



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:05 AM UTC

PDB ID : 7AZY / pdb_00007azy
EMDB ID : EMD-11951
Title : Context-specific inhibition of eukaryotic translation by macrolide antibiotics
Authors : Koller, T.O.; Wilson, D.N.
Deposited on : 2020-11-17
Resolution : 2.88 Å(reported)
Based on initial model : 6Q8Y

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

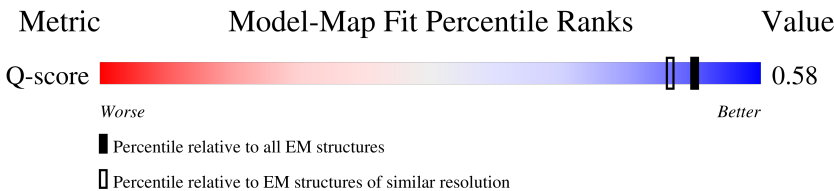
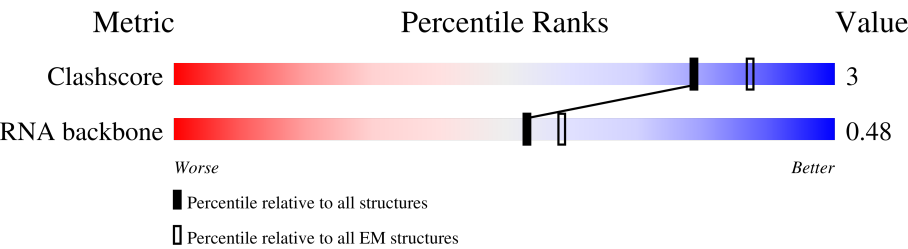
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.88 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	12040 (2.38 - 3.38)

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	b	256	27% 86% 5% 9%
2	c	137	9% 84% 15% .
3	d	100	27% 96% . .
4	e	191	15% 91% 9%
5	f	155	7% 37% 6% 57%

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Mol	Chain	Length	Quality of chain
6	g	88	
7	h	174	
8	I	142	
9	j	78	
10	k	199	
11	q	127	
12	M	51	
13	N	138	
14	O	136	
15	P	128	
16	Q	106	
17	R	204	
18	S	149	
19	U	92	
20	V	199	
21	W	59	
22	x	254	
23	y	184	
24	l	387	
25	m	186	
26	n	113	
27	o	221	
28	p	362	
29	r	130	
30	s	172	

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Mol	Chain	Length	Quality of chain
31	t	297	
32	u	160	
33	v	107	
34	w	121	
35	A	176	
36	B	121	
37	C	244	
38	D	120	
39	E	3396	
40	F	121	
41	G	158	
42	H	189	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
43	TEL	E	3401	X	-	-	-

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 210087 atoms, of which 87854 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 protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	b	233	Total	C	H	N	O	S	0	0
			3679	1151	1876	322	327	3		

- Molecule 2 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	c	136	Total	C	H	N	O	S	0	0
			2051	628	1048	189	179	7		

- Molecule 3 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	d	99	Total	C	H	N	O	S	0	0
			1620	481	849	156	132	2		

- Molecule 4 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	e	191	Total	C	H	N	O	S	0	0
			3105	963	1587	274	277	4		

- Molecule 5 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	f	67	Total	C	H	N	O	S	0	0
			1107	349	564	106	87	1		

- Molecule 6 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	g	87	Total	C	H	N	O	S	0	0
			1364	414	683	148	114	5		

- Molecule 7 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	h	169	Total	C	H	N	O	S	0	0
			2736	847	1383	253	249	4		

- Molecule 8 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	121	Total	C	H	N	O	S	0	0
			1990	620	1026	169	173	2		

- Molecule 9 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	77	Total	C	H	N	O	0	0
			1294	391	682	115	106		

- Molecule 10 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	193	Total	C	H	N	O	0	0
			3151	962	1608	315	266		

- Molecule 11 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	q	126	Total	C	H	N	O	0	0
			2074	625	1081	192	176		

- Molecule 12 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	M	50	Total	C	H	N	O	S	0	0
			911	272	475	97	65	2		

- Molecule 13 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	N	136	Total	C	H	N	O	S	0	0
			2202	675	1149	199	177	2		

- Molecule 14 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	135	Total	C	H	N	O	0	0
			2247	710	1155	202	180		

- Molecule 15 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace	
15	P	52	Total	C	H	N	O	S	0	0
			872	259	455	86	67	5		

- Molecule 16 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Q	105	Total	C	H	N	O	S	0	0
			1762	534	915	170	138	5		

- Molecule 17 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	203	Total	C	H	N	O	S	0	0
			3499	1077	1779	361	281	1		

- Molecule 18 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	S	148	Total	C	H	N	O	S	0	0
			2390	749	1217	231	190	3		

- Molecule 19 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	U	91	Total	C	H	N	O	S	0	0
			1431	429	737	138	121	6		

- Molecule 20 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	V	197	Total	C	H	N	O	S	0	0
			3215	1003	1660	289	262	1		

