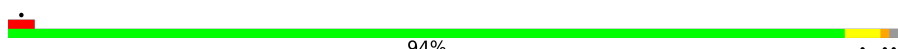
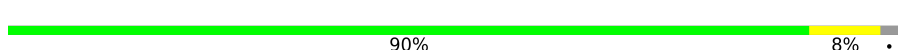
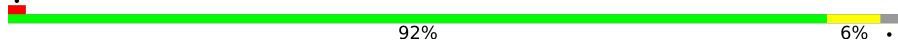
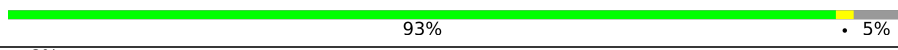
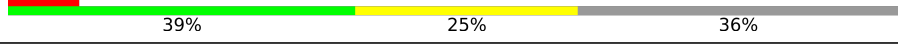
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13114 (2.45 - 3.45)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2886	
2	B	115	
3	C	274	

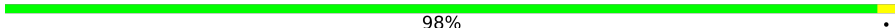
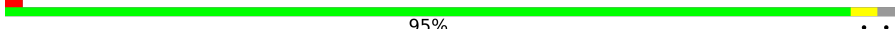
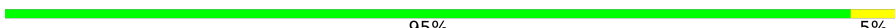
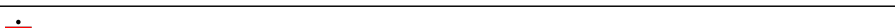
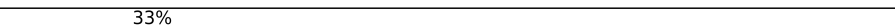
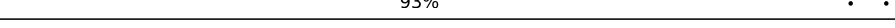
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Mol	Chain	Length	Quality of chain
4	D	210	
5	E	207	
6	F	179	
7	G	178	
8	H	151	
9	I	142	
10	J	122	
11	K	143	
12	L	137	
13	M	145	
14	N	117	
15	O	115	
16	P	118	
17	Q	104	
18	R	111	
19	S	99	
20	T	105	
21	U	96	
22	V	84	
23	W	78	
24	X	66	
25	Y	61	
26	Z	72	
27	0	60	
28	1	51	

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Mol	Chain	Length	Quality of chain
29	2	44	 98%
30	3	65	 95%
31	4	37	 95%
32	a	1528	 64% 27% 5%
33	b	222	 85% 64% 35%
34	d	205	 83% 17%
35	e	166	 79% 14% 6%
36	f	111	 6% 76% 17% 6%
37	g	157	 27% 86% 12%
38	h	132	 89% 11%
39	i	129	 46% 74% 23%
40	k	129	 84% 7% 9%
41	l	124	 87% 12%
42	m	118	 33% 65% 29% 5%
43	o	88	 91% 9%
44	p	82	 87% 13%
45	q	83	 93%
46	r	72	 62% 15% 22%
47	s	92	 52% 60% 26% 11%
48	t	90	 93% 6%
49	u	65	 51% 78% 12% 9%

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 132144 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2686	Total	C	N	O	P	0	0
			57663	25746	10590	18641	2686		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	115	Total	C	N	O	P	0	0
			2451	1097	445	794	115		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	273	Total	C	N	O	S	0	0
			2126	1322	428	367	9		

- Molecule 4 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	209	Total	C	N	O	S	0	0
			1559	970	287	297	5		

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	207	Total	C	N	O	S	0	0
			1584	1000	281	297	6		

- Molecule 6 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	178	Total	C	N	O	S	0	0
			1398	893	244	256	5		

- Molecule 7 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	174	Total	C	N	O	S	0	0
			1307	826	230	250	1		

- Molecule 8 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	50	Total	C	N	O	S	0	0
			385	250	66	68	1		

- Molecule 9 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	142	Total	C	N	O	S	0	0
			1121	715	205	196	5		

- Molecule 10 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	122	Total	C	N	O	S	0	0
			928	579	178	167	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	143	Total	C	N	O	S	0	0
			1061	666	200	192	3		

- Molecule 12 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	137	Total	C	N	O	S	0	0
			1106	701	218	183	4		

- Molecule 13 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	138	Total	C	N	O	S	0	0
			1126	710	218	193	5		

- Molecule 14 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	116	Total	C	N	O	S	0	0
			907	563	176	165	3		

- Molecule 15 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	115	Total	C	N	O	S	0	0
			936	591	178	163	4		

- Molecule 16 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	117	Total	C	N	O	S	0	0
			934	589	188	157			

- Molecule 17 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0
			812	517	148	143	4		

- Molecule 18 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	110	Total	C	N	O	S	0	0
			845	529	159	153	4		

- Molecule 19 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	94	Total	C	N	O	S	0	0
			753	480	138	135			

- Molecule 20 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	104	Total	C	N	O	S	0	0
			800	507	146	146	1		

- Molecule 21 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	94	Total	C	N	O	S	0	0
			754	479	137	137	1		

- Molecule 22 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	76	Total	C	N	O	S	0	0
			581	362	113	105	1		

- Molecule 23 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	77	Total	C	N	O	S	0	0
			619	386	126	105	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	65	Total	C	N	O	S	0	0
			538	338	103	96	1		

- Molecule 25 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	58	Total	C	N	O	S	0	0
			456	289	85	80	2		

- Molecule 26 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	46	Total	C	N	O	S	0	0
			363	224	62	71	6		

- Molecule 27 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	55	Total	C	N	O	S	0	0
			441	267	91	82	1		

- Molecule 28 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	49	Total	C	N	O	S	0	0
			411	263	75	70	3		

- Molecule 29 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	44	Total	C	N	O	S	0	0
			363	222	86	53	2		

- Molecule 30 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	64	Total	C	N	O	S	0	0
			505	313	106	82	4		

- Molecule 31 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	37	Total	C	N	O	S	0	0
			305	184	70	46	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1453	Total	C	N	O	P	0	0
			31185	13913	5721	10098	1453		

- Molecule 33 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	222	Total	C	N	O	S	0	0
			1733	1106	301	316	10		

- Molecule 34 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	205	Total	C	N	O	S	0	0
			1620	1003	309	300	8		

- Molecule 35 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	156	Total	C	N	O	S	0	0
			1146	716	213	212	5		

- Molecule 36 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	104	Total	C	N	O	S	0	0
			859	547	150	156	6		

- Molecule 37 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	154	Total	C	N	O	S	0	0
			1217	761	232	219	5		

- Molecule 38 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	131	Total	C	N	O	S	0	0
			1002	637	173	186	6		

- Molecule 39 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	125	Total	C	N	O	S	0	0
			999	623	195	177	4		

- Molecule 40 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	118	Total	C	N	O	S	0	0
			882	546	170	164	2		

- Molecule 41 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	123	Total	C	N	O	S	0	0
			963	594	201	166	2		

- Molecule 42 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	112	Total	C	N	O	S	0	0
			888	543	182	158	5		

- Molecule 43 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	88	Total	C	N	O	S	0	0
			729	451	145	132	1		

- Molecule 44 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	82	Total	C	N	O	S	0	0
			639	406	123	108	2		

- Molecule 45 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	80	Total	C	N	O	S	0	0
			670	429	119	119	3		

- Molecule 46 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	56	Total	C	N	O	S	0	0
			456	291	84	80	1		

- Molecule 47 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	82	Total	C	N	O	S	0	0
			660	420	124	112	4		

- Molecule 48 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	t	89	Total	C	N	O	S	0	0
			704	439	142	121	2		

- Molecule 49 is a protein called Small ribosomal subunit protein bS21B.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	59	Total	C	N	O	S	0	0
			500	313	105	81	1		

- Molecule 50 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
50	A	133	Total	Mg	0
			133	133	
50	B	3	Total	Mg	0
			3	3	
50	C	1	Total	Mg	0
			1	1	
50	0	1	Total	Mg	0
			1	1	
50	a	15	Total	Mg	0
			15	15	

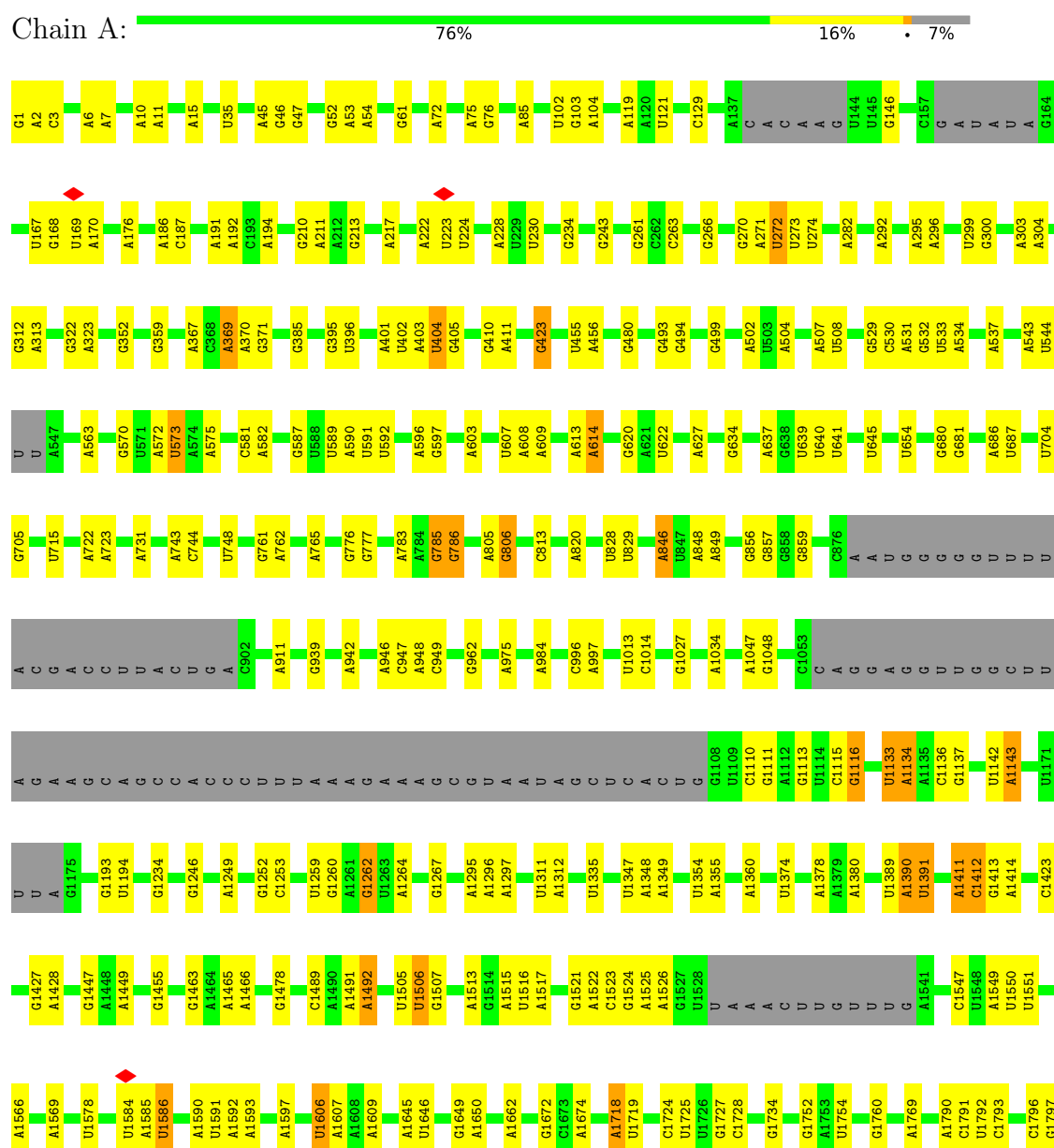
- Molecule 51 is ZINC ION (CCD ID: ZN) (formula: Zn).

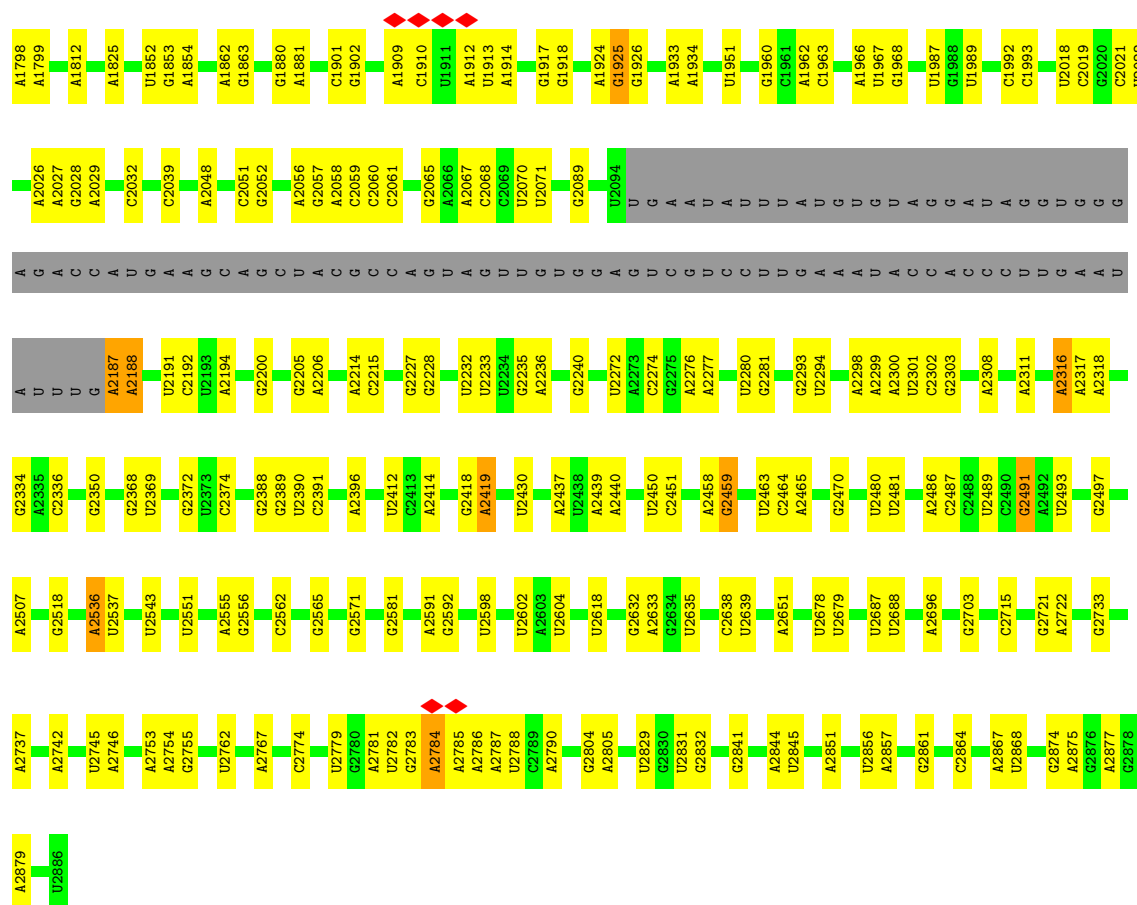
Mol	Chain	Residues	Atoms		AltConf
51	4	1	Total	Zn	0
			1	1	

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 ribosomal RNA





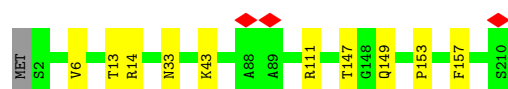
Chain B: 77% 22%



Chain C: 95%

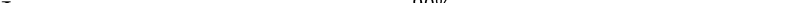


Chain D: 95% 5%



- Chain F: 

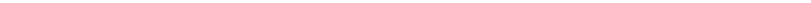
Amino Acid	Number of Mutations
MET	3
A2	2
E11	1
A30	2
L36	2
V40	2
G41	1
D42	1
A43	1
A44	1
K45	1
D46	1
K47	1
K48	1
T49	1
M50	1
F52	1
G62	1
V66	1
V67	1
S73	1
F77	1
R80	1
I85	1
V89	1
R95	1
L103	1
A107	1
R112	1
R115	1
G116	1
G126	1
P139	1
E140	1
I141	1
D142	1
Y143	1
D144	1
K145	1
V146	1
S148	1
I149	1
R150	1
G151	1
L152	1
T158	1
T159	1
A160	1
K161	1
Q165	1
K178	1
S179	1

- Chain G: 

Category	Count
MET	1
S2	1
S13	1
K31	1
V42	1
V46	1
A47	1
N61	1
Q65	1
E85	1
R86	1
R87	1
I90	1
E103	1
K117	1
I132	1
Y165	1
Y166	1
D167	1
E168	1
E174	1
A175	1
LYS	1
LYS	1
LYS	1
LYS	1

- Chain H: 24% 9% 67%

[illegible]

- Chain I: 

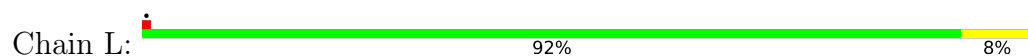
- Chain J: 90% 10%



- Molecule 11: Large ribosomal subunit protein uL15



- Molecule 12: Large ribosomal subunit protein uL16



- Molecule 13: Large ribosomal subunit protein bL17



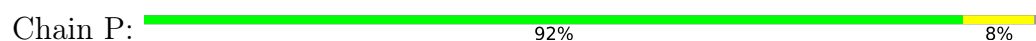
- Molecule 14: Large ribosomal subunit protein uL18



- Molecule 15: Large ribosomal subunit protein bL19



- Molecule 16: Large ribosomal subunit protein bL20



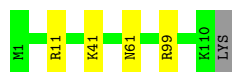
- Molecule 17: Large ribosomal subunit protein bL21





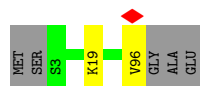
- Molecule 18: Large ribosomal subunit protein uL22

Chain R: 95%



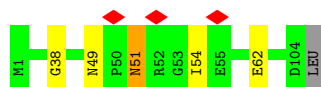
- Molecule 19: Large ribosomal subunit protein uL23

Chain S: 93%



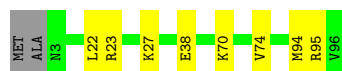
- Molecule 20: Large ribosomal subunit protein uL24

Chain T: 94%



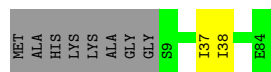
- Molecule 21: Large ribosomal subunit protein bL25

Chain U: 90%



- Molecule 22: Large ribosomal subunit protein bL27

Chain V: 88%



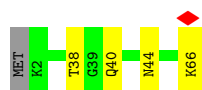
- Molecule 23: Large ribosomal subunit protein bL28

Chain W: 87%



- Molecule 24: Large ribosomal subunit protein uL29

Chain X: 92%



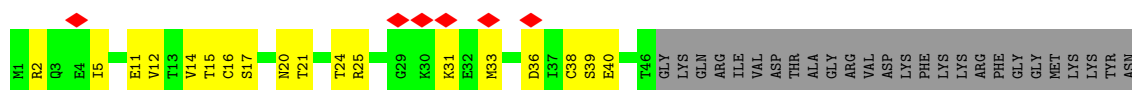
- Molecule 25: Large ribosomal subunit protein uL30

Chain Y: 93% 5%



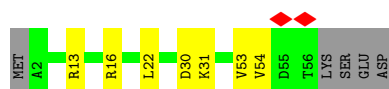
- Molecule 26: Large ribosomal subunit protein bL31

Chain Z: 8% 39% 25% 36%



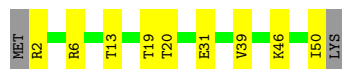
- Molecule 27: Large ribosomal subunit protein bL32