- Molecule 21 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	58	Total	C	H	N	O	0	0
			953	289	491	100	73		

- Molecule 22 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	x	252	Total	C	H	N	O	S	0	0
			3895	1191	1981	388	334	1		

- Molecule 23 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	y	183	Total	C	H	N	O	0	0
			2857	882	1437	281	257		

- Molecule 24 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	l	386	Total	C	H	N	O	S	0	0
			6217	1950	3142	584	533	8		

- Molecule 25 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	m	185	Total	C	H	N	O	S	0	0
			2985	908	1544	290	241	2		

- Molecule 26 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace	
26	n	109	Total	C	H	N	O	S	0	0
			1788	556	912	167	152	1		

- Molecule 27 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	o	220	Total	C	H	N	O	S	0	0
			3576	1121	1806	335	307	7		

- Molecule 28 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	p	361	Total	C	H	N	O	S	0	0
			5607	1729	2859	522	494	3		

- Molecule 29 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	r	127	Total	C	H	N	O	S	0	0
			2111	647	1091	205	167	1		

- Molecule 30 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	s	172	Total	C	H	N	O	S	0	0
			2932	930	1487	267	244	4		

- Molecule 31 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	t	296	Total	C	H	N	O	S	0	0
			4700	1501	2325	414	458	2		

- Molecule 32 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	u	159	Total	C	H	N	O	S	0	0
			2599	805	1323	246	221	4		

- Molecule 33 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	v	106	Total	C	H	N	O	S	0	0
			1730	540	880	165	144	1		

- Molecule 34 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	w	100	Total	C	H	N	O		0	0
			1608	516	812	131	149			

- Molecule 35 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	A	156	Total	C	H	N	O	S	0	0
			2565	800	1326	222	216	1		

- Molecule 36 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	B	112	Total	C	H	N	O	S	0	0
			1821	545	941	179	152	4		

- Molecule 37 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	C	222	Total	C	H	N	O	S	0	0
			3646	1151	1862	324	308	1		

- Molecule 38 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	D	119	Total	C	H	N	O	S	0	0
			2047	615	1078	186	167	1		

- Molecule 39 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	E	3161	Total	C	H	N	O	P	0	0
			101575	30200	33966	12186	22062	3161		

- Molecule 40 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	F	121	Total	C	H	N	O	P	0	0
			3883	1152	1304	461	845	121		

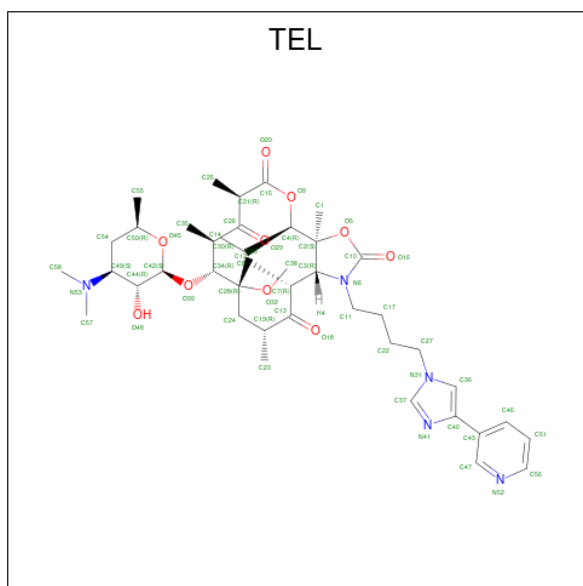
- Molecule 41 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	G	158	Total	C	H	N	O	P	0	0
			5046	1500	1694	586	1108	158		

- Molecule 42 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	H	188	Total	C	H	N	O	0	0
			3138	935	1617	326	260		

- Molecule 43 is TELITHROMYCIN (CCD ID: TEL) (formula: $C_{43}H_{65}N_5O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
43	E	1	Total	C	H	N	O	0
			105	43	47	5	10	

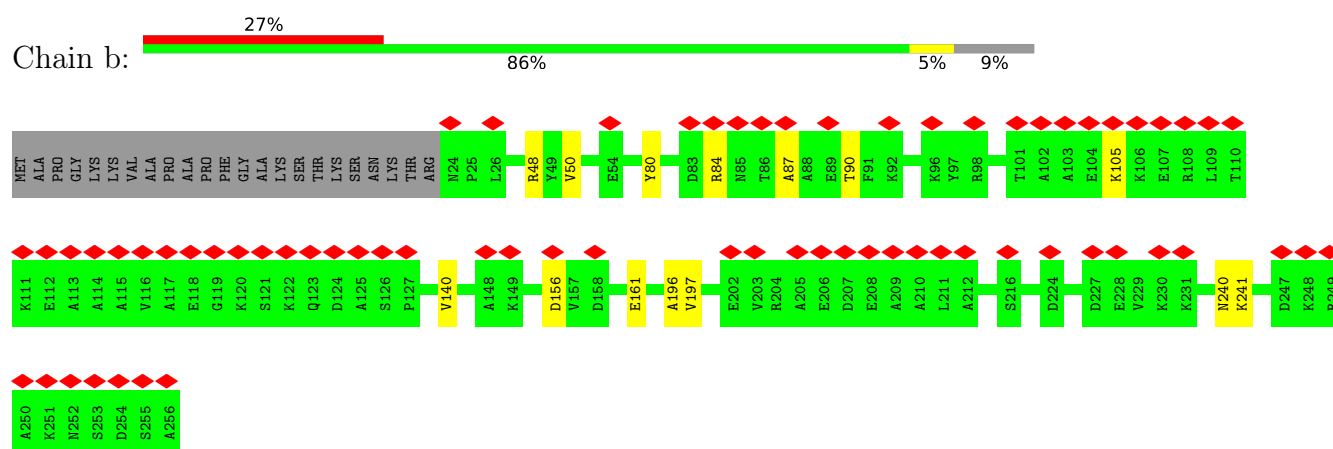
- Molecule 44 is water.