Chain 0: 80% 12% 8%



- Molecule 28: Large ribosomal subunit protein bL33

Chain 1: 78% 18%



- Molecule 29: Large ribosomal subunit protein bL34

Chain 2: 98%



- Molecule 30: Large ribosomal subunit protein bL35

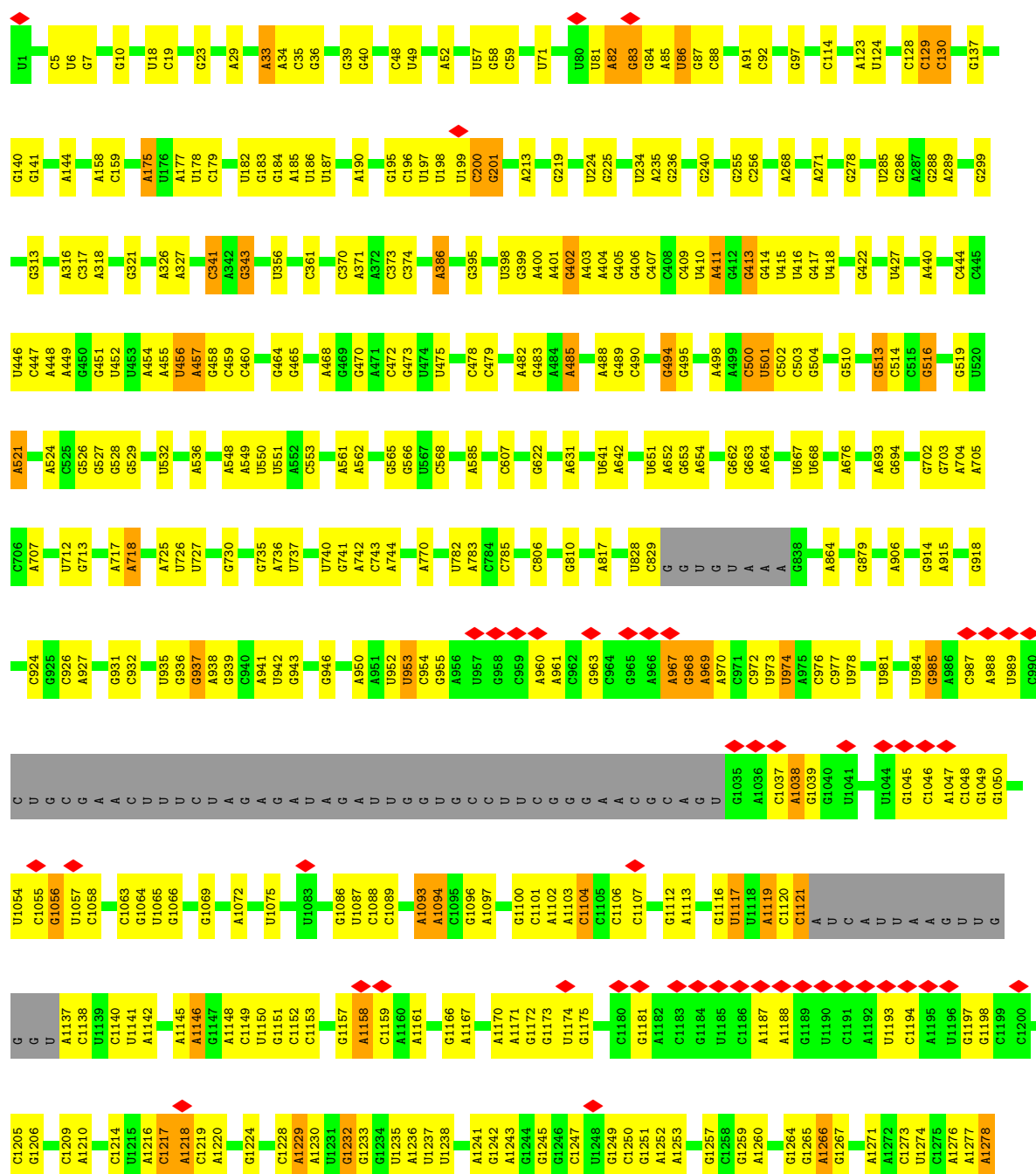
Chain 3: 95%

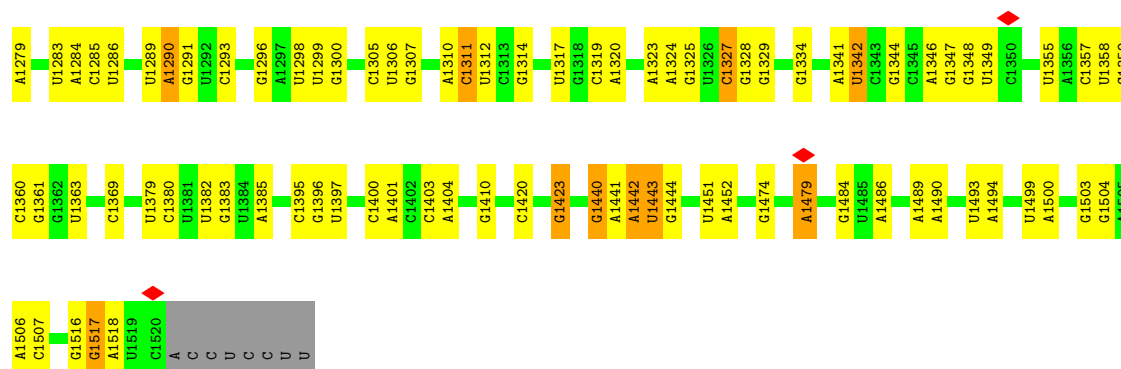


- Molecule 31: Large ribosomal subunit protein bL36

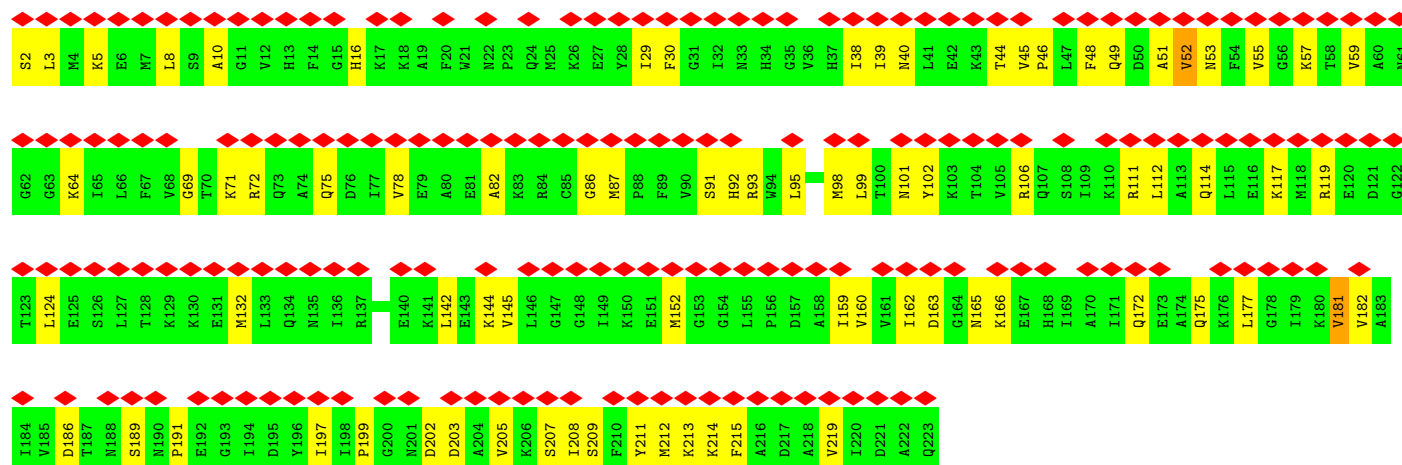
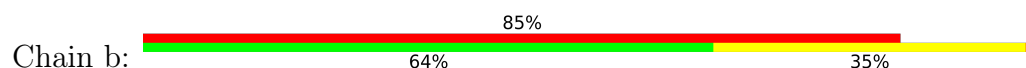
A diagram of a protein structure, likely a beta-strand, with four residues highlighted in yellow: M1, C27, T28, and G37. The residues are arranged in a linear sequence, with M1 and G37 at the ends and C27 and T28 in the middle. The highlighting is done with a yellow brushstroke effect.

Chain a: 64% 27% 5%

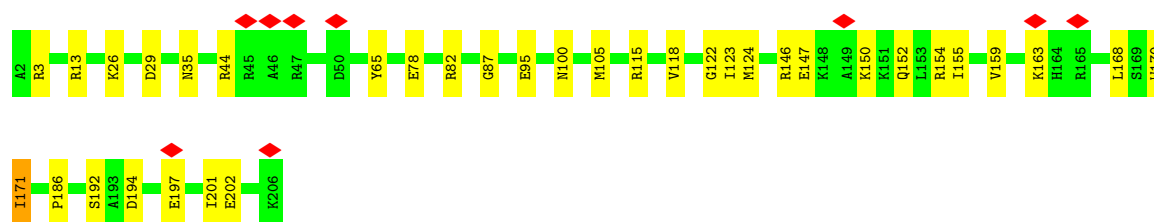
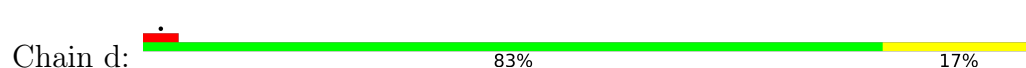




• Molecule 33: Small ribosomal subunit protein uS2



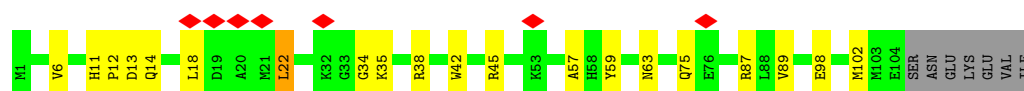
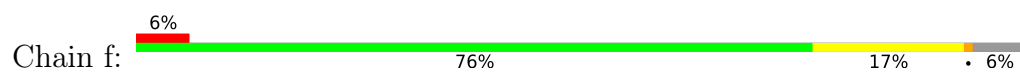
• Molecule 34: Small ribosomal subunit protein uS4



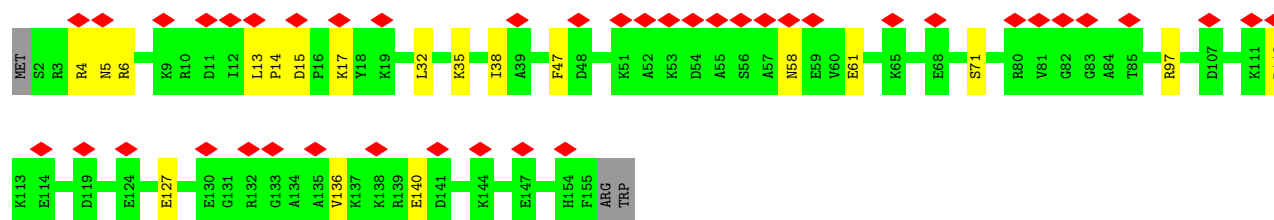
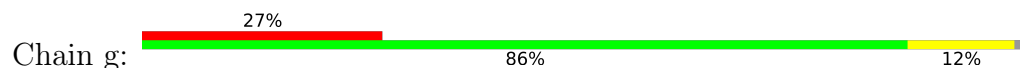
• Molecule 35: Small ribosomal subunit protein uS5



• Molecule 36: Small ribosomal subunit protein bS6



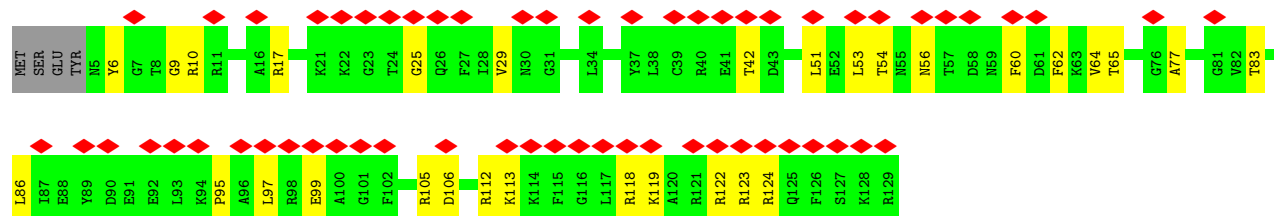
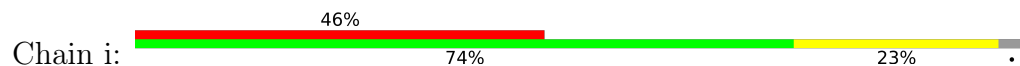
- Molecule 37: Small ribosomal subunit protein uS7



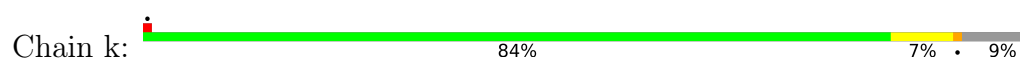
- Molecule 38: Small ribosomal subunit protein uS8



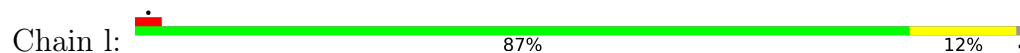
- Molecule 39: Small ribosomal subunit protein uS9



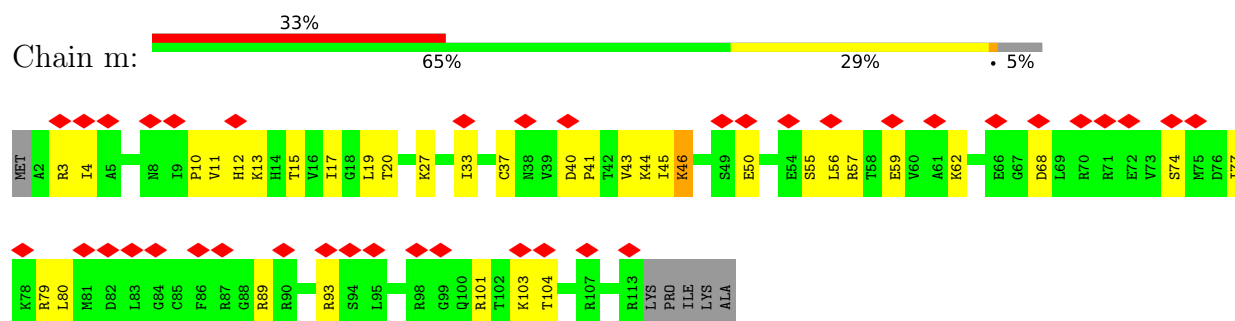
- Molecule 40: Small ribosomal subunit protein uS11



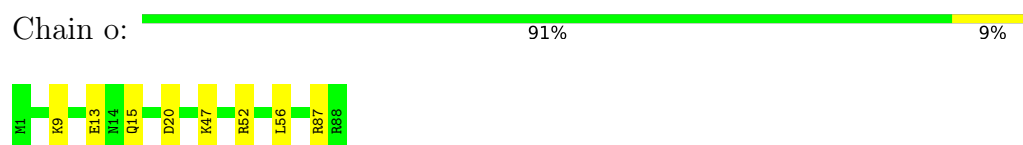
- Molecule 41: Small ribosomal subunit protein uS12



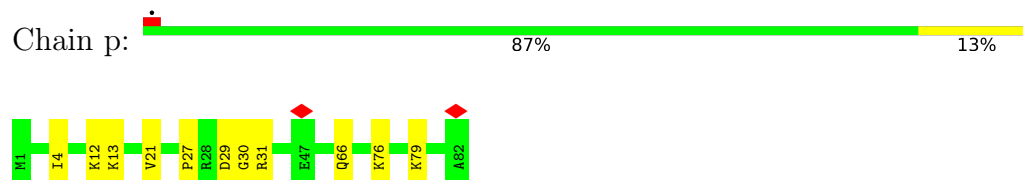
- Molecule 42: Small ribosomal subunit protein uS13



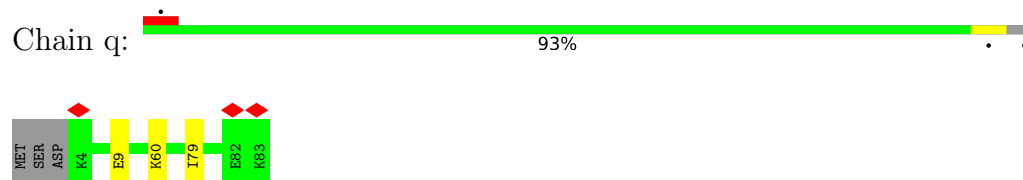
- Molecule 43: Small ribosomal subunit protein uS15



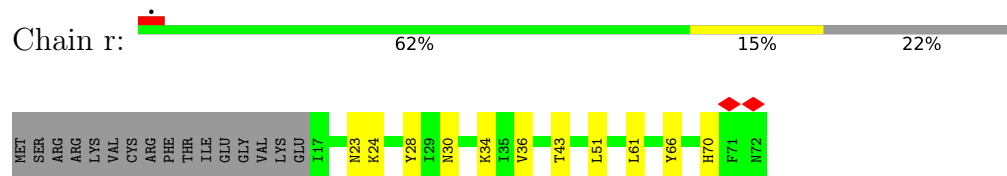
- Molecule 44: Small ribosomal subunit protein bS16



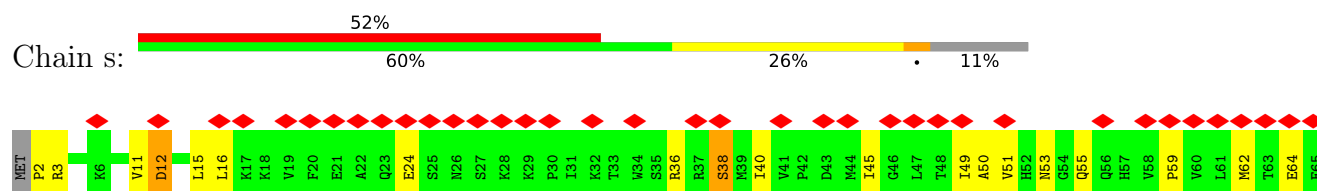
- Molecule 45: Small ribosomal subunit protein uS17

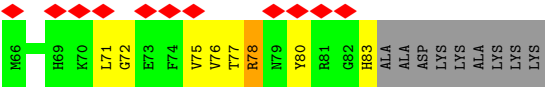


- Molecule 46: Small ribosomal subunit protein bS18

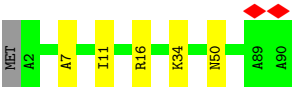
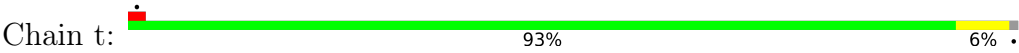


- Molecule 47: Small ribosomal subunit protein uS19

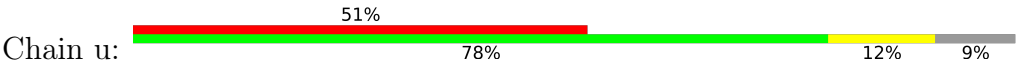




• Molecule 48: Small ribosomal subunit protein bS20



• Molecule 49: Small ribosomal subunit protein bS21B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33316	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.702	Depositor
Minimum map value	-0.305	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.104	Depositor
Map size ($\text{\AA}$)	456.0, 456.0, 456.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.76, 0.76, 0.76	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 2MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	0/64570	0.30	0/100702
2	B	0.20	0/2742	0.28	0/4270
3	C	0.22	0/2162	0.33	0/2898
4	D	0.21	0/1584	0.31	0/2135
5	E	0.21	0/1603	0.32	0/2150
6	F	0.17	0/1419	0.32	0/1900
7	G	0.16	0/1326	0.28	0/1790
8	H	0.27	0/390	0.40	0/525
9	I	0.21	0/1146	0.30	0/1545
10	J	0.20	0/937	0.31	0/1254
11	K	0.19	0/1074	0.29	0/1428
12	L	0.19	0/1125	0.31	0/1501
13	M	0.22	0/1145	0.35	0/1527
14	N	0.18	0/918	0.35	0/1227
15	O	0.20	0/950	0.30	0/1265
16	P	0.23	0/946	0.32	0/1266
17	Q	0.19	0/822	0.29	0/1090
18	R	0.21	0/852	0.31	0/1142
19	S	0.18	0/764	0.30	0/1024
20	T	0.18	0/810	0.30	0/1083
21	U	0.18	0/765	0.32	0/1023
22	V	0.22	0/590	0.36	0/789
23	W	0.20	0/629	0.29	0/841
24	X	0.21	0/541	0.31	0/714
25	Y	0.24	0/461	0.35	0/616
26	Z	0.15	0/370	0.33	0/499
27	0	0.20	0/448	0.31	0/599
28	1	0.18	0/418	0.36	0/554
29	2	0.25	0/366	0.37	0/477
30	3	0.22	0/512	0.37	0/676
31	4	0.19	0/306	0.26	0/401
32	a	0.17	0/34923	0.29	0/54472

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.23	0/1761	0.41	0/2365
34	d	0.18	0/1639	0.31	0/2191
35	e	0.17	0/1160	0.31	0/1559
36	f	0.21	0/876	0.37	0/1177
37	g	0.16	0/1235	0.32	0/1652
38	h	0.20	0/1020	0.30	0/1369
39	i	0.17	0/1012	0.33	0/1350
40	k	0.16	0/897	0.32	0/1214
41	l	0.21	0/978	0.31	0/1313
42	m	0.17	0/897	0.34	0/1201
43	o	0.17	0/736	0.27	0/980
44	p	0.19	0/648	0.35	0/860
45	q	0.16	0/683	0.29	0/912
46	r	0.16	0/464	0.29	0/623
47	s	0.14	0/676	0.31	0/908
48	t	0.25	0/711	0.33	0/943
49	u	0.14	0/509	0.26	0/674
All	All	0.20	0/143516	0.31	0/214674

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	A	57663	0	28947	162	0
2	B	2451	0	1242	12	0
3	C	2126	0	2242	6	0
4	D	1559	0	1570	7	0
5	E	1584	0	1660	6	0
6	F	1398	0	1461	16	0
7	G	1307	0	1365	8	0
8	H	385	0	408	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1121	0	1170	3	0
10	J	928	0	993	8	0
11	K	1061	0	1134	3	0
12	L	1106	0	1177	6	0
13	M	1126	0	1172	3	0
14	N	907	0	943	4	0
15	O	936	0	985	6	0
16	P	934	0	991	6	0
17	Q	812	0	867	6	0
18	R	845	0	901	3	0
19	S	753	0	785	2	0
20	T	800	0	845	3	0
21	U	754	0	783	6	0
22	V	581	0	596	1	0
23	W	619	0	651	6	0
24	X	538	0	586	2	0
25	Y	456	0	488	0	0
26	Z	363	0	352	14	0
27	0	441	0	447	6	0
28	1	411	0	443	5	0
29	2	363	0	411	0	0
30	3	505	0	549	1	0
31	4	305	0	343	1	0
32	a	31185	0	15677	274	0
33	b	1733	0	1788	55	0
34	d	1620	0	1673	24	0
35	e	1146	0	1201	14	0
36	f	859	0	870	14	0
37	g	1217	0	1263	14	0
38	h	1002	0	1031	9	0
39	i	999	0	1039	23	0
40	k	882	0	903	7	0
41	l	963	0	1025	9	0
42	m	888	0	936	24	0
43	o	729	0	769	5	0
44	p	639	0	686	8	0
45	q	670	0	699	2	0
46	r	456	0	474	6	0
47	s	660	0	680	22	0
48	t	704	0	762	4	0
49	u	500	0	532	6	0
50	0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	A	133	0	0	0	0
50	B	3	0	0	0	0
50	C	1	0	0	0	0
50	a	15	0	0	0	0
51	4	1	0	0	0	0
All	All	132144	0	88515	766	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 4.