Mol	Chain	Residues	Atoms	AltConf
44	E	3	Total O	0
			3 3	

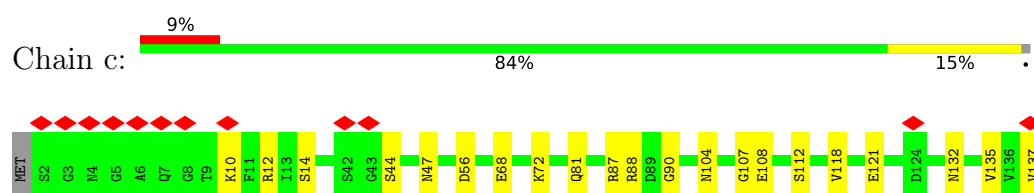
3 Residue-property plots

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

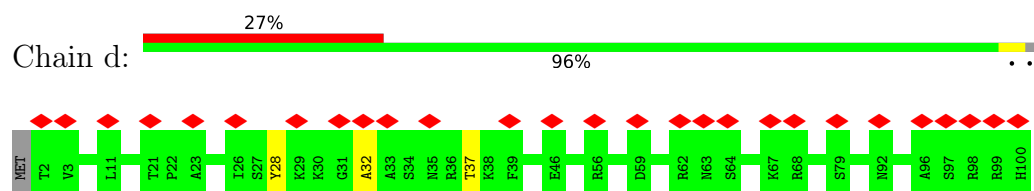
• Molecule 1: 60S ribosomal protein L8-A



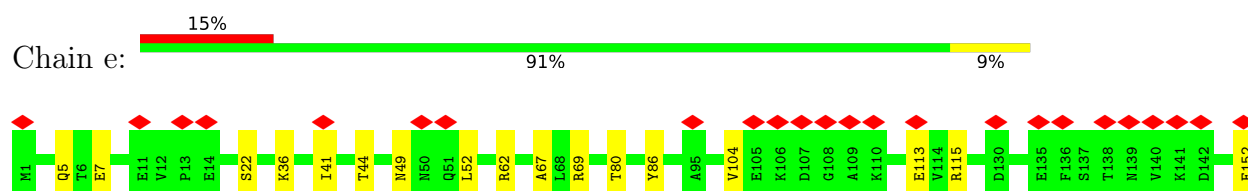
• Molecule 2: 60S ribosomal protein L23-A

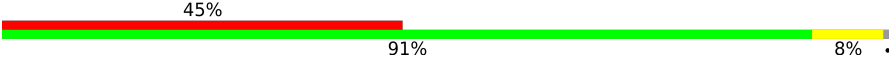


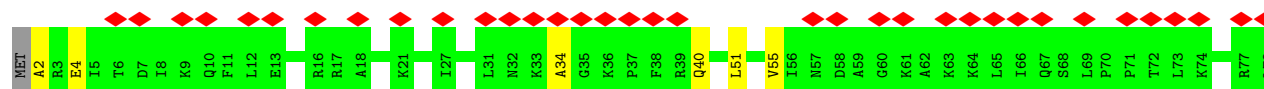
• Molecule 3: 60S ribosomal protein L36-A



• Molecule 4: 60S ribosomal protein L9-A

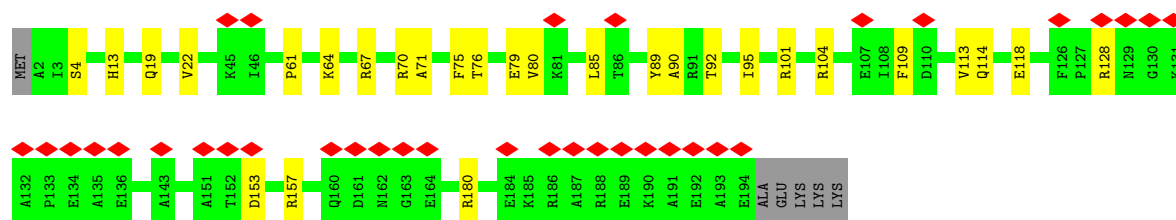


Chain j: 