All (766) 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)
26:Z:11:GLU:HA	26:Z:25:ARG:HA	1.63	0.78
1:A:2293:G:H22	1:A:2301:U:H3	1.29	0.78
2:B:20:U:H3	2:B:59:G:H1	1.30	0.77
32:a:662:G:H2'	32:a:663:G:C8	2.20	0.76
33:b:59:VAL:HG21	33:b:219:VAL:HG13	1.70	0.73
32:a:1278:A:N3	32:a:1344:G:O2'	2.20	0.73
35:e:55:GLU:HG3	35:e:57:PRO:HD2	1.71	0.73
1:A:2440:A:OP1	1:A:2486:A:N6	2.21	0.73
32:a:416:U:OP1	34:d:13:ARG:NH2	2.22	0.72
32:a:1278:A:H2'	32:a:1279:A:C8	2.25	0.72
1:A:2274:C:OP2	28:1:2:ARG:NH1	2.22	0.71
32:a:943:G:N7	42:m:101:ARG:NH2	2.38	0.71
32:a:1216:A:H1'	47:s:78:ARG:HH22	1.56	0.71
35:e:163:GLU:O	38:h:116:ARG:NH1	2.24	0.70
37:g:58:ASN:HB3	37:g:61:GLU:HG2	1.74	0.69
1:A:2301:U:H5'	6:F:85:ILE:HD11	1.73	0.69
32:a:1369:C:P	37:g:6:ARG:HH12	2.14	0.69
32:a:1172:G:O2'	32:a:1173:G:N7	2.25	0.69
32:a:81:U:H1'	32:a:82:A:H5''	1.75	0.69
32:a:1224:G:OP1	39:i:118:ARG:NH2	2.26	0.69
32:a:457:A:H3'	32:a:458:G:H8	1.58	0.69
32:a:924:C:H5''	37:g:4:ARG:HE	1.56	0.69
33:b:112:LEU:HB2	33:b:142:LEU:HD23	1.74	0.69
5:E:76:THR:HG22	5:E:78:ARG:H	1.56	0.68
37:g:35:LYS:HD3	37:g:38:ILE:HD12	1.75	0.68
33:b:165:ASN:HB2	33:b:189:SER:HB3	1.75	0.68
34:d:124:MET:HG3	34:d:146:ARG:HG2	1.76	0.68
32:a:97:G:OP1	48:t:16:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:88:ASN:HD21	10:J:92:GLN:HB2	1.57	0.67
1:A:2439:A:H2'	1:A:2440:A:H8	1.59	0.67
32:a:440:A:H61	32:a:470:G:H5''	1.59	0.67
33:b:163:ASP:HB3	33:b:166:LYS:HB3	1.76	0.67
34:d:202:GLU:OE1	35:e:112:ARG:NH1	2.27	0.67
26:Z:20:ASN:ND2	26:Z:40:GLU:OE1	2.28	0.66
32:a:130:C:OP1	44:p:66:GLN:NE2	2.29	0.66
21:U:74:VAL:HG12	21:U:95:ARG:HA	1.77	0.66
33:b:10:ALA:HB1	33:b:207:SER:HA	1.78	0.66
1:A:856:G:H2'	1:A:857:G:C8	2.32	0.65
32:a:1093:A:H4'	32:a:1094:A:O5'	1.96	0.65
32:a:1141:U:H2'	32:a:1142:A:H8	1.61	0.65
32:a:57:U:H2'	32:a:58:G:H8	1.62	0.64
45:q:9:GLU:HG3	45:q:60:LYS:HG2	1.80	0.64
42:m:93:ARG:NH1	47:s:80:TYR:OH	2.30	0.64
39:i:122:ARG:NH1	39:i:123:ARG:O	2.31	0.64
8:H:4:ILE:HG12	8:H:18:ILE:HG22	1.78	0.64
32:a:663:G:H2'	32:a:664:A:H8	1.62	0.63
32:a:1347:G:H2'	32:a:1348:G:C8	2.33	0.63
32:a:175:A:H62	32:a:187:U:H3	1.46	0.63
6:F:139:PRO:HB2	26:Z:33:MET:HE1	1.80	0.63
6:F:36:LEU:HD23	6:F:152:LEU:HD21	1.81	0.63
42:m:101:ARG:NH1	42:m:104:THR:OG1	2.32	0.63
32:a:84:G:H2'	32:a:85:A:C8	2.33	0.63
32:a:1341:A:OP2	39:i:119:LYS:NZ	2.32	0.63
1:A:715:U:OP2	43:o:87:ARG:NH2	2.31	0.63
32:a:1241:A:H2'	32:a:1242:G:C8	2.34	0.63
32:a:1341:A:H2'	32:a:1342:U:C6	2.33	0.63
1:A:213:G:H22	1:A:230:U:H4'	1.64	0.63
42:m:20:THR:HG21	42:m:27:LYS:HD3	1.80	0.62
32:a:985:G:H2'	32:a:987:C:H41	1.64	0.62
32:a:1395:C:H2'	32:a:1396:G:C8	2.34	0.62
36:f:38:ARG:HB3	36:f:63:ASN:HB2	1.81	0.62
1:A:2317:A:H2'	1:A:2318:A:C8	2.35	0.62
1:A:272:U:O2'	1:A:352:G:N2	2.30	0.62
47:s:12:ASP:OD1	47:s:12:ASP:N	2.33	0.61
39:i:118:ARG:HE	39:i:124:ARG:HA	1.65	0.61
42:m:79:ARG:HH21	42:m:80:LEU:HG	1.65	0.61
32:a:1479:A:H5'	41:l:44:LYS:HD3	1.82	0.61
46:r:30:ASN:HD21	46:r:34:LYS:HB2	1.65	0.61
1:A:591:U:H2'	1:A:592:U:C6	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:159:ILE:HD11	33:b:181:VAL:HG13	1.81	0.61
47:s:36:ARG:NH2	47:s:75:VAL:O	2.33	0.61
1:A:2459:G:OP1	12:L:56:ARG:NH2	2.34	0.61
32:a:735:G:H2'	32:a:736:A:C8	2.36	0.60
32:a:950:A:N7	47:s:55:GLN:NE2	2.49	0.60
32:a:1157:G:N2	32:a:1161:A:OP2	2.29	0.60
42:m:10:PRO:HB2	42:m:13:LYS:HD2	1.83	0.60
1:A:2635:U:OP2	1:A:2721:G:O2'	2.20	0.60
6:F:103:LEU:HD12	6:F:107:ALA:HB3	1.83	0.60
40:k:88:GLY:O	40:k:93:ARG:NH1	2.35	0.60
32:a:1319:C:H2'	32:a:1320:A:H8	1.67	0.60
34:d:152:GLN:HB2	34:d:155:ILE:HG13	1.83	0.60
26:Z:16:CYS:SG	26:Z:17:SER:N	2.75	0.60
32:a:1369:C:P	37:g:6:ARG:NH1	2.74	0.60
32:a:224:U:H2'	32:a:225:G:H8	1.66	0.60
33:b:52:VAL:HA	33:b:55:VAL:HG22	1.84	0.60
27:O:53:VAL:HG23	27:O:54:VAL:HG13	1.84	0.59
32:a:1209:C:H2'	32:a:1210:A:H8	1.67	0.59
32:a:976:C:H2'	32:a:977:C:H6	1.67	0.59
1:A:848:A:H2'	1:A:849:A:H8	1.67	0.59
46:r:66:TYR:HB2	46:r:70:HIS:NE2	2.17	0.59
32:a:326:A:H2'	32:a:327:A:C8	2.37	0.59
32:a:501:U:OP1	34:d:44:ARG:NH2	2.36	0.59
32:a:1347:G:H2'	32:a:1348:G:H8	1.68	0.59
32:a:1141:U:H2'	32:a:1142:A:C8	2.38	0.58
41:l:79:VAL:HG12	41:l:102:LEU:HD23	1.84	0.58
1:A:2389:G:H2'	1:A:2390:U:C6	2.38	0.58
32:a:938:A:H2'	32:a:939:G:C8	2.39	0.58
35:e:166:GLY:HA3	38:h:116:ARG:HD2	1.84	0.58
10:J:4:MET:HG2	10:J:5:GLN:HG2	1.84	0.58
34:d:65:TYR:OH	34:d:95:GLU:OE2	2.20	0.58
2:B:75:U:OP1	21:U:23:ARG:NH2	2.35	0.58
1:A:2551:U:OP1	10:J:40:LYS:NZ	2.36	0.58
8:H:6:LYS:HD2	8:H:37:VAL:HG13	1.84	0.58
32:a:1056:G:N2	32:a:1181:G:O2'	2.36	0.58
32:a:1382:U:H2'	32:a:1383:G:C8	2.38	0.58
1:A:2841:G:N2	1:A:2844:A:OP2	2.32	0.58
26:Z:38:CYS:SG	26:Z:39:SER:N	2.76	0.58
32:a:326:A:H2'	32:a:327:A:H8	1.69	0.58
2:B:11:A:N1	2:B:67:G:O2'	2.33	0.57
32:a:1440:G:O2'	32:a:1441:A:H2'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1158:A:H5'	32:a:1159:C:H5	1.68	0.57
32:a:946:G:O6	42:m:103:LYS:NZ	2.37	0.57
44:p:4:ILE:HG12	44:p:21:VAL:HG22	1.87	0.57
1:A:2439:A:H2'	1:A:2440:A:C8	2.40	0.57
32:a:1253:A:H62	32:a:1264:G:H21	1.53	0.57
37:g:71:SER:HB2	37:g:97:ARG:HG2	1.84	0.57
1:A:2187:A:H2'	1:A:2188:A:C8	2.40	0.57
32:a:470:G:O2'	32:a:472:C:N4	2.38	0.57
1:A:2787:A:H2'	1:A:2788:U:C6	2.40	0.57
39:i:29:VAL:HG22	39:i:64:VAL:HB	1.86	0.57
35:e:80:THR:HG22	35:e:122:ASN:HB2	1.87	0.56
1:A:2762:U:OP1	4:D:111:ARG:NH2	2.39	0.56
32:a:1045:G:H4'	32:a:1046:C:H5''	1.87	0.56
32:a:1116:G:N2	32:a:1117:U:O4	2.27	0.56
1:A:2187:A:H2'	1:A:2188:A:H8	1.70	0.56
6:F:73:SER:HB3	6:F:80:ARG:HD3	1.87	0.56
32:a:83:G:H2'	32:a:84:G:C8	2.41	0.56
32:a:186:U:H2'	32:a:187:U:C6	2.41	0.56
32:a:662:G:H2'	32:a:663:G:H8	1.69	0.56
33:b:162:ILE:HD12	33:b:163:ASP:HB2	1.87	0.56
34:d:118:VAL:HG22	34:d:123:ILE:HG13	1.86	0.56
36:f:42:TRP:CD2	36:f:102:MET:HG2	2.40	0.56
1:A:848:A:H2'	1:A:849:A:C8	2.40	0.56
1:A:2232:U:H2'	1:A:2233:U:C6	2.41	0.56
32:a:140:G:H2'	32:a:141:G:C8	2.41	0.56
32:a:1038:A:H3'	32:a:1039:G:H8	1.70	0.56
32:a:651:U:H2'	32:a:652:A:C8	2.40	0.56
22:V:37:ILE:HG22	22:V:38:ILE:HG13	1.86	0.56
32:a:663:G:H2'	32:a:664:A:C8	2.40	0.56
33:b:160:VAL:HA	33:b:182:VAL:O	2.05	0.56
1:A:295:A:H2'	1:A:296:A:H8	1.70	0.56
12:L:67:ARG:NH1	12:L:105:GLU:OE2	2.34	0.56
32:a:976:C:H2'	32:a:977:C:C6	2.41	0.55
39:i:53:LEU:HD23	39:i:97:LEU:HD23	1.87	0.55
41:l:68:GLY:O	41:l:99:ARG:NH1	2.38	0.55
1:A:1718:A:H2	1:A:1734:G:H21	1.54	0.55
32:a:85:A:O2'	32:a:86:U:O4'	2.24	0.55
32:a:702:G:H2'	32:a:703:G:C8	2.41	0.55
1:A:403:A:H4'	1:A:404:U:H5''	1.89	0.55
32:a:57:U:H2'	32:a:58:G:C8	2.41	0.55
32:a:401:A:C6	32:a:403:A:H1'	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:78:VAL:HG23	33:b:212:MET:HE1	1.89	0.55
45:q:60:LYS:HE3	45:q:79:ILE:HD11	1.89	0.55
32:a:18:U:H2'	32:a:19:C:C6	2.42	0.55
21:U:22:LEU:HG	21:U:27:LYS:HB2	1.89	0.55
23:W:17:ASN:OD1	23:W:27:ARG:HD2	2.08	0.54
32:a:1278:A:H2'	32:a:1279:A:H8	1.71	0.54
34:d:192:SER:OG	34:d:194:ASP:OD1	2.24	0.54
47:s:51:VAL:HB	47:s:75:VAL:HG21	1.89	0.54
33:b:48:PHE:HE1	33:b:214:LYS:HG2	1.71	0.54
32:a:406:G:H2'	32:a:407:C:C6	2.42	0.54
1:A:1465:A:H2'	1:A:1466:A:C8	2.43	0.54
18:R:11:ARG:NH1	18:R:99:ARG:O	2.40	0.54
28:1:31:GLU:HG2	28:1:46:LYS:HG3	1.89	0.54
5:E:16:LEU:HD22	5:E:196:LYS:HG3	1.89	0.54
32:a:1209:C:H2'	32:a:1210:A:C8	2.42	0.54
32:a:1400:C:H2'	32:a:1401:A:H8	1.73	0.54
34:d:3:ARG:HH12	34:d:115:ARG:HD3	1.72	0.54
1:A:6:A:H2'	1:A:7:A:C8	2.43	0.54
42:m:55:SER:O	42:m:59:GLU:HG2	2.08	0.54
10:J:7:GLU:HG2	10:J:20:GLU:HG3	1.88	0.53
33:b:99:LEU:HB3	33:b:177:LEU:HD12	1.90	0.53
37:g:15:ASP:OD1	37:g:17:LYS:N	2.36	0.53
26:Z:36:ASP:OD1	26:Z:36:ASP:N	2.41	0.53
32:a:490:C:OP1	41:l:114:ARG:NH2	2.40	0.53
1:A:1259:U:OP1	27:O:13:ARG:NH1	2.38	0.53
8:H:27:ARG:NH1	23:W:60:ASP:OD2	2.41	0.53
32:a:341:C:O2'	32:a:343:G:OP1	2.20	0.53
32:a:489:G:H2'	32:a:490:C:C6	2.44	0.53
35:e:79:ASP:HB3	35:e:121:HIS:HB2	1.91	0.53
32:a:398:U:H3	32:a:422:G:H1	1.55	0.53
32:a:503:C:H2'	32:a:504:G:H8	1.73	0.53
41:l:33:VAL:HG12	41:l:79:VAL:HG22	1.91	0.53
30:3:17:THR:HG22	30:3:18:GLY:H	1.74	0.53
44:p:12:LYS:HG2	44:p:13:LYS:HG2	1.91	0.53
8:H:38:GLN:O	8:H:43:ASN:ND2	2.33	0.53
36:f:6:VAL:HG13	36:f:89:VAL:HG22	1.91	0.53
1:A:1505:U:H4'	1:A:1506:U:H5'	1.91	0.53
42:m:4:ILE:HG23	42:m:57:ARG:HG2	1.90	0.53
1:A:1335:U:OP1	19:S:19:LYS:NZ	2.41	0.52
32:a:1361:G:OP2	39:i:112:ARG:NH2	2.43	0.52
42:m:40:ASP:HB3	42:m:43:VAL:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:p:27:PRO:HG2	44:p:30:GLY:HA3	1.90	0.52
46:r:23:ASN:OD1	46:r:24:LYS:N	2.42	0.52
1:A:1311:U:H2'	1:A:1312:A:H8	1.75	0.52
32:a:1230:A:H62	32:a:1290:A:N6	2.07	0.52
1:A:270:G:H2'	1:A:271:A:C8	2.45	0.52
1:A:805:A:H5'	1:A:806:G:OP1	2.10	0.52
32:a:1054:U:H2'	32:a:1055:C:C6	2.45	0.52
33:b:30:PHE:HB2	33:b:40:ASN:HB2	1.91	0.52
1:A:1133:U:H3'	1:A:1134:A:H5''	1.92	0.52
32:a:446:U:H3	32:a:464:G:H1	1.57	0.52
32:a:1299:U:H2'	32:a:1300:G:H8	1.74	0.52
42:m:11:VAL:HB	42:m:46:LYS:HG3	1.92	0.52
1:A:1798:A:H2'	1:A:1799:A:C8	2.44	0.52
32:a:288:G:H2'	32:a:289:A:C8	2.44	0.52
32:a:1307:G:N1	32:a:1310:A:OP2	2.42	0.52
1:A:2632:G:H2'	1:A:2633:A:H8	1.76	0.51
39:i:51:LEU:HD11	39:i:62:PHE:HZ	1.75	0.51
39:i:83:THR:HG23	39:i:97:LEU:HD13	1.93	0.51
16:P:107:ALA:O	16:P:111:GLU:HG2	2.09	0.51
32:a:1204:A:O2'	32:a:1206:G:N7	2.34	0.51
43:o:9:LYS:O	43:o:13:GLU:HG2	2.11	0.51
47:s:53:ASN:HB2	47:s:77:THR:HG22	1.93	0.51
6:F:147:ASP:OD1	6:F:147:ASP:N	2.43	0.51
1:A:1142:U:H4'	1:A:1143:A:O4'	2.11	0.51
1:A:1853:G:H1'	1:A:1881:A:N6	2.25	0.51
1:A:639:U:H2'	1:A:640:U:H6	1.76	0.51
23:W:72:ARG:NH1	23:W:78:ILE:O	2.42	0.51
46:r:28:TYR:O	46:r:36:VAL:HG12	2.11	0.51
1:A:369:A:O2'	1:A:423:G:OP1	2.21	0.51
1:A:2067:A:H2'	1:A:2068:C:C6	2.46	0.51
12:L:63:LYS:HB3	12:L:107:THR:HG22	1.92	0.51
32:a:1119:A:H2'	32:a:1120:C:C6	2.45	0.51
32:a:972:C:H2'	32:a:973:U:O4'	2.10	0.51
32:a:1219:C:H2'	32:a:1220:A:H8	1.76	0.51
33:b:69:GLY:HA2	33:b:162:ILE:HG12	1.93	0.51
1:A:295:A:H2'	1:A:296:A:C8	2.45	0.50
41:l:39:THR:HG22	41:l:51:LYS:HG3	1.93	0.50
1:A:1853:G:H1'	1:A:1881:A:H61	1.75	0.50
4:D:13:THR:OG1	4:D:14:ARG:N	2.44	0.50
6:F:116:GLY:HA3	6:F:178:LYS:HB2	1.93	0.50
14:N:8:LEU:O	14:N:12:LYS:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:34:GLU:HG2	17:Q:61:VAL:HG22	1.93	0.50
32:a:717:A:H2'	32:a:718:A:H8	1.77	0.50
32:a:717:A:H2'	32:a:718:A:C8	2.46	0.50
32:a:931:G:H2'	32:a:932:C:C6	2.46	0.50
32:a:1121:C:O4'	32:a:1137:A:N6	2.44	0.50
33:b:16:HIS:ND1	33:b:186:ASP:OD2	2.38	0.50
15:O:107:LYS:HG2	32:a:1423:G:H5'	1.93	0.50
32:a:29:A:O2'	32:a:285:U:OP1	2.28	0.50
8:H:14:VAL:HG22	8:H:15:LEU:H	1.76	0.50
12:L:43:THR:HG22	12:L:94:VAL:HG12	1.93	0.50
26:Z:14:VAL:HG22	26:Z:33:MET:HB3	1.93	0.50
32:a:1112:G:H2'	32:a:1113:A:H8	1.76	0.50
41:l:29:GLN:HB3	41:l:81:LEU:HD21	1.92	0.50
1:A:300:G:N1	1:A:303:A:OP2	2.40	0.50
1:A:2187:A:O2'	1:A:2188:A:OP1	2.28	0.50
1:A:2388:G:H2'	1:A:2389:G:C8	2.47	0.50
32:a:1152:C:H2'	32:a:1153:C:H6	1.77	0.50
32:a:1305:C:H2'	32:a:1306:U:C6	2.45	0.50
38:h:115:ASP:N	38:h:115:ASP:OD1	2.45	0.50
1:A:1516:U:H2'	1:A:1517:A:H8	1.77	0.50
20:T:38:GLY:N	20:T:62:GLU:OE2	2.24	0.50
32:a:513:G:H2'	32:a:514:C:C6	2.47	0.50
7:G:61:ASN:O	7:G:65:GLN:HG2	2.11	0.50
32:a:1283:U:H2'	32:a:1284:A:C8	2.47	0.50
38:h:96:LYS:HG2	38:h:119:ARG:NH2	2.27	0.50
33:b:112:LEU:HD22	33:b:142:LEU:HB3	1.92	0.49
32:a:1357:C:H2'	32:a:1358:U:C6	2.47	0.49
34:d:197:GLU:CD	34:d:197:GLU:H	2.21	0.49
1:A:494:G:N3	18:R:61:ASN:ND2	2.49	0.49
1:A:2280:U:H2'	1:A:2281:G:C8	2.47	0.49
15:O:31:LEU:HD11	15:O:75:PHE:HE2	1.77	0.49
32:a:1323:A:H2'	32:a:1324:A:C8	2.47	0.49
1:A:2419:A:H2'	1:A:2419:A:N3	2.28	0.49
3:C:1:MET:N	3:C:23:THR:OG1	2.42	0.49
32:a:400:A:OP2	34:d:26:LYS:NZ	2.45	0.49
32:a:1229:A:H2	32:a:1232:G:N3	2.10	0.49
32:a:1259:G:N3	32:a:1317:U:O2'	2.44	0.49
1:A:1412:C:HO2'	1:A:1586:U:HO2'	1.57	0.49
12:L:116:GLU:O	12:L:120:ARG:HG2	2.12	0.49
37:g:5:ASN:OD1	37:g:5:ASN:N	2.44	0.49
47:s:49:ILE:HG21	47:s:62:MET:HE2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:703:G:H2'	32:a:704:A:C8	2.48	0.49
32:a:1145:A:O2'	32:a:1146:A:OP1	2.30	0.49
47:s:45:ILE:HD13	47:s:64:GLU:HG2	1.95	0.49
4:D:6:VAL:H	4:D:33:ASN:HD21	1.61	0.49
14:N:80:ASP:O	14:N:84:GLU:HG3	2.13	0.49
39:i:6:TYR:HE1	39:i:17:ARG:HB3	1.77	0.49
7:G:103:GLU:HG2	7:G:117:LYS:HD2	1.94	0.49
31:4:27:CYS:SG	31:4:28:THR:N	2.85	0.49
32:a:1152:C:H2'	32:a:1153:C:C6	2.48	0.49
32:a:1245:G:N2	32:a:1250:C:O2'	2.46	0.49
1:A:589:U:H2'	1:A:590:A:H8	1.78	0.48
42:m:15:THR:OG1	42:m:41:PRO:HA	2.13	0.48
1:A:722:A:H2'	1:A:723:A:C8	2.47	0.48
1:A:1962:A:N3	1:A:2581:G:O2'	2.37	0.48
1:A:2389:G:C2	1:A:2390:U:C4	3.01	0.48
32:a:1047:A:H2'	32:a:1048:C:O4'	2.12	0.48
32:a:1283:U:H2'	32:a:1284:A:H8	1.77	0.48
39:i:54:THR:HB	39:i:86:LEU:HD21	1.95	0.48
6:F:30:ALA:N	6:F:159:THR:OG1	2.43	0.48
6:F:62:GLY:O	6:F:95:ARG:NH1	2.46	0.48
32:a:953:U:OP2	32:a:1214:C:O2'	2.25	0.48
1:A:1550:U:H2'	1:A:1551:U:C6	2.49	0.48
8:H:6:LYS:HG2	8:H:47:PHE:HZ	1.79	0.48
32:a:373:C:H2'	32:a:374:C:H6	1.78	0.48
32:a:938:A:H2'	32:a:939:G:H8	1.75	0.48
32:a:968:G:OP2	32:a:1349:U:O2'	2.29	0.48
1:A:639:U:H2'	1:A:640:U:C6	2.48	0.48
32:a:516:G:H8	32:a:524:A:H2	1.60	0.48
32:a:1055:C:OP2	32:a:1056:G:O2'	2.28	0.48
32:a:1289:U:H4'	32:a:1290:A:C4	2.48	0.48
32:a:1341:A:H2'	32:a:1342:U:H6	1.78	0.48
37:g:136:VAL:O	37:g:140:GLU:HG2	2.13	0.48
1:A:1411:A:H4'	1:A:1412:C:OP1	2.13	0.48
1:A:2021:C:H2'	1:A:2022:U:C6	2.48	0.48
32:a:1166:G:H2'	32:a:1167:A:H8	1.79	0.48
40:k:19:ALA:O	40:k:82:VAL:HA	2.14	0.48
1:A:2696:A:O2'	13:M:85:ASP:OD1	2.27	0.48
1:A:2783:G:C4	1:A:2784:A:H1'	2.49	0.48
32:a:526:G:H2'	32:a:527:G:H8	1.79	0.48
32:a:1299:U:H2'	32:a:1300:G:C8	2.49	0.48
32:a:1369:C:OP2	37:g:6:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:205:VAL:O	33:b:209:SER:OG	2.24	0.48
42:m:50:GLU:OE1	42:m:50:GLU:N	2.28	0.48
37:g:13:LEU:HD12	37:g:14:PRO:HD2	1.96	0.48
1:A:2458:A:N6	1:A:2470:G:O2'	2.43	0.48
32:a:451:G:H2'	32:a:452:U:C6	2.49	0.48
44:p:76:LYS:HA	44:p:79:LYS:HZ3	1.78	0.48
33:b:2:SER:OG	33:b:3:LEU:N	2.46	0.48
1:A:2280:U:OP1	1:A:2369:U:O2'	2.31	0.47
36:f:42:TRP:HB2	36:f:59:TYR:HB2	1.96	0.47
1:A:1:G:H2'	1:A:2:A:C8	2.49	0.47
1:A:2205:G:H2'	1:A:2206:A:C8	2.50	0.47
32:a:184:G:H2'	32:a:185:A:H8	1.79	0.47
32:a:1120:C:O2'	32:a:1121:C:O5'	2.32	0.47
33:b:172:GLN:HA	33:b:175:GLN:HG2	1.96	0.47
2:B:29:C:H2'	2:B:51:A:H61	1.79	0.47
3:C:162:PHE:HB3	3:C:195:VAL:HG13	1.95	0.47
39:i:9:GLY:HA3	39:i:77:ALA:O	2.13	0.47
32:a:175:A:H2	32:a:213:A:H5'	1.78	0.47
32:a:1273:C:H2'	32:a:1274:U:C6	2.49	0.47
9:I:74:TYR:O	9:I:86:SER:HA	2.13	0.47
32:a:1106:C:H2'	32:a:1107:C:C6	2.49	0.47
47:s:62:MET:HE1	47:s:71:LEU:HD21	1.96	0.47
14:N:73:ILE:O	14:N:77:ILE:HG12	2.14	0.47
36:f:11:HIS:ND1	36:f:12:PRO:HD2	2.30	0.47
36:f:13:ASP:OD1	36:f:14:GLN:N	2.46	0.47
47:s:11:VAL:HG13	47:s:38:SER:HB3	1.96	0.47
1:A:543:A:H2'	1:A:544:U:C6	2.50	0.47
1:A:596:A:H2'	1:A:597:G:H8	1.79	0.47
1:A:680:G:H2'	1:A:681:G:C8	2.50	0.47
1:A:1427:G:H2'	1:A:1428:A:C8	2.50	0.47
19:S:96:VAL:HG22	24:X:40:GLN:OE1	2.15	0.47
32:a:370:C:H2'	32:a:371:A:O4'	2.15	0.47
32:a:448:A:H2'	32:a:449:A:H8	1.79	0.47
32:a:1232:G:H2'	32:a:1233:G:H8	1.79	0.47
33:b:44:THR:HG22	33:b:199:PRO:HB2	1.97	0.47
33:b:64:LYS:HG2	33:b:87:MET:HE1	1.96	0.47
1:A:640:U:H2'	1:A:641:U:C6	2.50	0.47
32:a:1236:A:H2'	32:a:1237:U:C6	2.50	0.47
35:e:41:ASP:CG	35:e:45:ARG:HG2	2.40	0.47
3:C:158:SER:O	3:C:161:THR:OG1	2.31	0.47
32:a:1064:G:H2'	32:a:1065:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1106:C:H2'	32:a:1107:C:H6	1.79	0.47
32:a:1369:C:H5''	37:g:6:ARG:HH22	1.80	0.47
49:u:40:LYS:H	49:u:43:TRP:HE3	1.63	0.47
1:A:1389:U:H2'	1:A:1390:A:O4'	2.15	0.46
1:A:2632:G:H2'	1:A:2633:A:C8	2.51	0.46
5:E:45:GLN:HG2	5:E:47:THR:HG23	1.96	0.46
11:K:108:VAL:HG13	11:K:125:ILE:HG23	1.97	0.46
34:d:87:GLY:N	34:d:201:ILE:HD11	2.30	0.46
38:h:91:HIS:CE1	38:h:122:GLY:HA2	2.50	0.46
1:A:581:C:H2'	1:A:582:A:C8	2.50	0.46
32:a:1216:A:H1'	47:s:78:ARG:NH2	2.27	0.46
46:r:61:LEU:HA	46:r:61:LEU:HD23	1.83	0.46
1:A:1348:A:H2'	1:A:1349:A:C8	2.51	0.46
1:A:1592:A:H2'	1:A:1593:A:C8	2.50	0.46
17:Q:36:ASP:OD1	17:Q:36:ASP:N	2.45	0.46
33:b:117:LYS:HE2	33:b:117:LYS:HB3	1.79	0.46
47:s:15:LEU:HD21	47:s:49:ILE:HD11	1.96	0.46
1:A:785:G:H5'	1:A:786:G:OP1	2.16	0.46
1:A:1852:U:H2'	1:A:1853:G:O4'	2.15	0.46
1:A:2536:A:H2'	1:A:2537:U:C6	2.50	0.46
28:l:13:THR:HG21	28:l:39:VAL:HG23	1.97	0.46
32:a:1063:C:H2'	32:a:1064:G:H8	1.80	0.46
32:a:1197:G:H2'	32:a:1198:G:O4'	2.15	0.46
1:A:704:U:H2'	1:A:705:G:O4'	2.15	0.46
32:a:454:A:H2'	32:a:455:A:C8	2.50	0.46
32:a:937:G:C2	32:a:938:A:C8	3.04	0.46
35:e:76:LEU:HD11	35:e:118:VAL:HG12	1.95	0.46
41:l:30:ARG:HA	41:l:30:ARG:HD2	1.73	0.46
47:s:2:PRO:HB2	47:s:3:ARG:H	1.57	0.46
1:A:1311:U:H2'	1:A:1312:A:C8	2.51	0.46
32:a:1242:G:H2'	32:a:1243:A:C8	2.51	0.46
1:A:2317:A:H2'	1:A:2318:A:H8	1.79	0.46
7:G:85:GLU:OE2	7:G:87:LYS:NZ	2.48	0.46
32:a:448:A:H2'	32:a:449:A:C8	2.51	0.46
32:a:1311:C:C2	47:s:72:GLY:HA3	2.50	0.46
1:A:299:U:H2'	1:A:300:G:O4'	2.15	0.46
1:A:591:U:H2'	1:A:592:U:H6	1.80	0.46
32:a:653:G:H22	32:a:730:G:H1	1.64	0.46
47:s:50:ALA:HA	47:s:59:PRO:HA	1.98	0.46
48:t:34:LYS:HB3	48:t:50:ASN:HD22	1.81	0.46
32:a:447:C:H2'	32:a:448:A:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:967:A:O4'	32:a:1348:G:N2	2.47	0.46
32:a:1228:C:H4'	32:a:1291:G:H22	1.81	0.46
1:A:2299:A:H2'	6:F:77:PHE:HE2	1.81	0.45
7:G:167:ASP:OD1	7:G:167:ASP:N	2.49	0.45
35:e:143:GLY:O	35:e:147:ILE:HG13	2.16	0.45
1:A:608:A:H2'	1:A:609:A:C8	2.51	0.45
32:a:219:G:OP1	44:p:31:ARG:NH2	2.49	0.45
32:a:482:A:H2'	32:a:483:G:C8	2.51	0.45
32:a:1101:C:H2'	32:a:1102:A:O4'	2.17	0.45
2:B:47:C:H2'	2:B:48:A:H8	1.82	0.45
26:Z:12:VAL:HG13	26:Z:14:VAL:HG23	1.97	0.45
34:d:78:GLU:O	34:d:82:ARG:HG2	2.16	0.45
48:t:34:LYS:HB3	48:t:50:ASN:ND2	2.31	0.45
1:A:2048:A:OP1	4:D:147:THR:OG1	2.29	0.45
17:Q:27:LEU:O	17:Q:67:GLN:NE2	2.50	0.45
32:a:1298:U:H2'	32:a:1299:U:C6	2.52	0.45
41:l:114:ARG:HB3	41:l:119:THR:HB	1.99	0.45
49:u:33:ARG:O	49:u:36:GLU:HG2	2.16	0.45
1:A:596:A:H2'	1:A:597:G:C8	2.51	0.45
1:A:2070:U:H2'	1:A:2071:U:C6	2.51	0.45
32:a:489:G:H2'	32:a:490:C:H6	1.80	0.45
32:a:631:A:C8	38:h:109:SER:HA	2.52	0.45
33:b:53:ASN:O	33:b:57:LYS:HG2	2.17	0.45
42:m:33:ILE:HG23	42:m:59:GLU:HB2	1.97	0.45
1:A:6:A:H2'	1:A:7:A:H8	1.79	0.45
1:A:1260:G:OP1	27:0:16:ARG:NH2	2.35	0.45
6:F:148:SER:HB3	6:F:150:ARG:NH1	2.32	0.45
6:F:161:LYS:HD2	6:F:165:GLN:HE22	1.81	0.45
7:G:90:ILE:HD11	7:G:132:ILE:HD11	1.97	0.45
18:R:41:LYS:HE3	27:0:22:LEU:HD21	1.98	0.45
32:a:457:A:H3'	32:a:458:G:C8	2.46	0.45
32:a:935:U:H2'	32:a:936:G:C8	2.51	0.45
32:a:1148:A:H4'	32:a:1149:C:O4'	2.16	0.45
42:m:44:LYS:HD3	42:m:46:LYS:NZ	2.31	0.45
1:A:607:U:C5	1:A:620:G:C5	3.05	0.45
1:A:1465:A:H2'	1:A:1466:A:H8	1.82	0.45
34:d:122:GLY:C	34:d:146:ARG:HG3	2.41	0.45
32:a:39:G:H22	32:a:386:A:H5'	1.81	0.45
32:a:84:G:H2'	32:a:85:A:H8	1.81	0.45
32:a:175:A:C4	32:a:177:A:C8	3.05	0.45
32:a:1228:C:H3'	32:a:1327:C:H41	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1257:G:N2	32:a:1260:A:OP2	2.47	0.45
48:t:7:ALA:O	48:t:11:ILE:HG13	2.16	0.45
1:A:2060:C:H2'	1:A:2061:C:C6	2.51	0.45
9:I:107:GLY:HA2	9:I:111:ARG:NH2	2.32	0.45
23:W:18:VAL:HG22	23:W:24:LYS:HD3	1.99	0.45
28:l:6:ARG:HD3	28:l:50:ILE:HA	1.97	0.45
33:b:102:TYR:CE1	33:b:106:ARG:HD2	2.52	0.45
6:F:126:GLY:O	6:F:158:THR:OG1	2.33	0.45
32:a:1140:C:H2'	32:a:1141:U:C6	2.51	0.45
32:a:1252:A:OP2	32:a:1265:G:N2	2.50	0.45
32:a:1252:A:N6	32:a:1265:G:O2'	2.50	0.45
33:b:92:HIS:CD2	33:b:145:VAL:HA	2.52	0.45
39:i:95:PRO:O	39:i:99:GLU:HG2	2.16	0.45
24:X:66:LYS:HA	24:X:66:LYS:HD2	1.82	0.44
32:a:1251:G:H2'	32:a:1265:G:H21	1.82	0.44
32:a:1341:A:O2'	32:a:1342:U:OP1	2.30	0.44
36:f:42:TRP:HE3	36:f:59:TYR:HB3	1.81	0.44
39:i:54:THR:HG23	39:i:56:ASN:H	1.82	0.44
42:m:89:ARG:HH12	47:s:76:VAL:HG11	1.82	0.44
1:A:1354:U:H2'	1:A:1355:A:H8	1.82	0.44
6:F:139:PRO:CB	26:Z:33:MET:HE1	2.47	0.44
10:J:105:GLU:N	10:J:105:GLU:OE1	2.50	0.44
32:a:35:C:H2'	32:a:36:G:H8	1.83	0.44
32:a:1157:G:O2'	32:a:1161:A:N6	2.50	0.44
32:a:1289:U:H5''	32:a:1290:A:OP1	2.17	0.44
32:a:1359:G:P	39:i:113:LYS:HZ1	2.40	0.44
39:i:105:ARG:NH1	39:i:106:ASP:O	2.50	0.44
40:k:123:PRO:HG2	49:u:38:PHE:HB2	1.98	0.44
1:A:313:A:N3	5:E:169:ASN:ND2	2.62	0.44
6:F:52:PHE:HB3	6:F:147:ASP:OD2	2.17	0.44
32:a:1069:G:N2	32:a:1072:A:OP2	2.45	0.44
34:d:159:VAL:HG12	34:d:163:LYS:HE3	1.98	0.44
42:m:37:CYS:SG	42:m:56:LEU:HD12	2.58	0.44
47:s:11:VAL:HB	47:s:16:LEU:HD13	1.99	0.44
1:A:1525:A:H2'	1:A:1526:A:C8	2.52	0.44
32:a:1235:U:H2'	32:a:1236:A:C8	2.53	0.44
32:a:1369:C:C5'	37:g:6:ARG:HH12	2.27	0.44
32:a:1395:C:H2'	32:a:1396:G:H8	1.78	0.44
37:g:112:ARG:NH1	37:g:127:GLU:OE1	2.51	0.44
43:o:52:ARG:O	43:o:56:LEU:HG	2.17	0.44
2:B:58:C:H2'	2:B:59:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:41:GLN:O	8:H:45:LYS:HG2	2.17	0.44
15:O:2:LYS:HG3	15:O:7:GLU:HG3	2.00	0.44
32:a:1088:C:H2'	32:a:1089:C:C6	2.52	0.44
32:a:1097:A:OP1	33:b:111:ARG:NH1	2.50	0.44
32:a:1517:G:O6	49:u:46:LYS:NZ	2.51	0.44
1:A:1549:A:H2'	1:A:1550:U:C6	2.53	0.44
1:A:2774:C:OP1	4:D:43:LYS:NZ	2.35	0.44
17:Q:40:MET:HE2	17:Q:40:MET:HB2	1.94	0.44
32:a:1232:G:H2'	32:a:1233:G:C8	2.53	0.44
33:b:2:SER:O	33:b:5:LYS:HG2	2.18	0.44
1:A:401:A:H2'	1:A:402:U:O4'	2.18	0.44
1:A:1590:A:H2'	1:A:1591:U:C6	2.53	0.44
32:a:667:U:H2'	32:a:668:U:C6	2.53	0.44
32:a:704:A:H2'	32:a:705:A:C8	2.53	0.44
32:a:969:A:H1'	32:a:974:U:O4	2.16	0.44
32:a:1249:G:H2'	32:a:1250:C:C6	2.53	0.44
33:b:75:GLN:O	33:b:78:VAL:HG12	2.16	0.44
39:i:25:GLY:HA2	39:i:60:PHE:O	2.17	0.44
1:A:1349:A:OP1	3:C:39:LYS:NZ	2.41	0.44
2:B:28:C:H1'	2:B:55:A:H61	1.83	0.44
23:W:56:MET:HE3	23:W:56:MET:HB2	1.87	0.44
26:Z:2:ARG:O	26:Z:5:ILE:HG12	2.17	0.44
32:a:526:G:H2'	32:a:527:G:C8	2.53	0.44
32:a:1112:G:H2'	32:a:1113:A:C8	2.52	0.44
32:a:1252:A:C6	32:a:1266:A:H1'	2.53	0.44
39:i:10:ARG:HB3	39:i:105:ARG:HH21	1.83	0.44
13:M:36:THR:OG1	13:M:37:THR:N	2.51	0.44
32:a:195:G:H2'	32:a:196:C:C6	2.52	0.44
32:a:502:C:H2'	32:a:503:C:C6	2.53	0.44
17:Q:67:GLN:OE1	17:Q:95:THR:OG1	2.30	0.43
1:A:581:C:H2'	1:A:582:A:H8	1.83	0.43
10:J:35:ILE:HG21	10:J:103:THR:HG21	2.00	0.43
33:b:92:HIS:ND1	33:b:144:LYS:HE2	2.33	0.43
32:a:498:A:N3	32:a:532:U:O2'	2.50	0.43
32:a:828:U:C4	32:a:829:C:C4	3.06	0.43
32:a:1285:C:H2'	32:a:1286:U:C6	2.53	0.43
34:d:105:MET:HG2	34:d:171:ILE:HD11	2.00	0.43
1:A:45:A:H2'	1:A:46:G:O4'	2.18	0.43
1:A:846:A:H8	1:A:846:A:OP2	2.02	0.43
32:a:693:A:C4	32:a:694:G:C8	3.07	0.43
32:a:941:A:H2'	32:a:942:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1442:A:H5'	32:a:1444:G:O4'	2.18	0.43
42:m:11:VAL:O	42:m:45:ILE:HB	2.18	0.43
1:A:1913:U:O4	1:A:1914:A:N6	2.51	0.43
26:Z:31:LYS:HE2	26:Z:31:LYS:HB2	1.85	0.43
32:a:158:A:H2'	32:a:159:C:C6	2.54	0.43
34:d:168:LEU:HD13	34:d:170:TRP:CZ2	2.54	0.43
34:d:170:TRP:CD2	34:d:186:PRO:HA	2.54	0.43
1:A:1380:A:O2'	1:A:1391:U:O2	2.35	0.43
32:a:200:C:H4'	32:a:201:G:C8	2.54	0.43
32:a:414:G:H2'	32:a:415:U:C6	2.54	0.43
32:a:736:A:H2'	32:a:737:U:C6	2.53	0.43
32:a:1358:U:H2'	32:a:1359:G:O4'	2.18	0.43
32:a:1403:C:H2'	32:a:1404:A:C8	2.53	0.43
39:i:112:ARG:HE	39:i:112:ARG:HA	1.83	0.43
40:k:53:ARG:HH21	40:k:57:LYS:HD3	1.83	0.43
42:m:37:CYS:SG	42:m:59:GLU:HG3	2.58	0.43
47:s:40:ILE:HD12	47:s:40:ILE:H	1.83	0.43
1:A:570:G:H2'	1:A:2026:A:N7	2.33	0.43
1:A:1516:U:H2'	1:A:1517:A:C8	2.54	0.43
1:A:1649:G:H2'	1:A:1650:A:C8	2.53	0.43
32:a:478:C:H2'	32:a:479:C:C6	2.53	0.43
33:b:92:HIS:CD2	33:b:93:ARG:HB3	2.53	0.43
35:e:160:SER:O	35:e:164:ILE:HG23	2.18	0.43
1:A:1790:A:H2'	1:A:1791:C:C6	2.53	0.43
1:A:2048:A:H4'	4:D:149:GLN:O	2.19	0.43
1:A:2638:C:H2'	1:A:2639:U:H6	1.82	0.43
32:a:196:C:H2'	32:a:197:U:O4'	2.19	0.43
32:a:977:C:H2'	32:a:978:U:C6	2.54	0.43
33:b:51:ALA:O	33:b:55:VAL:HG13	2.19	0.43
33:b:75:GLN:NE2	33:b:91:SER:OG	2.44	0.43
33:b:119:ARG:O	33:b:119:ARG:NH1	2.35	0.43
40:k:93:ARG:NH2	40:k:112:ASP:OD2	2.42	0.43
16:P:104:ASP:OD1	16:P:105:ALA:N	2.52	0.43
32:a:954:C:H2'	32:a:955:G:H8	1.84	0.43
32:a:1056:G:H1'	32:a:1181:G:N2	2.34	0.43
32:a:1324:A:H2'	32:a:1325:G:O4'	2.18	0.43
33:b:69:GLY:O	33:b:91:SER:HA	2.18	0.43
36:f:12:PRO:HD3	36:f:57:ALA:HA	2.00	0.43
1:A:613:A:H5''	1:A:614:A:C8	2.54	0.43
7:G:165:TYR:HB2	7:G:168:GLU:HB2	2.00	0.43
16:P:105:ALA:O	16:P:109:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:464:G:H2'	32:a:465:G:H8	1.84	0.43
32:a:726:U:H2'	32:a:727:U:H6	1.84	0.43
32:a:1311:C:H42	47:s:36:ARG:HG3	1.84	0.43
32:a:1379:U:H2'	32:a:1380:C:H6	1.83	0.43
39:i:51:LEU:HD11	39:i:62:PHE:CZ	2.54	0.43
1:A:2316:A:H2'	1:A:2317:A:C8	2.54	0.42
2:B:1:A:H8	2:B:2:U:C5	2.36	0.42
32:a:91:A:H2'	32:a:92:C:C6	2.54	0.42
32:a:399:G:OP1	34:d:26:LYS:HD2	2.19	0.42
32:a:459:C:H2'	32:a:460:C:H6	1.83	0.42
32:a:1103:A:O2'	32:a:1104:C:H6	2.02	0.42
1:A:1115:C:H2'	1:A:1116:G:C8	2.54	0.42
15:O:31:LEU:O	15:O:41:ILE:HA	2.18	0.42
32:a:494:G:H2'	32:a:495:G:C8	2.54	0.42
32:a:1066:G:H4'	33:b:101:ASN:HB2	2.00	0.42
32:a:1266:A:N3	32:a:1266:A:H2'	2.35	0.42
1:A:1193:G:H2'	1:A:1194:U:H6	1.85	0.42
3:C:212:LYS:HD2	3:C:217:ILE:HD12	2.01	0.42
32:a:1145:A:H2'	32:a:1146:A:C8	2.54	0.42
32:a:1236:A:H2'	32:a:1237:U:H6	1.84	0.42
33:b:177:LEU:HD23	33:b:177:LEU:HA	1.84	0.42
34:d:95:GLU:O	34:d:100:ASN:ND2	2.52	0.42
36:f:45:ARG:HB2	36:f:59:TYR:CE1	2.54	0.42
1:A:1792:U:H2'	1:A:1793:C:C6	2.54	0.42
1:A:1792:U:H2'	1:A:1793:C:H6	1.83	0.42
13:M:87:LEU:HD23	13:M:87:LEU:HA	1.84	0.42
32:a:33:A:H2'	32:a:34:A:C8	2.54	0.42
32:a:178:U:H2'	32:a:179:C:C6	2.54	0.42
32:a:413:G:H2'	32:a:414:G:C8	2.54	0.42
32:a:1334:G:O2'	39:i:122:ARG:NH1	2.52	0.42
33:b:82:ALA:HB1	33:b:87:MET:O	2.19	0.42
42:m:13:LYS:HD3	42:m:17:ILE:HG22	2.02	0.42
42:m:15:THR:HG23	42:m:43:VAL:O	2.19	0.42
1:A:1515:A:C5	1:A:1516:U:C5	3.08	0.42
1:A:2783:G:N3	1:A:2784:A:H1'	2.34	0.42
8:H:1:MET:O	8:H:20:ASN:HA	2.19	0.42
12:L:31:GLU:OE2	12:L:107:THR:OG1	2.29	0.42
32:a:485:A:N3	32:a:485:A:H2'	2.34	0.42
32:a:1066:G:H1	32:a:1075:U:H3	1.67	0.42
32:a:1305:C:H2'	32:a:1306:U:H6	1.83	0.42
33:b:86:GLY:O	33:b:87:MET:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:h:11:PHE:CD1	38:h:77:ILE:HD11	2.54	0.42
1:A:192:A:N6	1:A:2419:A:O2'	2.52	0.42
1:A:1917:G:H2'	1:A:1918:G:H8	1.83	0.42
1:A:2638:C:H2'	1:A:2639:U:C6	2.54	0.42
26:Z:12:VAL:HG12	26:Z:24:THR:O	2.20	0.42
26:Z:36:ASP:OD1	42:m:3:ARG:NH2	2.48	0.42
32:a:299:G:H5''	44:p:31:ARG:HG3	2.02	0.42
32:a:528:G:H2'	32:a:529:G:C8	2.54	0.42
32:a:1311:C:H2'	32:a:1312:U:C6	2.55	0.42
33:b:45:VAL:HB	33:b:46:PRO:HD3	2.02	0.42
33:b:191:PRO:HB2	33:b:197:ILE:HD13	2.01	0.42
1:A:186:A:H2'	1:A:187:C:C6	2.55	0.42
32:a:129:C:O2'	32:a:130:C:OP1	2.37	0.42
32:a:286:G:N2	32:a:289:A:OP2	2.48	0.42
32:a:416:U:OP2	32:a:417:G:O2'	2.25	0.42
32:a:502:C:H2'	32:a:503:C:H6	1.84	0.42
32:a:1049:G:H3'	32:a:1050:G:H8	1.85	0.42
32:a:1216:A:H2'	32:a:1217:C:C5	2.55	0.42
32:a:1237:U:H2'	32:a:1238:U:C6	2.55	0.42
32:a:1451:U:H2'	32:a:1452:A:H8	1.84	0.42
33:b:30:PHE:HB3	33:b:38:ILE:O	2.20	0.42
1:A:222:A:C2	1:A:2396:A:H1'	2.55	0.42
1:A:533:U:H2'	1:A:534:A:C8	2.55	0.42
1:A:2450:U:H2'	1:A:2451:C:C6	2.54	0.42
7:G:174:GLU:OE1	7:G:174:GLU:N	2.52	0.42
20:T:49:ASN:HB3	20:T:54:ILE:HB	2.01	0.42
32:a:1382:U:H2'	32:a:1383:G:H8	1.82	0.42
36:f:75:GLN:OE1	36:f:87:ARG:NH1	2.53	0.42
1:A:53:A:H2'	1:A:54:A:C8	2.55	0.42
1:A:743:A:H2'	1:A:744:C:C6	2.55	0.42
11:K:19:LEU:HB3	11:K:31:SER:HB3	2.02	0.42
32:a:528:G:H2'	32:a:529:G:H8	1.84	0.42
1:A:1348:A:H2'	1:A:1349:A:H8	1.85	0.42
32:a:1151:G:O6	32:a:1173:G:O6	2.38	0.42
33:b:71:LYS:O	33:b:75:GLN:HG3	2.20	0.42
33:b:124:LEU:HD23	33:b:132:MET:HG2	2.01	0.42
32:a:373:C:H2'	32:a:374:C:C6	2.54	0.41
32:a:402:G:N2	32:a:417:G:H1'	2.35	0.41
32:a:406:G:H2'	32:a:407:C:H6	1.85	0.41
32:a:1170:A:H2'	32:a:1171:A:O4'	2.19	0.41
42:m:74:SER:HA	42:m:77:ILE:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1491:A:H2'	1:A:1492:A:C8	2.55	0.41
1:A:2390:U:C4	1:A:2391:C:C4	3.09	0.41
5:E:63:PRO:HB2	5:E:64:TRP:CE3	2.55	0.41
17:Q:59:LYS:HE2	17:Q:59:LYS:HB3	1.83	0.41
32:a:409:C:H2'	32:a:411:A:C2	2.54	0.41
32:a:785:C:H5''	40:k:129:VAL:HG22	2.02	0.41
32:a:1503:G:N2	32:a:1506:A:OP2	2.47	0.41
33:b:30:PHE:HD2	33:b:38:ILE:HB	1.85	0.41
35:e:47:GLY:HA3	35:e:70:ASN:O	2.20	0.41
36:f:38:ARG:NH1	36:f:98:GLU:O	2.44	0.41
43:o:47:LYS:HA	43:o:47:LYS:HD3	1.87	0.41
1:A:2491:G:C6	1:A:2565:G:C6	3.09	0.41
4:D:153:PRO:HG3	4:D:157:PHE:CZ	2.54	0.41
15:O:15:ARG:NH1	15:O:79:SER:O	2.53	0.41
16:P:86:ALA:HB2	16:P:116:ALA:HB2	2.01	0.41
20:T:51:ASN:OD1	20:T:51:ASN:N	2.53	0.41
32:a:1360:C:OP1	39:i:112:ARG:NH1	2.53	0.41
32:a:1442:A:H4'	32:a:1443:U:O5'	2.18	0.41
11:K:104:ASP:N	11:K:104:ASP:OD1	2.50	0.41
32:a:988:A:H2'	32:a:989:U:C6	2.55	0.41
33:b:213:LYS:HG3	33:b:214:LYS:N	2.35	0.41
36:f:42:TRP:CE3	36:f:59:TYR:HB3	2.56	0.41
43:o:15:GLN:HB2	43:o:20:ASP:HB3	2.01	0.41
1:A:948:A:H2'	1:A:949:C:C6	2.55	0.41
1:A:1523:C:H2'	1:A:1524:G:O4'	2.19	0.41
5:E:83:ARG:HG2	5:E:84:LYS:HG2	2.02	0.41
27:O:30:ASP:OD1	27:O:31:LYS:N	2.54	0.41
32:a:500:C:C2	32:a:501:U:C5	3.08	0.41
32:a:1137:A:H3'	32:a:1138:C:H6	1.86	0.41
32:a:1140:C:H2'	32:a:1141:U:H6	1.86	0.41
33:b:202:ASP:CG	33:b:203:ASP:H	2.28	0.41
38:h:76:MET:HE2	38:h:132:ALA:HB3	2.01	0.41
40:k:97:ILE:HG22	49:u:12:PHE:HZ	1.85	0.41
1:A:761:G:H2'	1:A:762:A:O4'	2.20	0.41
26:Z:15:THR:HB	26:Z:21:THR:HG22	2.02	0.41
32:a:313:G:N1	32:a:316:A:OP2	2.50	0.41
32:a:549:A:H4'	32:a:550:U:H5''	2.03	0.41
32:a:740:U:H2'	32:a:741:G:O4'	2.20	0.41
32:a:1096:G:H4'	33:b:111:ARG:HH22	1.85	0.41
32:a:1396:G:H2'	32:a:1397:U:H6	1.85	0.41
33:b:92:HIS:CD2	33:b:145:VAL:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1924:A:H2'	1:A:1925:G:O4'	2.21	0.41
33:b:64:LYS:HE3	33:b:64:LYS:HB2	1.91	0.41
33:b:95:LEU:H	33:b:98:MET:HE3	1.86	0.41
34:d:159:VAL:O	34:d:163:LYS:HG3	2.20	0.41
36:f:18:LEU:O	36:f:22:LEU:HB2	2.20	0.41
38:h:30:SER:HB3	38:h:33:LYS:HG3	2.02	0.41
1:A:1412:C:H2'	1:A:1413:G:O4'	2.19	0.41
1:A:1724:C:O2'	1:A:1725:U:O5'	2.35	0.41
2:B:11:A:O2'	2:B:13:A:OP2	2.38	0.41
32:a:235:A:C2	32:a:271:A:C5	3.09	0.41
32:a:413:G:H2'	32:a:414:G:H8	1.85	0.41
32:a:1346:A:H2'	32:a:1347:G:H8	1.85	0.41
35:e:53:SER:HB3	35:e:59:ALA:HB2	2.02	0.41
35:e:56:VAL:O	35:e:60:ILE:HG13	2.21	0.41
1:A:2:A:H2'	1:A:3:C:C6	2.55	0.41
1:A:2191:U:H2'	1:A:2192:C:H6	1.86	0.41
1:A:2651:A:O5'	1:A:2651:A:H8	2.04	0.41
2:B:101:A:H4'	21:U:94:MET:HE1	2.03	0.41
3:C:81:ARG:NE	3:C:83:GLU:OE2	2.53	0.41
10:J:109:GLU:CD	10:J:109:GLU:H	2.29	0.41
10:J:122:LEU:HD23	10:J:122:LEU:HA	1.91	0.41
14:N:69:GLU:O	14:N:73:ILE:HG13	2.21	0.41
32:a:129:C:O2'	44:p:66:GLN:NE2	2.53	0.41
32:a:725:A:H2'	32:a:726:U:C6	2.56	0.41
33:b:29:ILE:HD13	33:b:29:ILE:HA	1.93	0.41
33:b:64:LYS:NZ	33:b:152:MET:HA	2.35	0.41
34:d:147:GLU:HA	34:d:150:LYS:HD2	2.03	0.41
35:e:46:ILE:HG12	35:e:47:GLY:N	2.36	0.41
46:r:51:LEU:HD23	46:r:51:LEU:HA	1.88	0.41
49:u:54:LYS:HE3	49:u:54:LYS:HB3	1.82	0.41
1:A:2:A:H2'	1:A:3:C:H6	1.86	0.41
1:A:85:A:C2	1:A:104:A:C5	3.09	0.41
1:A:533:U:O2'	16:P:49:ASP:OD2	2.21	0.41
1:A:1790:A:H2'	1:A:1791:C:H6	1.86	0.41
6:F:50:MET:HE2	6:F:67:VAL:HG23	2.02	0.41
32:a:641:U:O4	32:a:741:G:O2'	2.28	0.41
32:a:1193:U:H2'	32:a:1194:C:O4'	2.20	0.41
34:d:87:GLY:HA3	34:d:197:GLU:HG3	2.03	0.41
1:A:572:A:H5''	1:A:573:U:OP2	2.22	0.40
1:A:1662:A:H61	1:A:1992:C:H42	1.69	0.40
2:B:47:C:H2'	2:B:48:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:117:LYS:HE3	7:G:117:LYS:HB3	1.91	0.40
32:a:18:U:H2'	32:a:19:C:H6	1.85	0.40
32:a:726:U:H2'	32:a:727:U:C6	2.56	0.40
32:a:1379:U:H2'	32:a:1380:C:C6	2.56	0.40
1:A:1262:G:OP1	27:0:16:ARG:NE	2.53	0.40
32:a:456:U:H3'	32:a:457:A:H5''	2.02	0.40
32:a:503:C:H2'	32:a:504:G:C8	2.56	0.40
32:a:742:A:H4'	32:a:743:C:O5'	2.21	0.40
32:a:914:G:H2'	32:a:915:A:C8	2.56	0.40
32:a:1218:A:O4'	47:s:83:HIS:HB2	2.21	0.40
32:a:1499:U:H2'	32:a:1500:A:C8	2.56	0.40
1:A:499:G:N1	1:A:502:A:OP2	2.52	0.40
1:A:2235:G:H2'	1:A:2236:A:H8	1.86	0.40
2:B:26:C:H2'	2:B:27:A:H8	1.86	0.40
16:P:106:PHE:O	16:P:109:VAL:HG22	2.20	0.40
32:a:1400:C:H2'	32:a:1401:A:C8	2.54	0.40
33:b:49:GLN:O	33:b:52:VAL:HG22	2.21	0.40
34:d:152:GLN:HB3	34:d:154:ARG:HG2	2.04	0.40
47:s:15:LEU:HD12	47:s:15:LEU:HA	1.94	0.40
1:A:396:U:OP2	23:W:10:LYS:HE2	2.22	0.40
1:A:722:A:H2'	1:A:723:A:H8	1.86	0.40
1:A:1297:A:H5''	1:A:1606:U:O2	2.20	0.40
1:A:1649:G:H2'	1:A:1650:A:H8	1.87	0.40
1:A:2497:G:HO2'	1:A:2543:U:HO2'	1.69	0.40
1:A:2829:U:H5''	15:O:53:ASN:O	2.22	0.40
9:I:31:GLU:HG3	9:I:142:ILE:HD11	2.02	0.40
28:1:19:THR:OG1	28:1:20:THR:N	2.54	0.40
32:a:404:A:C4	32:a:405:G:C8	3.10	0.40
32:a:967:A:H8	32:a:1348:G:O2'	2.04	0.40
32:a:970:A:C2	32:a:1310:A:C4	3.10	0.40
33:b:211:TYR:HB3	33:b:215:PHE:CE2	2.57	0.40
36:f:34:GLY:O	36:f:35:LYS:HD2	2.22	0.40
1:A:292:A:N3	1:A:312:G:O2'	2.53	0.40
1:A:2687:U:H2'	1:A:2688:U:C6	2.56	0.40
1:A:2831:U:H2'	1:A:2832:G:O4'	2.22	0.40
21:U:38:GLU:OE1	21:U:38:GLU:N	2.38	0.40
21:U:70:LYS:HB3	21:U:70:LYS:HE2	1.80	0.40
32:a:521:A:N6	32:a:1197:G:O2'	2.55	0.40
33:b:208:ILE:HD13	33:b:208:ILE:HA	1.92	0.40
39:i:17:ARG:HB2	39:i:65:THR:OG1	2.22	0.40
42:m:12:HIS:HA	42:m:46:LYS:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	271/274 (99%)	264 (97%)	7 (3%)	0	100	100
4	D	207/210 (99%)	198 (96%)	9 (4%)	0	100	100
5	E	205/207 (99%)	200 (98%)	5 (2%)	0	100	100
6	F	176/179 (98%)	170 (97%)	6 (3%)	0	100	100
7	G	172/178 (97%)	165 (96%)	7 (4%)	0	100	100
8	H	48/151 (32%)	46 (96%)	2 (4%)	0	100	100
9	I	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
10	J	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
11	K	141/143 (99%)	135 (96%)	6 (4%)	0	100	100
12	L	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
13	M	136/145 (94%)	132 (97%)	4 (3%)	0	100	100
14	N	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
15	O	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
16	P	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
17	Q	102/104 (98%)	101 (99%)	1 (1%)	0	100	100
18	R	108/111 (97%)	104 (96%)	4 (4%)	0	100	100
19	S	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
20	T	102/105 (97%)	101 (99%)	1 (1%)	0	100	100
21	U	92/96 (96%)	89 (97%)	3 (3%)	0	100	100
22	V	74/84 (88%)	74 (100%)	0	0	100	100
23	W	75/78 (96%)	75 (100%)	0	0	100	100
24	X	63/66 (96%)	63 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Y	56/61 (92%)	55 (98%)	1 (2%)	0	100	100
26	Z	44/72 (61%)	41 (93%)	3 (7%)	0	100	100
27	0	53/60 (88%)	52 (98%)	1 (2%)	0	100	100
28	1	47/51 (92%)	46 (98%)	1 (2%)	0	100	100
29	2	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
30	3	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	4	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	b	220/222 (99%)	207 (94%)	13 (6%)	0	100	100
34	d	203/205 (99%)	199 (98%)	4 (2%)	0	100	100
35	e	154/166 (93%)	150 (97%)	4 (3%)	0	100	100
36	f	102/111 (92%)	99 (97%)	3 (3%)	0	100	100
37	g	152/157 (97%)	148 (97%)	4 (3%)	0	100	100
38	h	129/132 (98%)	129 (100%)	0	0	100	100
39	i	123/129 (95%)	117 (95%)	6 (5%)	0	100	100
40	k	116/129 (90%)	110 (95%)	6 (5%)	0	100	100
41	l	121/124 (98%)	117 (97%)	4 (3%)	0	100	100
42	m	110/118 (93%)	106 (96%)	4 (4%)	0	100	100
43	o	86/88 (98%)	86 (100%)	0	0	100	100
44	p	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
45	q	78/83 (94%)	73 (94%)	5 (6%)	0	100	100
46	r	54/72 (75%)	52 (96%)	2 (4%)	0	100	100
47	s	80/92 (87%)	80 (100%)	0	0	100	100
48	t	87/90 (97%)	86 (99%)	1 (1%)	0	100	100
49	u	57/65 (88%)	56 (98%)	1 (2%)	0	100	100
All	All	5092/5436 (94%)	4944 (97%)	148 (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	
3	C	226/227 (100%)	225 (100%)	1 (0%)	84	92
4	D	167/168 (99%)	167 (100%)	0	100	100
5	E	171/171 (100%)	170 (99%)	1 (1%)	78	89
6	F	148/149 (99%)	145 (98%)	3 (2%)	48	71
7	G	140/144 (97%)	138 (99%)	2 (1%)	59	77
8	H	40/115 (35%)	40 (100%)	0	100	100
9	I	118/118 (100%)	118 (100%)	0	100	100
10	J	99/99 (100%)	99 (100%)	0	100	100
11	K	108/108 (100%)	107 (99%)	1 (1%)	70	83
12	L	112/112 (100%)	111 (99%)	1 (1%)	70	83
13	M	117/122 (96%)	117 (100%)	0	100	100
14	N	95/96 (99%)	91 (96%)	4 (4%)	26	53
15	O	101/101 (100%)	101 (100%)	0	100	100
16	P	90/91 (99%)	90 (100%)	0	100	100
17	Q	85/85 (100%)	85 (100%)	0	100	100
18	R	91/92 (99%)	91 (100%)	0	100	100
19	S	81/84 (96%)	81 (100%)	0	100	100
20	T	86/87 (99%)	85 (99%)	1 (1%)	63	79
21	U	81/82 (99%)	81 (100%)	0	100	100
22	V	61/65 (94%)	61 (100%)	0	100	100
23	W	68/69 (99%)	68 (100%)	0	100	100
24	X	60/61 (98%)	58 (97%)	2 (3%)	33	58
25	Y	49/52 (94%)	48 (98%)	1 (2%)	48	71
26	Z	43/64 (67%)	43 (100%)	0	100	100
27	0	51/56 (91%)	51 (100%)	0	100	100
28	1	46/48 (96%)	46 (100%)	0	100	100
29	2	36/36 (100%)	35 (97%)	1 (3%)	38	62
30	3	53/54 (98%)	53 (100%)	0	100	100
31	4	35/35 (100%)	35 (100%)	0	100	100
33	b	186/186 (100%)	180 (97%)	6 (3%)	34	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	d	172/172 (100%)	169 (98%)	3 (2%)	53	73
35	e	120/130 (92%)	118 (98%)	2 (2%)	53	73
36	f	93/100 (93%)	92 (99%)	1 (1%)	65	80
37	g	126/129 (98%)	124 (98%)	2 (2%)	55	75
38	h	109/110 (99%)	108 (99%)	1 (1%)	70	83
39	i	105/109 (96%)	104 (99%)	1 (1%)	68	82
40	k	94/104 (90%)	93 (99%)	1 (1%)	65	80
41	l	106/107 (99%)	104 (98%)	2 (2%)	50	71
42	m	98/103 (95%)	94 (96%)	4 (4%)	27	53
43	o	80/80 (100%)	80 (100%)	0	100	100
44	p	62/62 (100%)	61 (98%)	1 (2%)	55	75
45	q	75/78 (96%)	75 (100%)	0	100	100
46	r	48/63 (76%)	47 (98%)	1 (2%)	47	69
47	s	74/81 (91%)	70 (95%)	4 (5%)	20	44
48	t	71/72 (99%)	71 (100%)	0	100	100
49	u	52/58 (90%)	52 (100%)	0	100	100
All	All	4329/4535 (96%)	4282 (99%)	47 (1%)	63	80