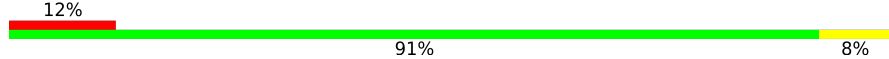


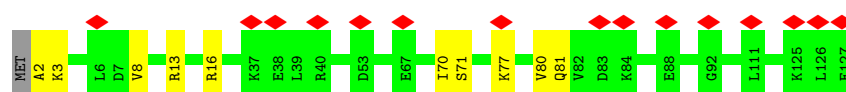
- Molecule 10: 60S ribosomal protein L13-A

Chain k: 



- Molecule 11: 60S ribosomal protein L26-A

Chain q: 



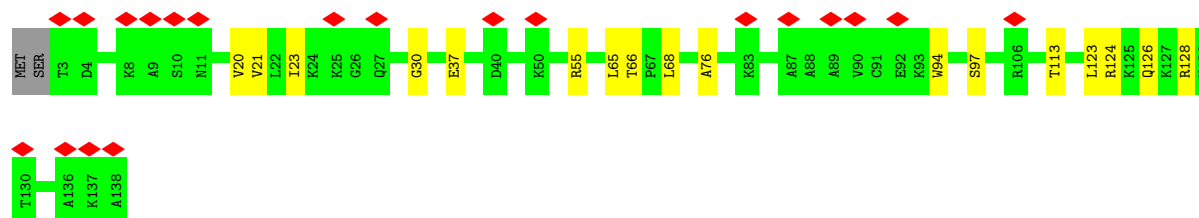
- Molecule 12: 60S ribosomal protein L39

Chain M: 

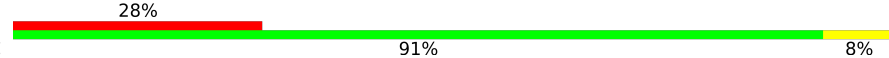


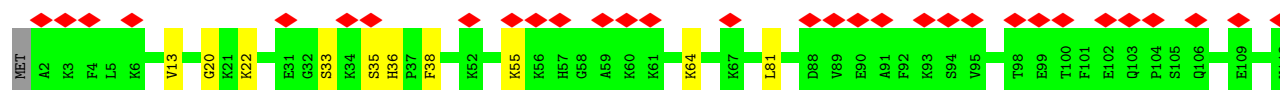
- Molecule 13: 60S ribosomal protein L14-A

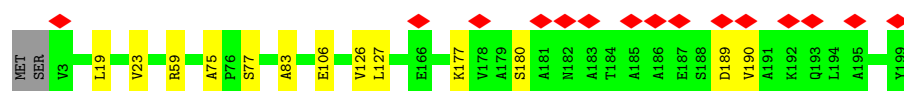
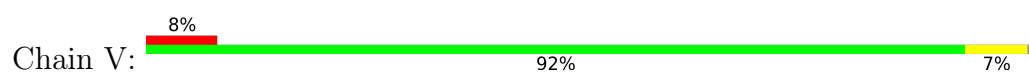
Chain N: 



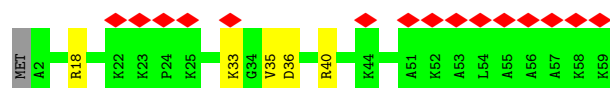
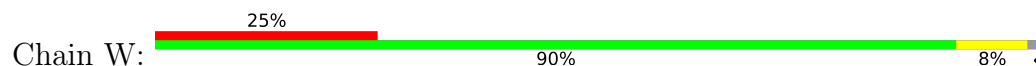
- Molecule 14: 60S ribosomal protein L27-A

Chain O: 

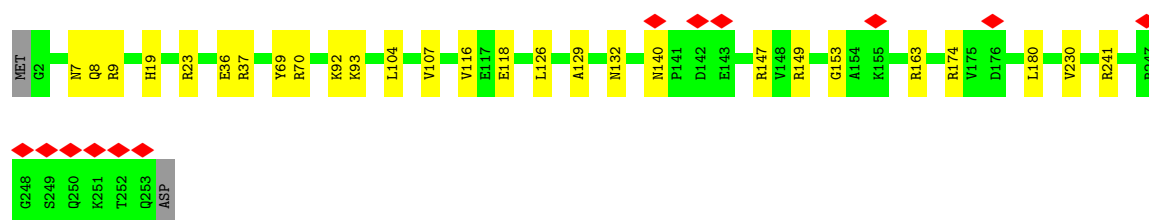
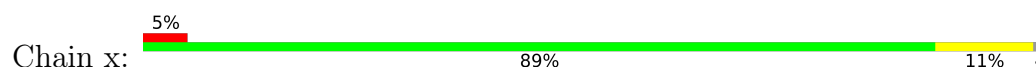




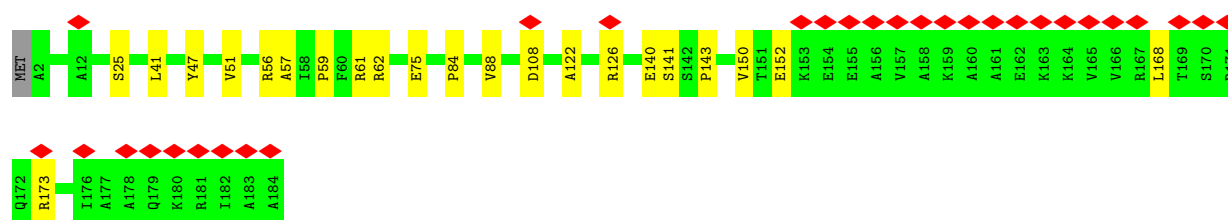
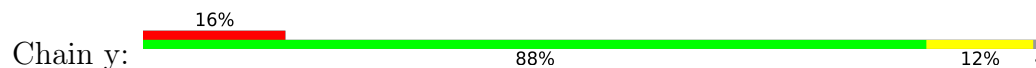
- Molecule 21: 60S ribosomal protein L29



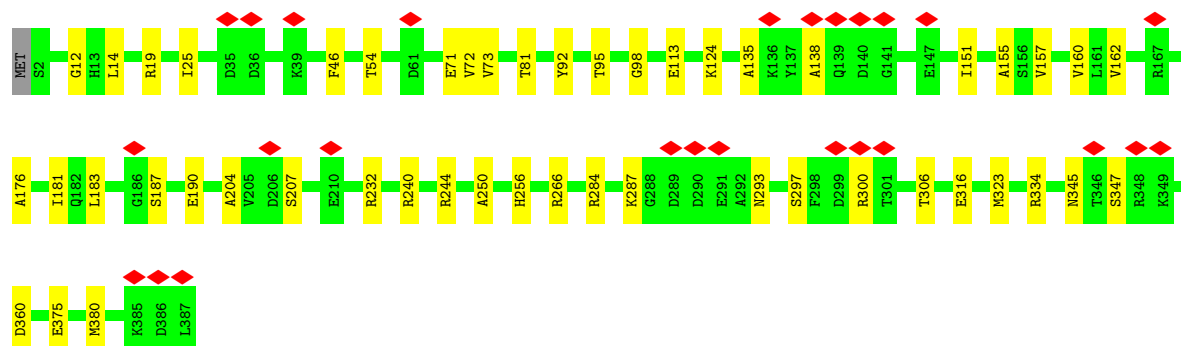
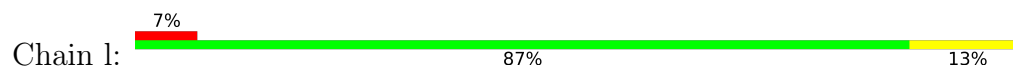
- Molecule 22: 60S ribosomal protein L2-A



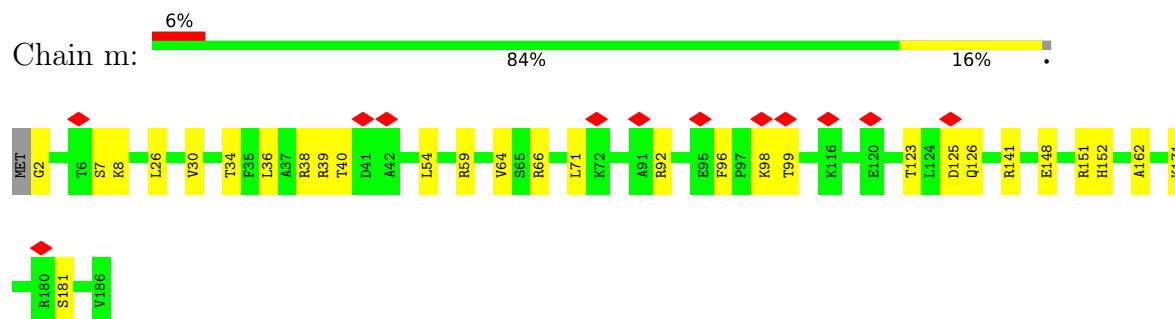
- Molecule 23: 60S ribosomal protein L17-A