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	51	THR
5	E	179	VAL
6	F	40	VAL
6	F	66	VAL
6	F	89	VAL
7	G	42	VAL
7	G	46	VAL
11	K	116	ILE
12	L	112	GLU
14	N	49	VAL
14	N	53	THR
14	N	57	ASP
14	N	113	HIS
20	T	51	ASN
24	X	38	THR

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Mol	Chain	Res	Type
24	X	44	ASN
25	Y	37	THR
29	2	21	ARG
33	b	8	LEU
33	b	39	ILE
33	b	52	VAL
33	b	72	ARG
33	b	114	GLN
33	b	181	VAL
34	d	29	ASP
34	d	35	ASN
34	d	171	ILE
35	e	46	ILE
35	e	85	VAL
36	f	22	LEU
37	g	32	LEU
37	g	47	PHE
38	h	3	MET
39	i	42	THR
40	k	129	VAL
41	l	21	VAL
41	l	82	ILE
42	m	19	LEU
42	m	46	LYS
42	m	62	LYS
42	m	68	ASP
44	p	29	ASP
46	r	43	THR
47	s	12	ASP
47	s	24	GLU
47	s	38	SER
47	s	78	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	87	ASN
4	D	50	GLN
4	D	137	ASN
4	D	149	GLN
5	E	45	GLN
6	F	37	ASN