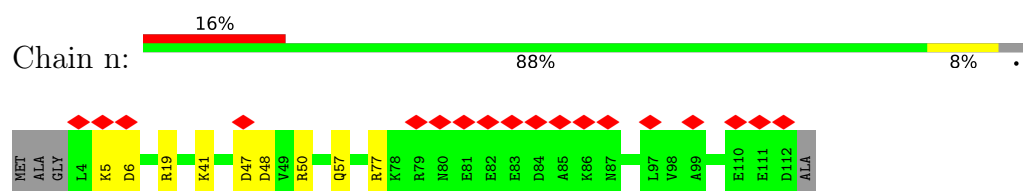
- Molecule 24: 60S ribosomal protein L3



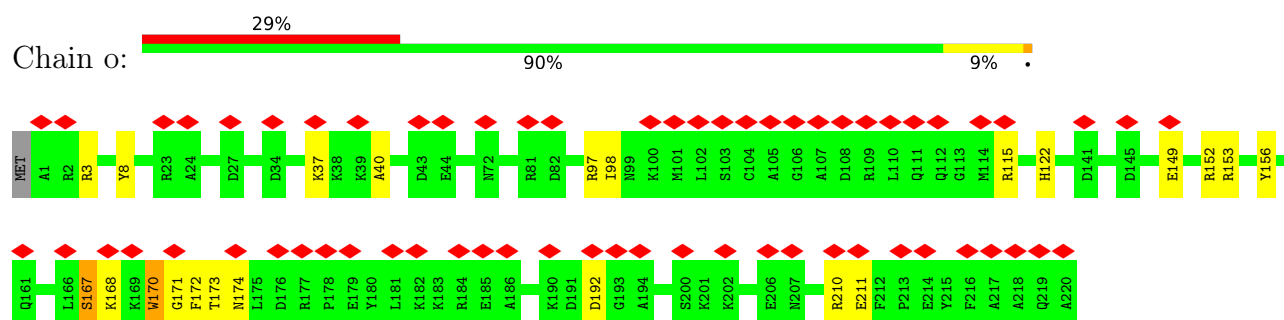
- Molecule 25: 60S ribosomal protein L18-A



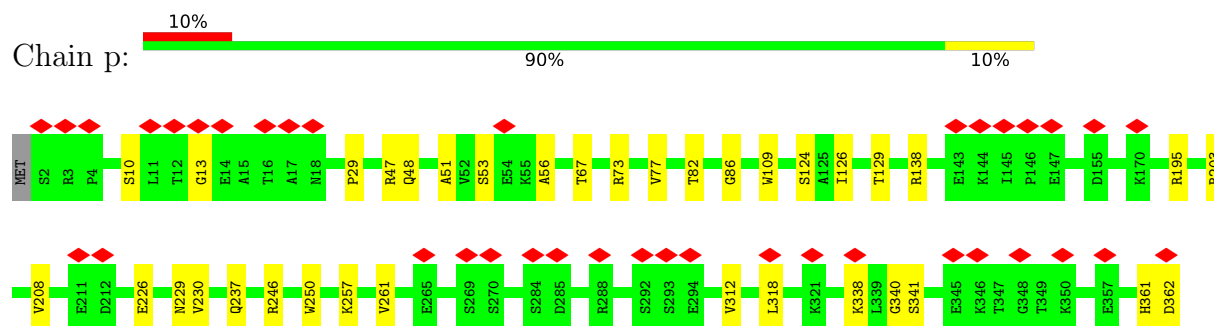
- Molecule 26: 60S ribosomal protein L31-A



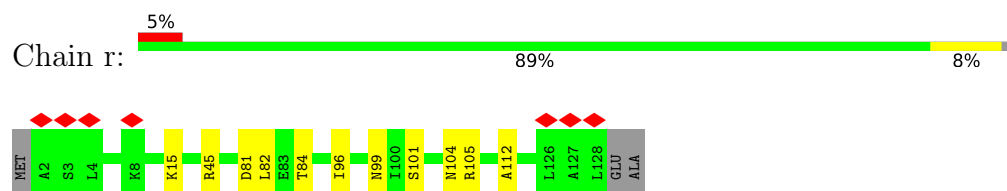
- Molecule 27: 60S ribosomal protein L10



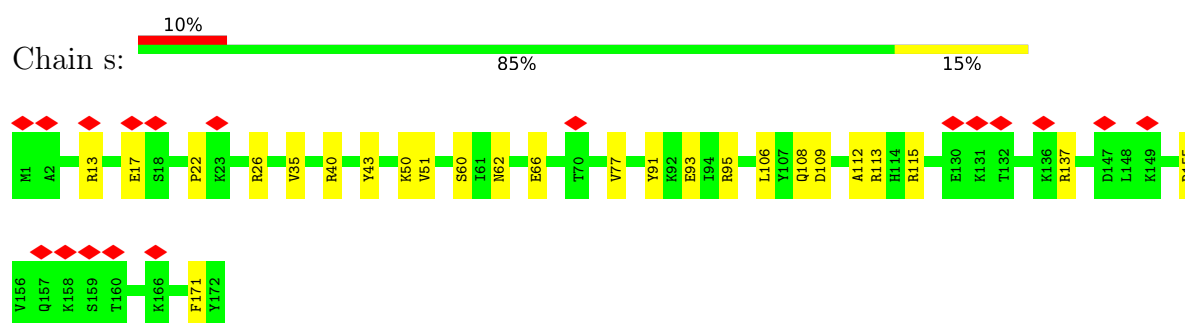
- Molecule 28: 60S ribosomal protein L4-A