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Mol	Chain	Res	Type
6	F	165	GLN
10	J	29	HIS
10	J	82	ASN
12	L	57	HIS
14	N	100	HIS
15	O	13	GLN
15	O	30	ASN
18	R	23	GLN
23	W	34	HIS
27	0	19	HIS
31	4	34	GLN
34	d	54	GLN
34	d	198	GLN
36	f	14	GLN
37	g	149	ASN
37	g	154	HIS
39	i	5	ASN
43	o	41	HIS
43	o	49	ASN
47	s	55	GLN
48	t	3	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2678/2886 (92%)	302 (11%)	7 (0%)
2	B	114/115 (99%)	11 (9%)	0
32	a	1449/1528 (94%)	181 (12%)	0
All	All	4241/4529 (93%)	494 (11%)	7 (0%)

All (494) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	11	A
1	A	15	A
1	A	35	U
1	A	47	G
1	A	52	G
1	A	61	G
1	A	72	A

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Mol	Chain	Res	Type
1	A	75	A
1	A	76	G
1	A	102	U
1	A	103	G
1	A	119	A
1	A	121	U
1	A	146	G
1	A	167	U
1	A	168	G
1	A	169	U
1	A	170	A
1	A	176	A
1	A	191	A
1	A	194	A
1	A	210	G
1	A	211	A
1	A	217	A
1	A	223	U
1	A	224	U
1	A	228	A
1	A	234	G
1	A	243	G
1	A	261	G
1	A	263	C
1	A	266	G
1	A	272	U
1	A	273	U
1	A	274	U
1	A	282	A
1	A	304	A
1	A	322	G
1	A	323	A
1	A	359	G
1	A	367	A
1	A	369	A
1	A	370	A
1	A	371	G
1	A	385	G
1	A	395	G
1	A	404	U
1	A	405	G
1	A	410	G

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Mol	Chain	Res	Type
1	A	411	A
1	A	423	G
1	A	455	U
1	A	456	A
1	A	480	G
1	A	493	G
1	A	504	A
1	A	507	A
1	A	508	U
1	A	529	G
1	A	530	C
1	A	531	A
1	A	532	G
1	A	537	A
1	A	563	A
1	A	573	U
1	A	575	A
1	A	587	G
1	A	603	A
1	A	614	A
1	A	622	U
1	A	627	A
1	A	634	G
1	A	637	A
1	A	645	U
1	A	654	U
1	A	686	A
1	A	687	U
1	A	731	A
1	A	748	U
1	A	765	A
1	A	776	G
1	A	777	G
1	A	783	A
1	A	785	G
1	A	786	G
1	A	806	G
1	A	813	C
1	A	820	A
1	A	828	U
1	A	829	U
1	A	846	A

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Mol	Chain	Res	Type
1	A	859	G
1	A	911	A
1	A	939	G
1	A	942	A
1	A	946	A
1	A	947	C
1	A	962	G
1	A	975	A
1	A	984	A
1	A	996	C
1	A	997	A
1	A	1013	U
1	A	1014	C
1	A	1027	G
1	A	1034	A
1	A	1047	A
1	A	1048	G
1	A	1110	C
1	A	1111	G
1	A	1113	G
1	A	1116	G
1	A	1133	U
1	A	1134	A
1	A	1136	C
1	A	1137	G
1	A	1143	A
1	A	1234	G
1	A	1246	G
1	A	1249	A
1	A	1252	G
1	A	1253	C
1	A	1262	G
1	A	1264	A
1	A	1267	G
1	A	1295	A
1	A	1296	A
1	A	1347	U
1	A	1360	A
1	A	1374	U
1	A	1378	A
1	A	1390	A
1	A	1391	U

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Mol	Chain	Res	Type
1	A	1411	A
1	A	1412	C
1	A	1414	A
1	A	1423	C
1	A	1447	G
1	A	1449	A
1	A	1455	G
1	A	1463	G
1	A	1478	G
1	A	1489	C
1	A	1492	A
1	A	1506	U
1	A	1507	G
1	A	1513	A
1	A	1521	G
1	A	1522	A
1	A	1547	C
1	A	1566	A
1	A	1569	A
1	A	1578	U
1	A	1584	U
1	A	1585	A
1	A	1586	U
1	A	1597	A
1	A	1606	U
1	A	1607	A
1	A	1609	A
1	A	1645	A
1	A	1646	U
1	A	1672	G
1	A	1674	A
1	A	1718	A
1	A	1719	U
1	A	1727	G
1	A	1728	C
1	A	1752	G
1	A	1754	U
1	A	1760	G
1	A	1769	A
1	A	1796	C
1	A	1797	G
1	A	1812	A

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Mol	Chain	Res	Type
1	A	1825	A
1	A	1854	A
1	A	1862	A
1	A	1863	G
1	A	1880	G
1	A	1901	C
1	A	1902	G
1	A	1909	A
1	A	1910	C
1	A	1912	A
1	A	1925	G
1	A	1926	G
1	A	1933	A
1	A	1934	A
1	A	1951	U
1	A	1960	G
1	A	1963	C
1	A	1966	A
1	A	1967	U
1	A	1968	G
1	A	1987	U
1	A	1989	U
1	A	1993	C
1	A	2018	U
1	A	2019	C
1	A	2027	A
1	A	2028	G
1	A	2029	A
1	A	2032	C
1	A	2039	C
1	A	2051	C
1	A	2052	G
1	A	2056	A
1	A	2057	G
1	A	2058	A
1	A	2059	C
1	A	2065	G
1	A	2089	G
1	A	2188	A
1	A	2194	A
1	A	2200	G
1	A	2214	A

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Mol	Chain	Res	Type
1	A	2215	C
1	A	2227	G
1	A	2228	G
1	A	2240	G
1	A	2272	U
1	A	2276	A
1	A	2277	A
1	A	2294	U
1	A	2298	A
1	A	2300	A
1	A	2302	C
1	A	2303	G
1	A	2308	A
1	A	2311	A
1	A	2316	A
1	A	2334	G
1	A	2336	C
1	A	2350	G
1	A	2368	G
1	A	2372	G
1	A	2374	C
1	A	2412	U
1	A	2414	A
1	A	2418	G
1	A	2419	A
1	A	2430	U
1	A	2437	A
1	A	2459	G
1	A	2463	U
1	A	2464	C
1	A	2465	A
1	A	2480	U
1	A	2481	U
1	A	2487	C
1	A	2489	U
1	A	2491	G
1	A	2493	U
1	A	2507	A
1	A	2518	G
1	A	2536	A
1	A	2555	A
1	A	2556	G

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Mol	Chain	Res	Type
1	A	2562	C
1	A	2571	G
1	A	2591	A
1	A	2592	G
1	A	2598	U
1	A	2602	U
1	A	2604	U
1	A	2618	U
1	A	2678	U
1	A	2679	U
1	A	2703	G
1	A	2715	C
1	A	2722	A
1	A	2733	G
1	A	2737	A
1	A	2742	A
1	A	2746	A
1	A	2753	A
1	A	2754	A
1	A	2755	G
1	A	2767	A
1	A	2779	U
1	A	2781	A
1	A	2782	U
1	A	2784	A
1	A	2785	A
1	A	2786	A
1	A	2790	A
1	A	2804	G
1	A	2805	A
1	A	2845	U
1	A	2851	A
1	A	2856	U
1	A	2857	A
1	A	2861	G
1	A	2864	C
1	A	2867	A
1	A	2868	U
1	A	2874	G
1	A	2875	A
1	A	2877	A
1	A	2879	A

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Mol	Chain	Res	Type
2	B	11	A
2	B	12	U
2	B	34	C
2	B	51	A
2	B	54	G
2	B	64	C
2	B	87	G
2	B	89	C
2	B	102	G
2	B	106	A
2	B	114	A
32	a	5	C
32	a	6	U
32	a	7	G
32	a	10	G
32	a	23	G
32	a	33	A
32	a	40	G
32	a	48	C
32	a	49	U
32	a	52	A
32	a	59	C
32	a	71	U
32	a	82	A
32	a	83	G
32	a	86	U
32	a	87	G
32	a	88	C
32	a	114	C
32	a	123	A
32	a	124	U
32	a	128	C
32	a	129	C
32	a	130	C
32	a	137	G
32	a	144	A
32	a	175	A
32	a	182	U
32	a	183	G
32	a	190	A
32	a	198	U
32	a	199	U

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Mol	Chain	Res	Type
32	a	200	C
32	a	201	G
32	a	234	U
32	a	236	G
32	a	240	G
32	a	255	G
32	a	256	C
32	a	268	A
32	a	278	G
32	a	317	C
32	a	318	A
32	a	321	G
32	a	341	C
32	a	343	G
32	a	356	U
32	a	361	C
32	a	386	A
32	a	395	G
32	a	402	G
32	a	410	U
32	a	411	A
32	a	413	G
32	a	418	U
32	a	427	U
32	a	444	C
32	a	456	U
32	a	457	A
32	a	468	A
32	a	473	G
32	a	475	U
32	a	485	A
32	a	488	A
32	a	494	G
32	a	500	C
32	a	501	U
32	a	510	G
32	a	513	G
32	a	516	G
32	a	519	G
32	a	521	A
32	a	536	A
32	a	548	A

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Mol	Chain	Res	Type
32	a	551	U
32	a	553	C
32	a	561	A
32	a	562	A
32	a	565	G
32	a	566	G
32	a	568	C
32	a	585	A
32	a	607	C
32	a	622	G
32	a	642	A
32	a	654	A
32	a	676	A
32	a	707	A
32	a	712	U
32	a	713	G
32	a	718	A
32	a	744	A
32	a	770	A
32	a	782	U
32	a	783	A
32	a	806	C
32	a	810	G
32	a	817	A
32	a	864	A
32	a	879	G
32	a	906	A
32	a	918	G
32	a	926	C
32	a	927	A
32	a	937	G
32	a	952	U
32	a	953	U
32	a	960	A
32	a	961	A
32	a	963	G
32	a	967	A
32	a	968	G
32	a	969	A
32	a	974	U
32	a	981	U
32	a	984	U

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Mol	Chain	Res	Type
32	a	985	G
32	a	1037	C
32	a	1038	A
32	a	1056	G
32	a	1057	U
32	a	1058	C
32	a	1086	G
32	a	1087	U
32	a	1093	A
32	a	1094	A
32	a	1100	G
32	a	1104	C
32	a	1117	U
32	a	1119	A
32	a	1121	C
32	a	1146	A
32	a	1150	U
32	a	1158	A
32	a	1174	U
32	a	1175	G
32	a	1187	A
32	a	1188	A
32	a	1203	U
32	a	1205	C
32	a	1217	C
32	a	1218	A
32	a	1229	A
32	a	1232	G
32	a	1247	C
32	a	1266	A
32	a	1267	G
32	a	1271	A
32	a	1276	A
32	a	1277	A
32	a	1278	A
32	a	1290	A
32	a	1293	C
32	a	1296	G
32	a	1311	C
32	a	1314	G
32	a	1327	C
32	a	1328	G

Continued on next page...

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Mol	Chain	Res	Type
32	a	1329	G
32	a	1342	U
32	a	1355	U
32	a	1363	U
32	a	1385	A
32	a	1410	G
32	a	1420	C
32	a	1423	G
32	a	1440	G
32	a	1442	A
32	a	1443	U
32	a	1474	G
32	a	1479	A
32	a	1484	G
32	a	1486	A
32	a	1489	A
32	a	1490	A
32	a	1493	U
32	a	1494	A
32	a	1504	G
32	a	1507	C
32	a	1516	G
32	a	1517	G
32	a	1518	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	129	C
1	A	785	G
1	A	1411	A
1	A	1606	U
1	A	2028	G
1	A	2187	A
1	A	2745	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	2MG	A	2434	1	23,26,27	0.41	0	32,38,41	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	2434	1	-	0/9/27/28	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 154 ligands modelled in this entry, 154 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

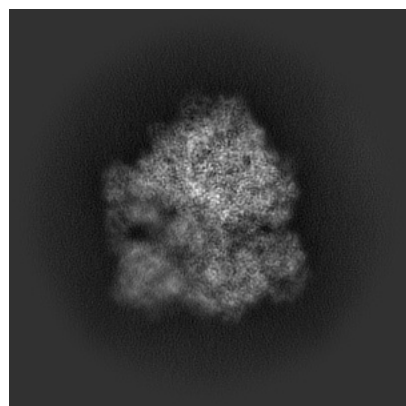
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56659. These allow visual inspection of the internal detail of the map and identification of artifacts.

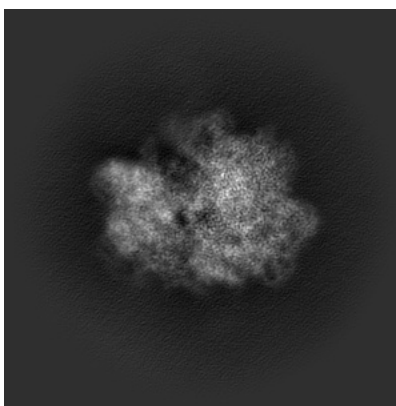
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

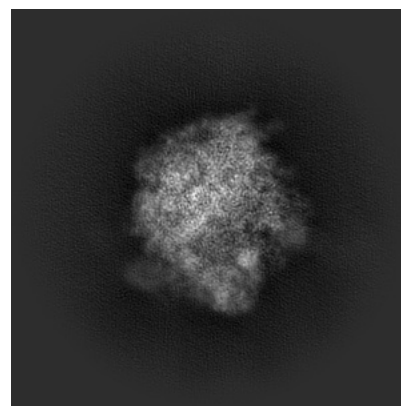
6.1.1 Primary map



X

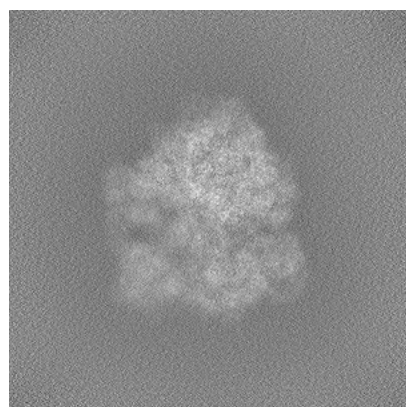


Y

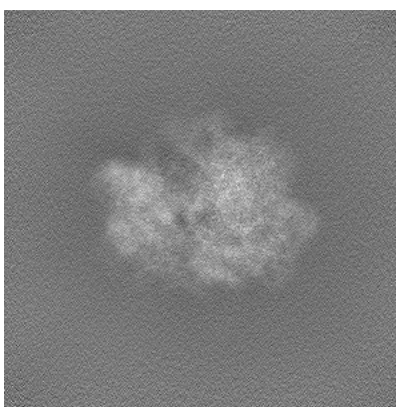


Z

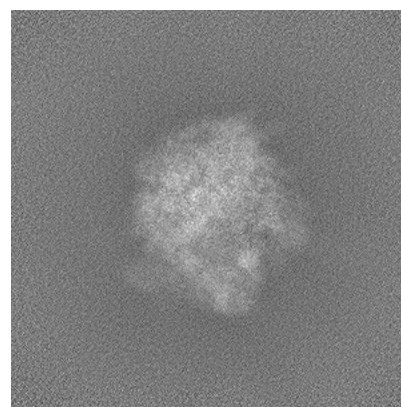
6.1.2 Raw map



X



Y

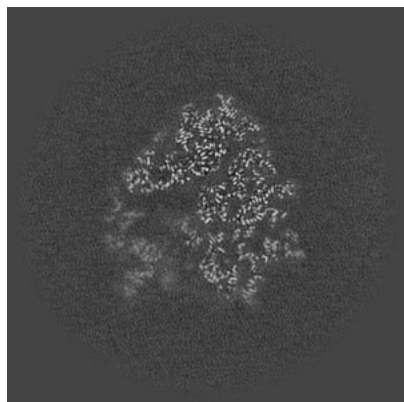


Z

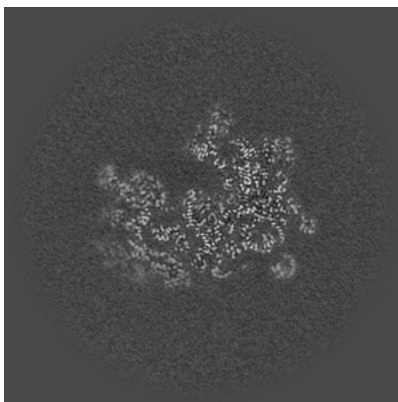
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

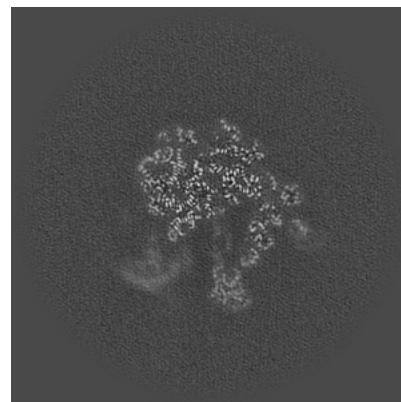
6.2.1 Primary map



X Index: 300

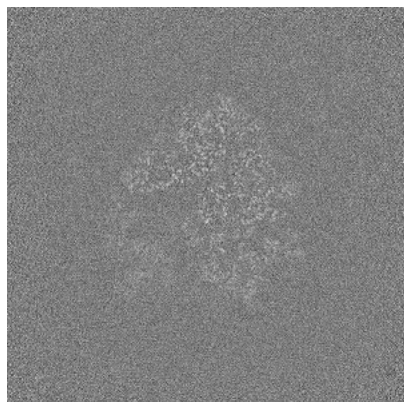


Y Index: 300

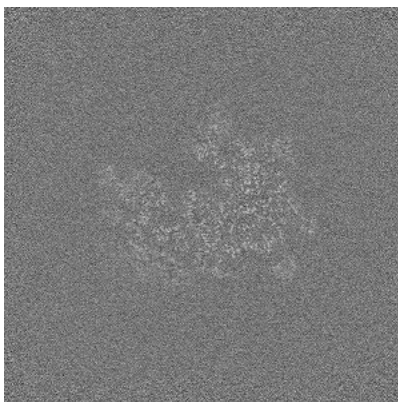


Z Index: 300

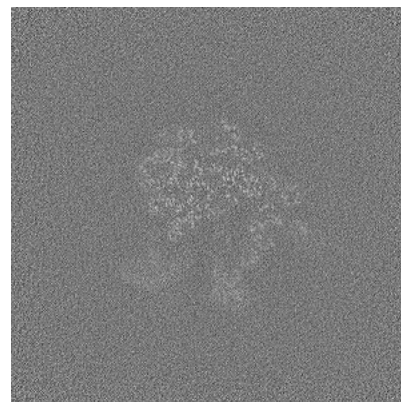
6.2.2 Raw map



X Index: 300



Y Index: 300

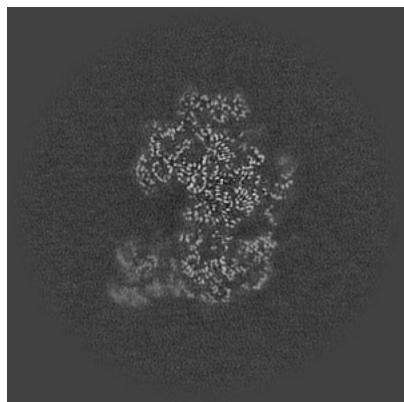


Z Index: 300

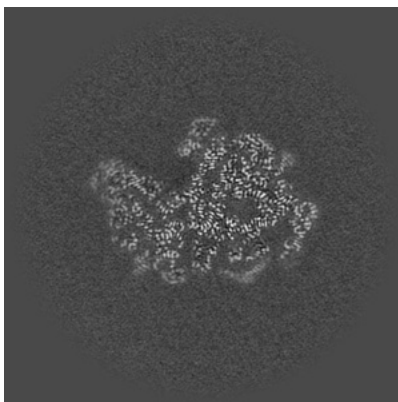
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

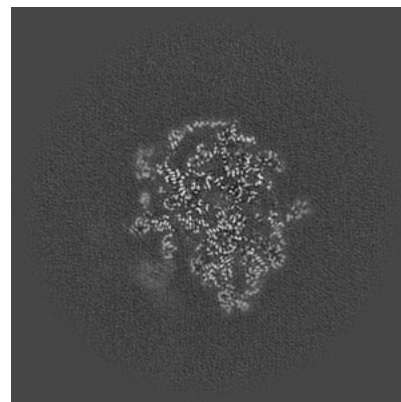
6.3.1 Primary map



X Index: 278

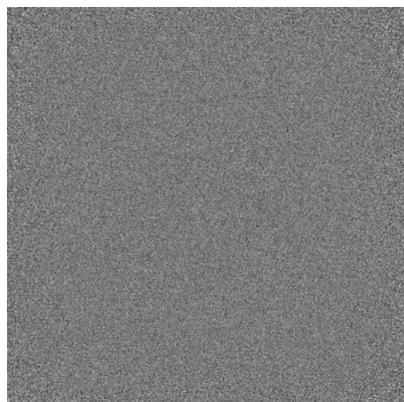


Y Index: 321

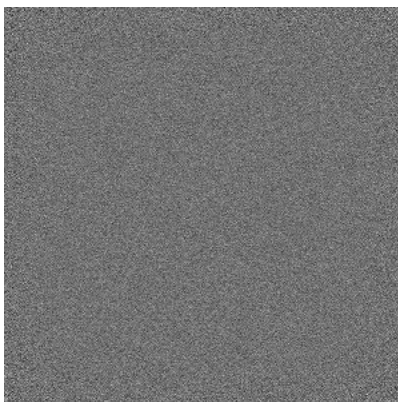


Z Index: 337

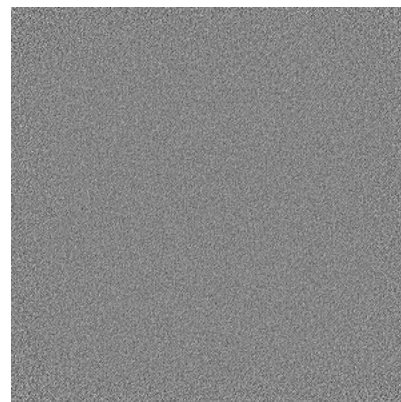
6.3.2 Raw map



X Index: 0



Y Index: 0

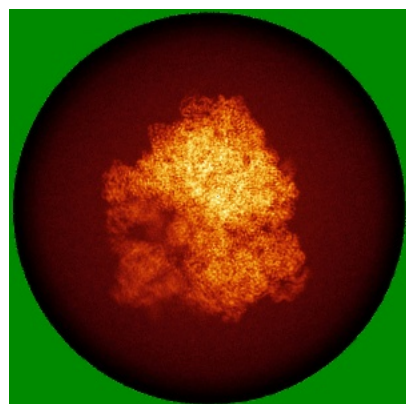


Z Index: 0

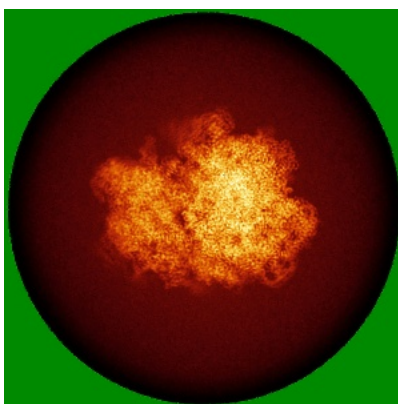
The images above show the largest variance slices of the map in three orthogonal directions.

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

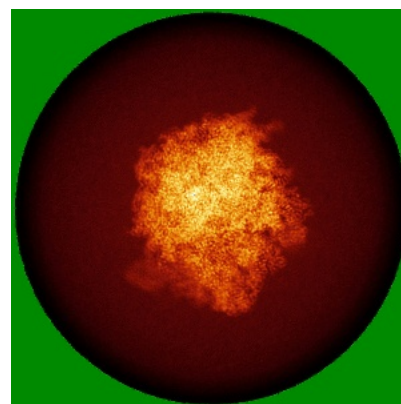
6.4.1 Primary map



X

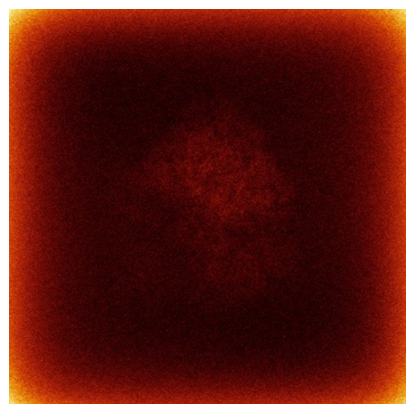


Y

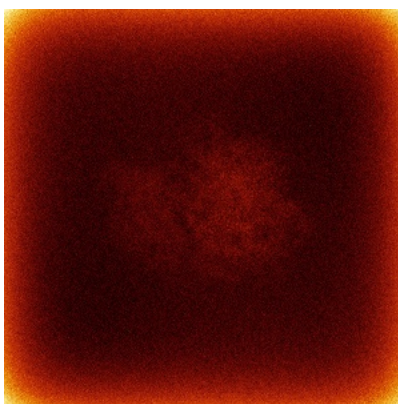


Z

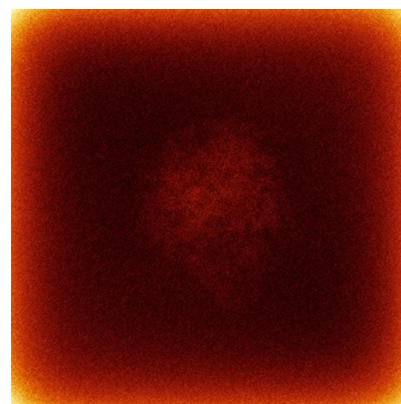
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

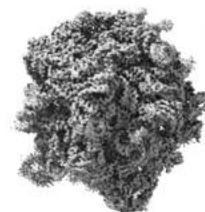
6.5.1 Primary map



X



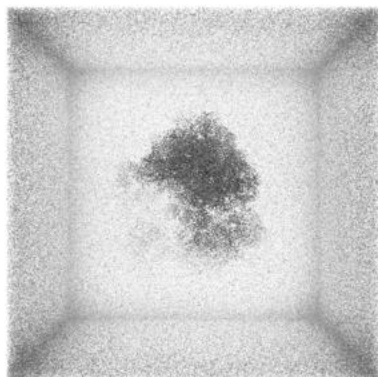
Y



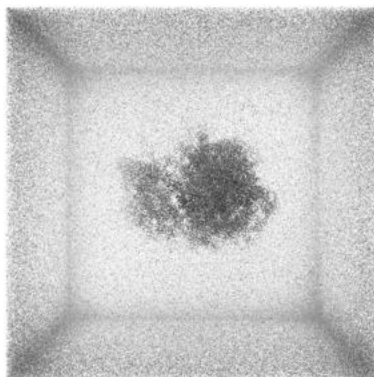
Z

The images above show the 3D surface view of the map at the recommended contour level 0.104. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

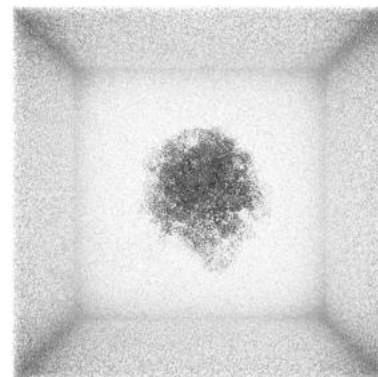
6.5.2 Raw map



X



Y



Z

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

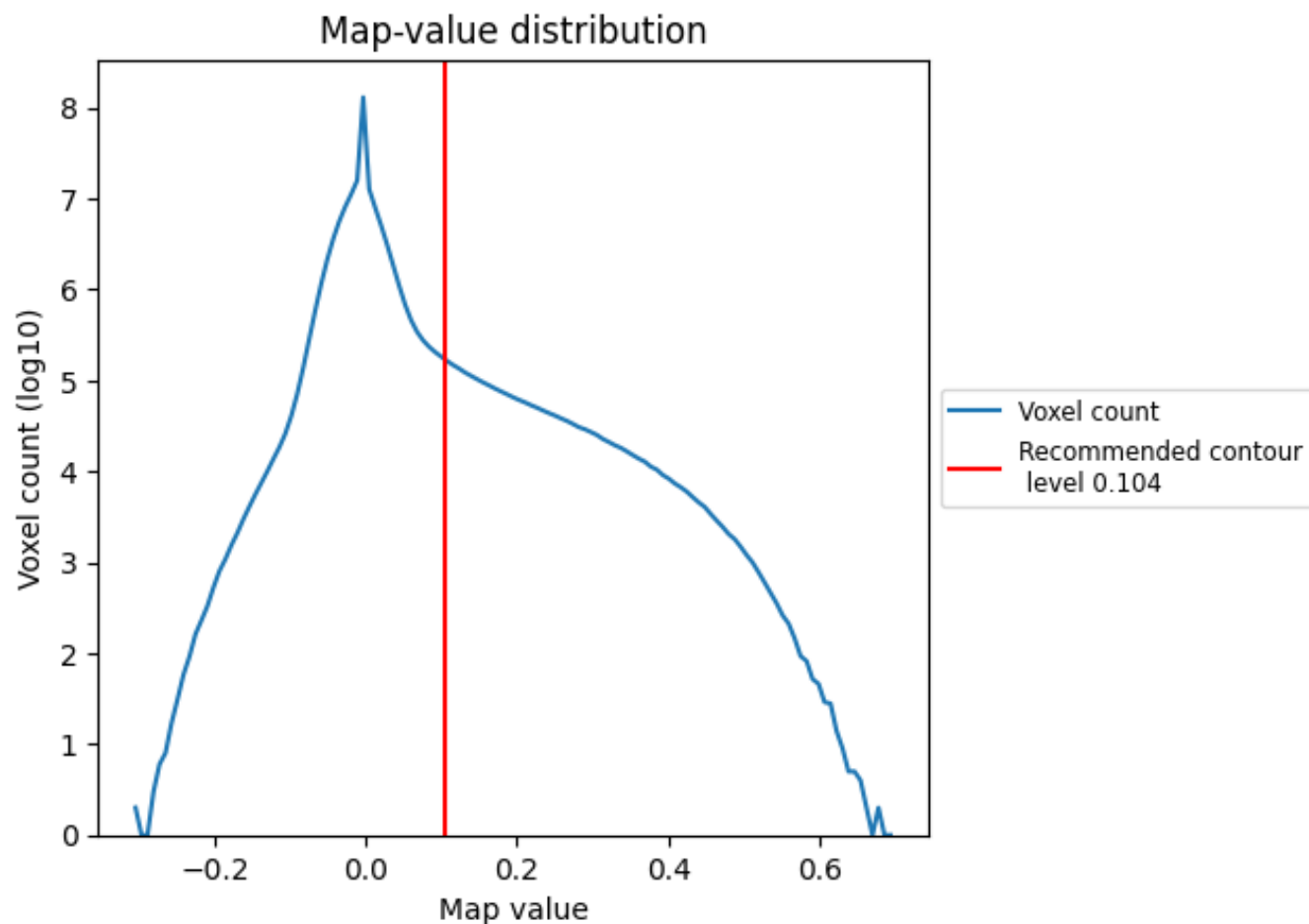
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