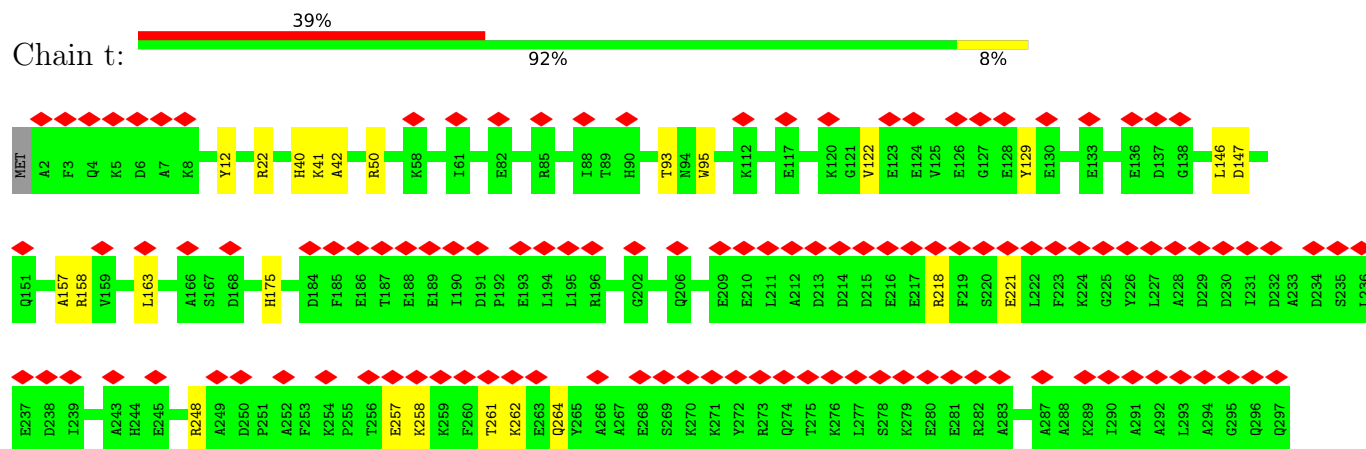
- Molecule 29: 60S ribosomal protein L32



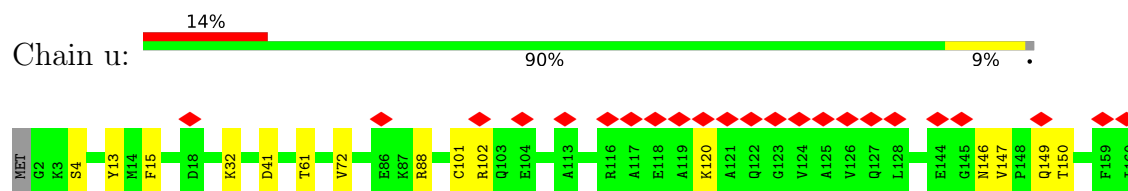
- Molecule 30: 60S ribosomal protein L20-A



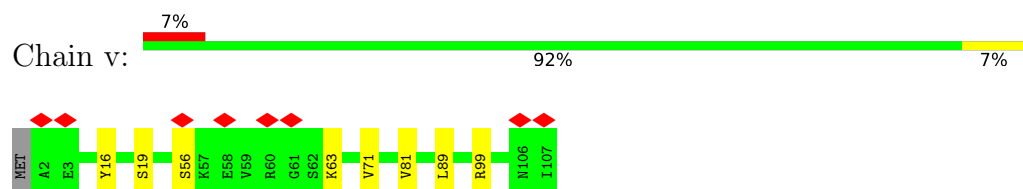
• Molecule 31: 60S ribosomal protein L5



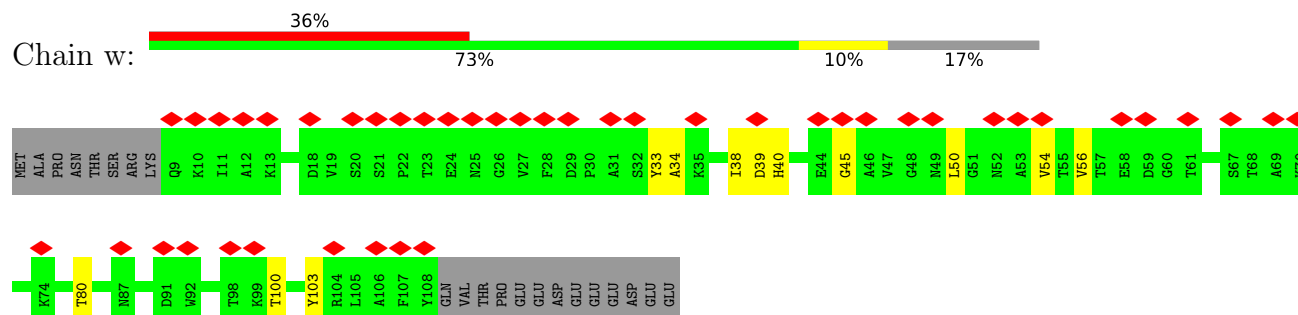
• Molecule 32: 60S ribosomal protein L21-A