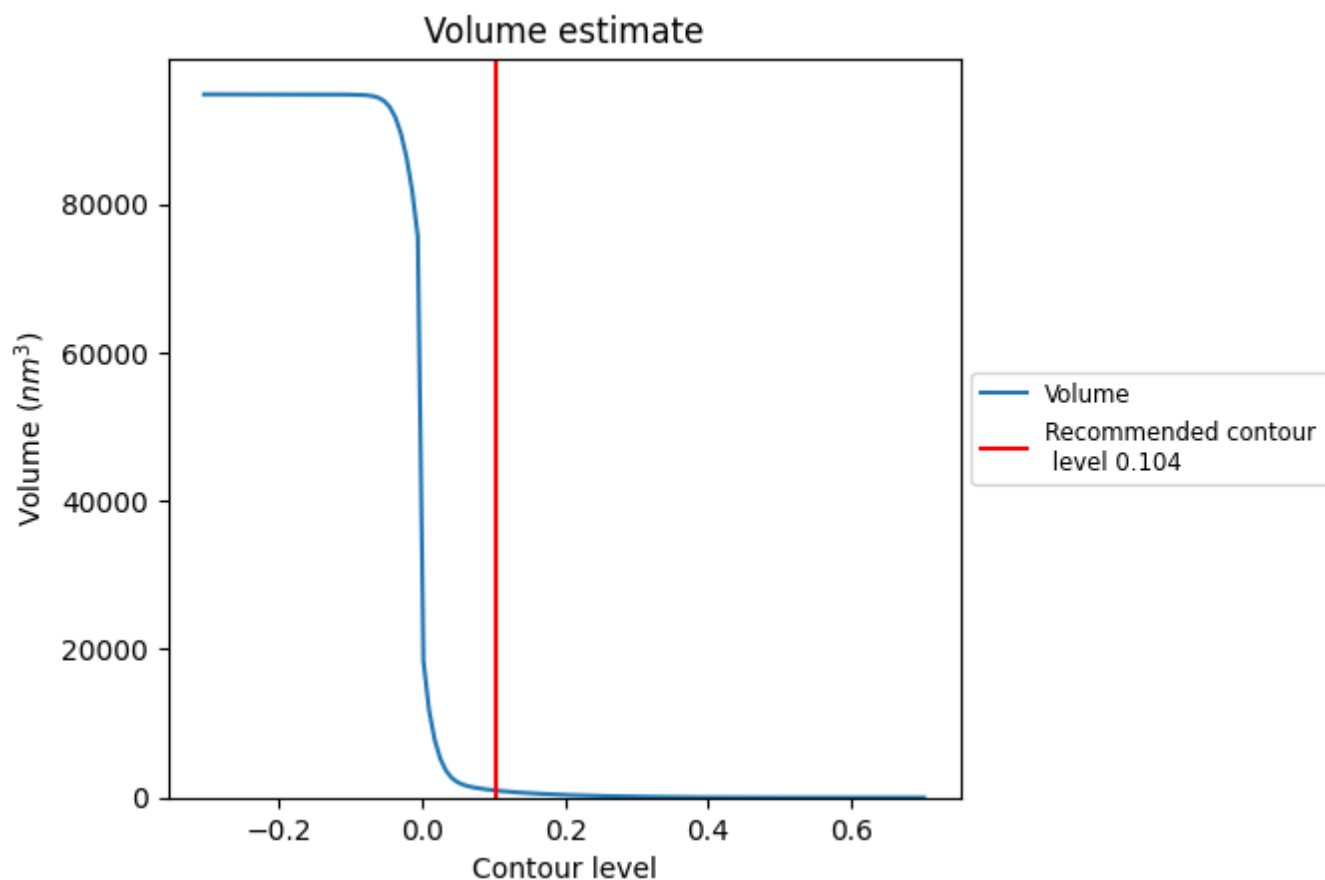
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

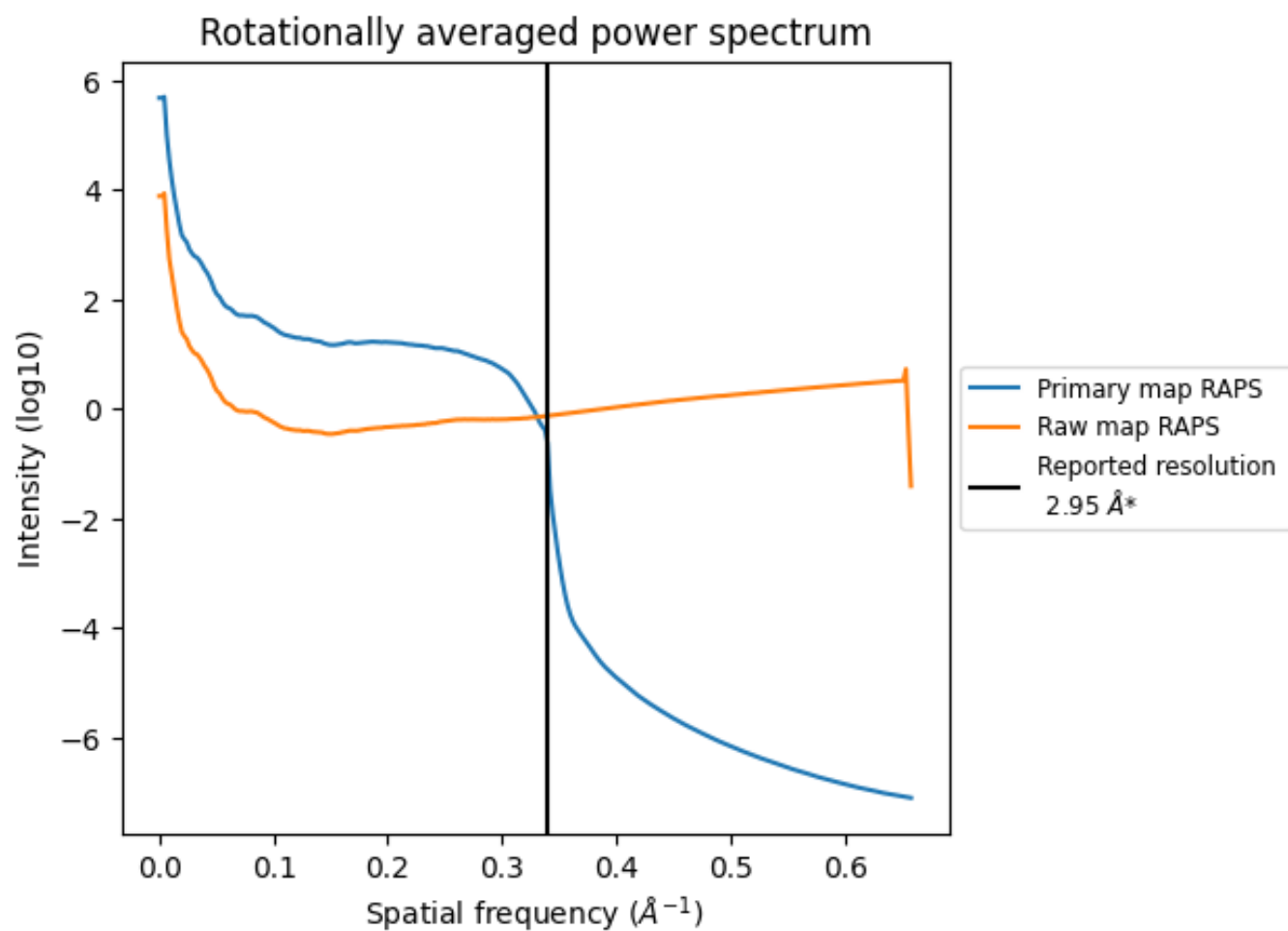
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 944 nm³; this corresponds to an approximate mass of 853 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

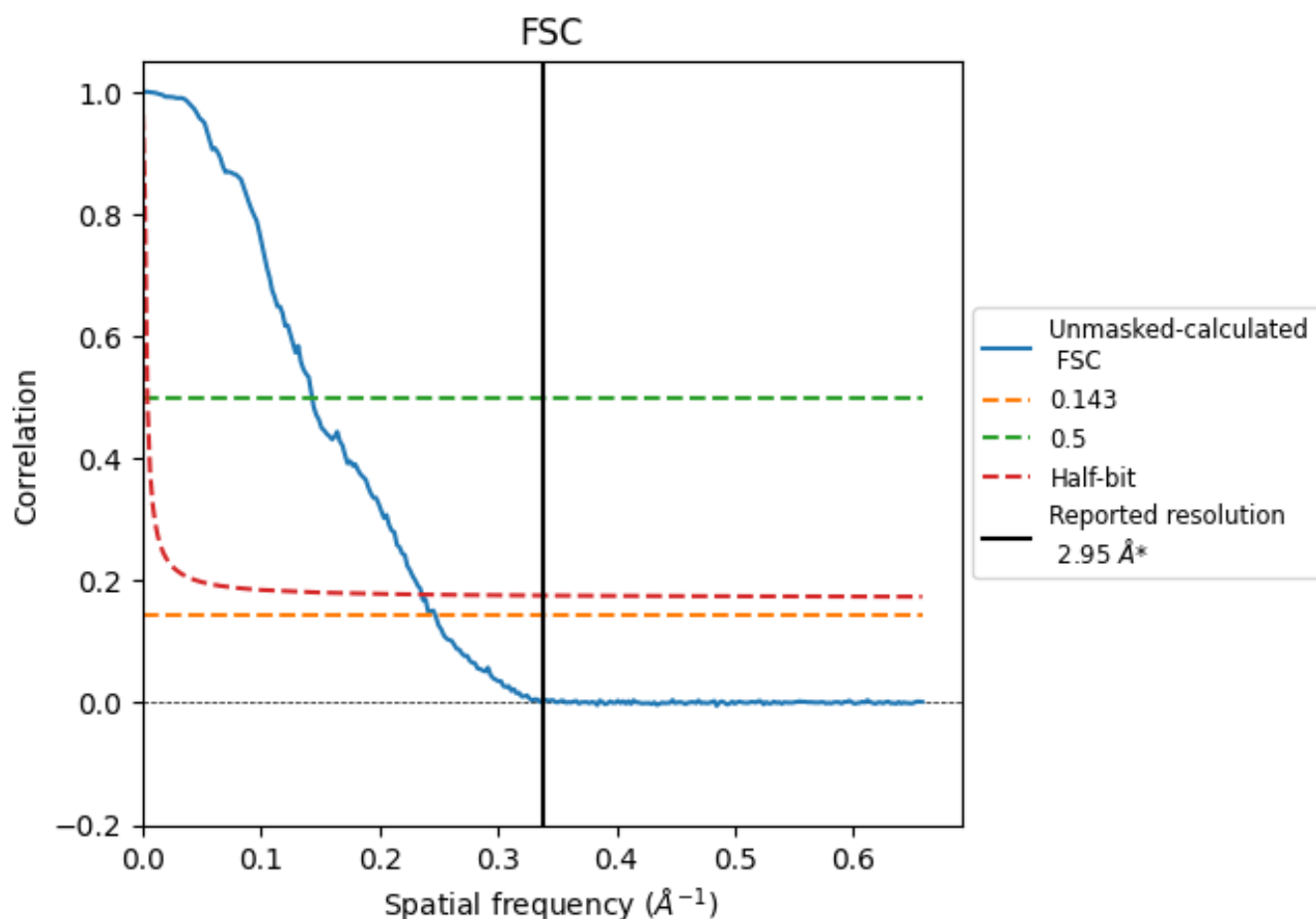


*Reported resolution corresponds to spatial frequency of 0.339 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.339 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

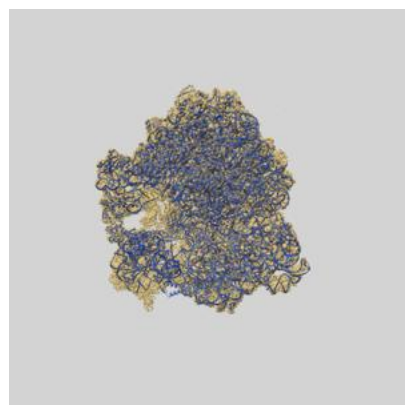
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.05	6.98	4.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 2.95 by more than 10 %

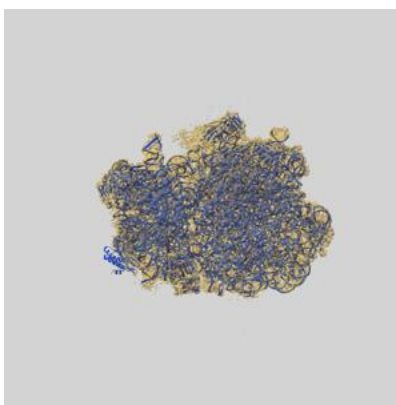
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56659 and PDB model 28NT. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

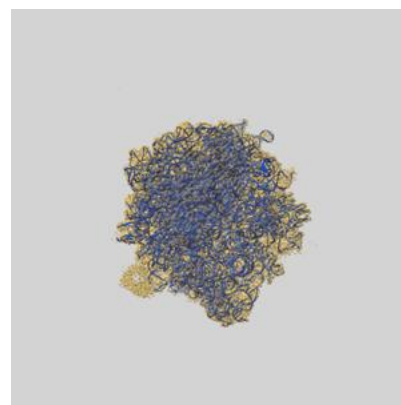
9.1 Map-model overlay [i](#)



X



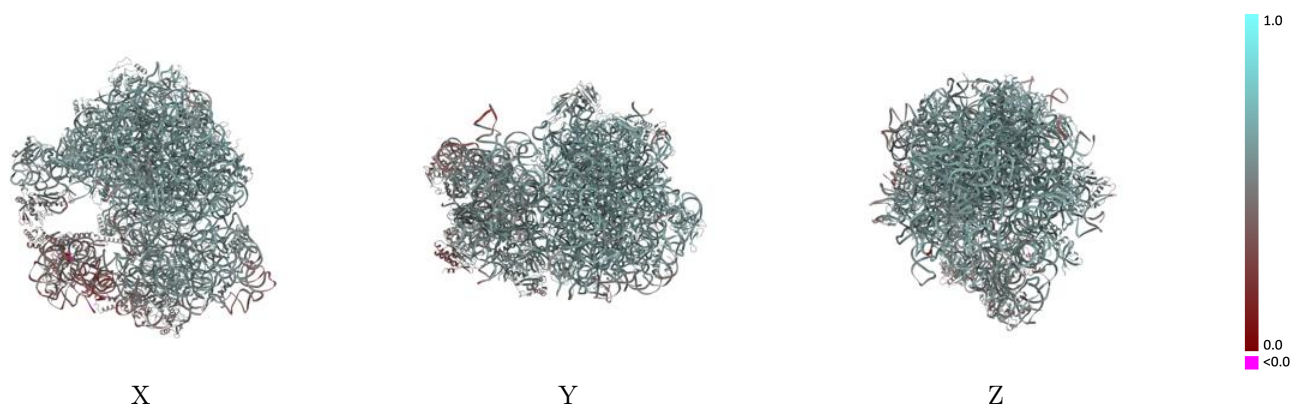
Y



Z

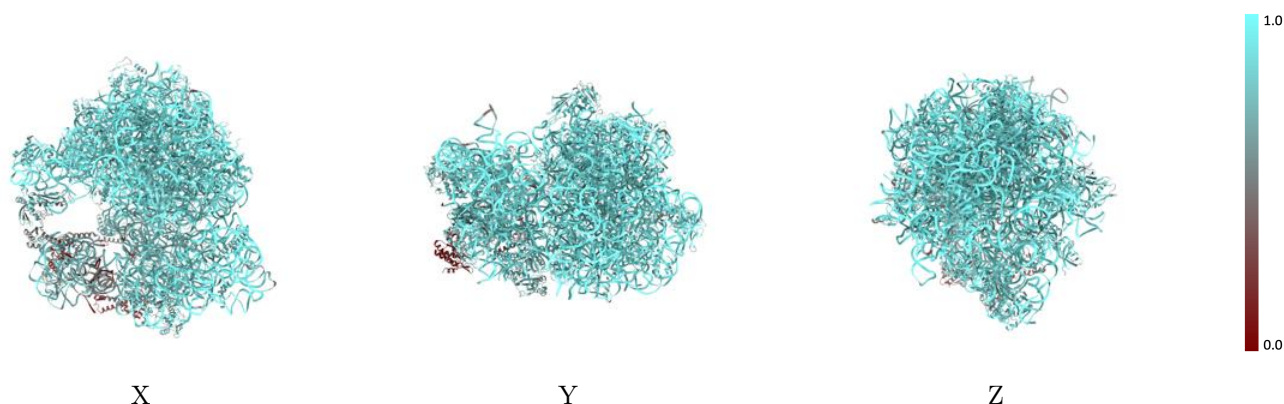
The images above show the 3D surface view of the map at the recommended contour level 0.104 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



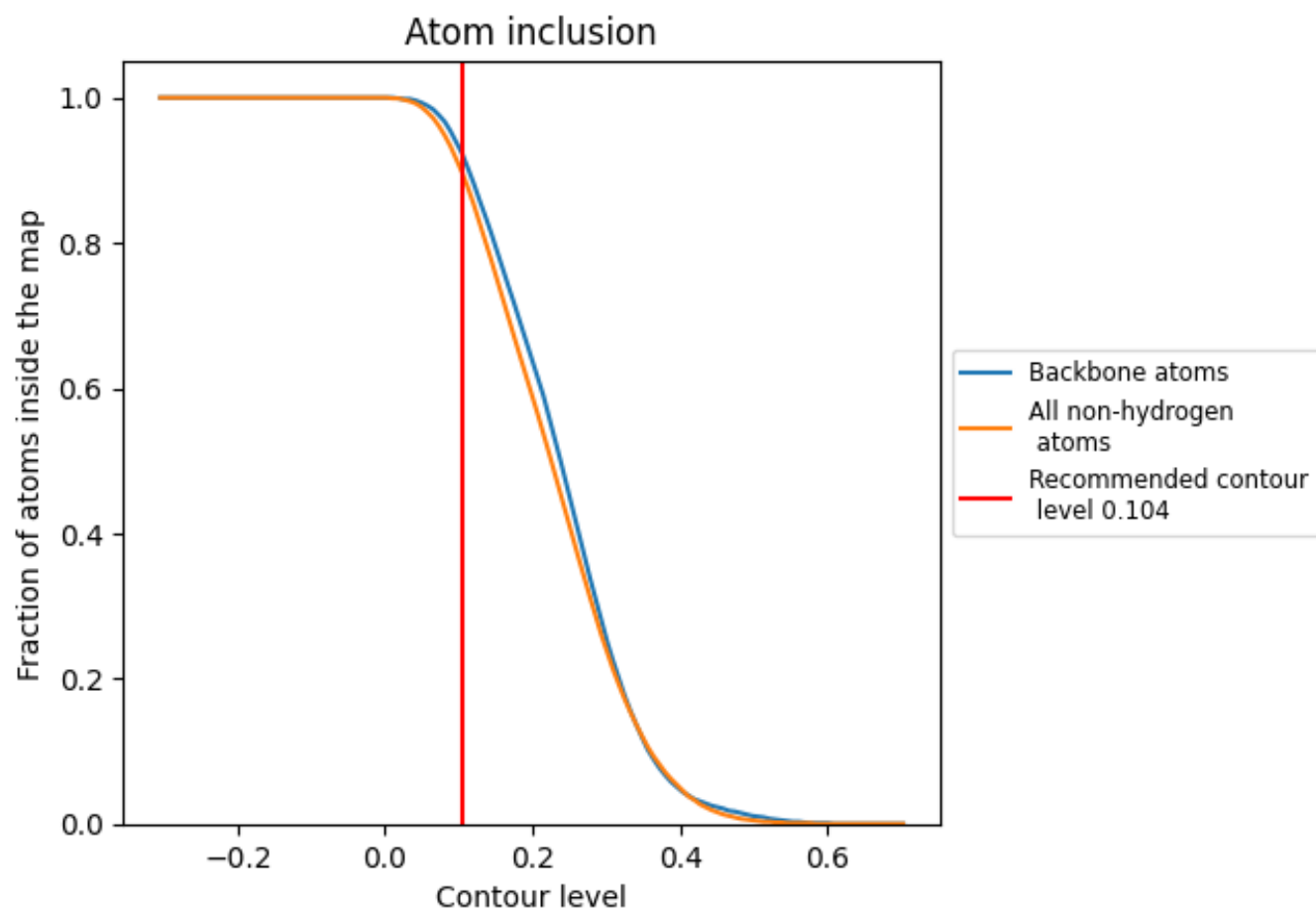
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.104).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.104) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8980	 0.5510
0	 0.9070	 0.5940
1	 0.8560	 0.5800
2	 0.9450	 0.6150
3	 0.9390	 0.6010
4	 0.9450	 0.6110
A	 0.9770	 0.5870
B	 0.9470	 0.5390
C	 0.9310	 0.6100
D	 0.9330	 0.6020
E	 0.8610	 0.5750
F	 0.6620	 0.4650
G	 0.8030	 0.5340
H	 0.7880	 0.5330
I	 0.9220	 0.5990
J	 0.9070	 0.6030
K	 0.9190	 0.5920
L	 0.8870	 0.5910
M	 0.9200	 0.5950
N	 0.8360	 0.5290
O	 0.9020	 0.6070
P	 0.9310	 0.5950
Q	 0.9190	 0.5950
R	 0.9170	 0.5970
S	 0.8500	 0.5750
T	 0.8490	 0.5600
U	 0.8510	 0.5690
V	 0.9120	 0.6030
W	 0.9070	 0.5910
X	 0.8560	 0.5460
Y	 0.9130	 0.5910
Z	 0.6440	 0.4420
a	 0.8910	 0.5020
b	 0.2060	 0.3600
d	 0.7370	 0.4760



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Chain	Atom inclusion	Q-score
e	 0.8110	 0.5390
f	 0.7180	 0.4910
g	 0.5370	 0.4120
h	 0.8620	 0.5560
i	 0.4240	 0.4020
k	 0.7950	 0.5250
l	 0.8120	 0.5540
m	 0.5010	 0.4130
o	 0.8330	 0.5440
p	 0.8400	 0.5470
q	 0.8140	 0.5530
r	 0.7920	 0.5300
s	 0.3600	 0.3230
t	 0.8560	 0.5410
u	 0.3910	 0.4560