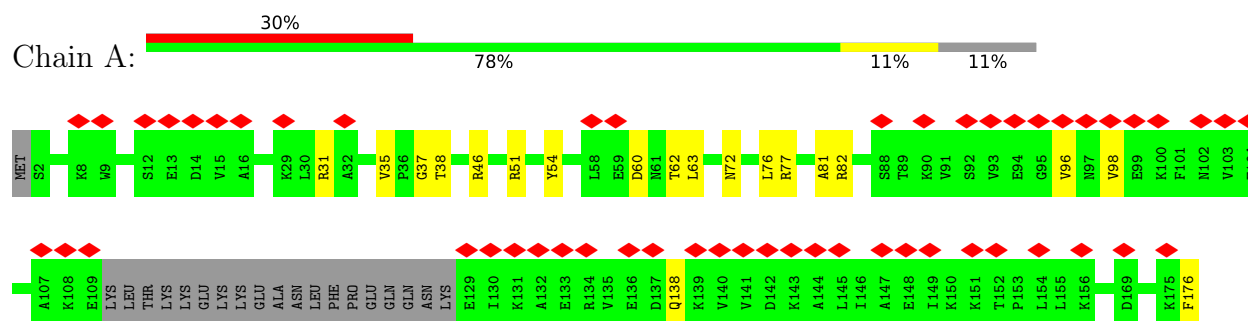
• Molecule 33: 60S ribosomal protein L33-A



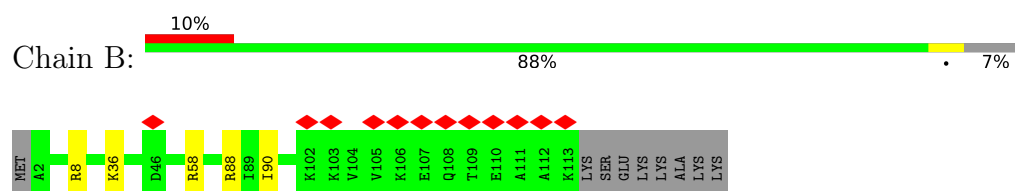
• Molecule 34: 60S ribosomal protein L22-A



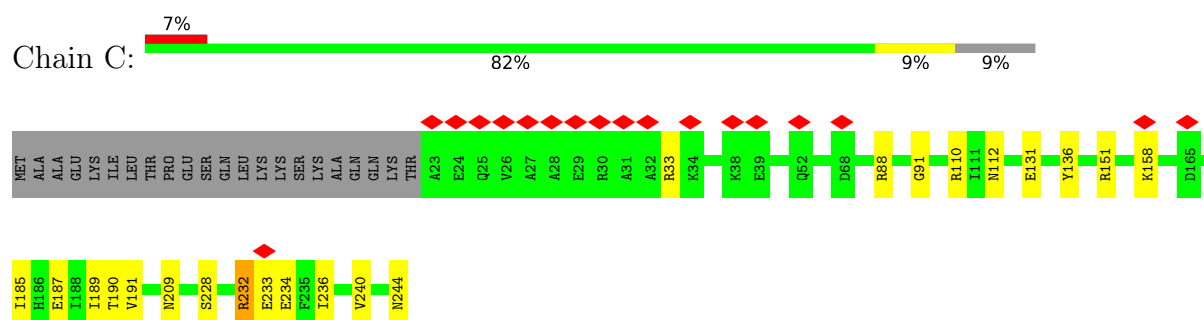
- Molecule 35: 60S ribosomal protein L6-A



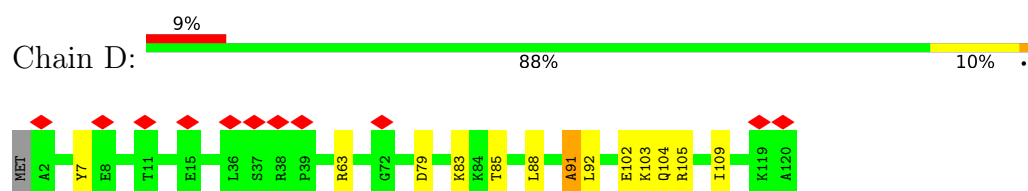
- Molecule 36: 60S ribosomal protein L34-A



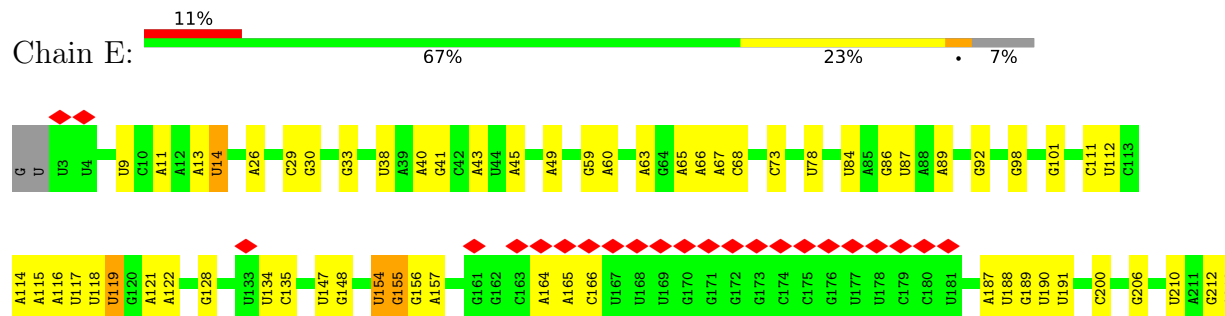
- Molecule 37: 60S ribosomal protein L7-A



- Molecule 38: 60S ribosomal protein L35-A

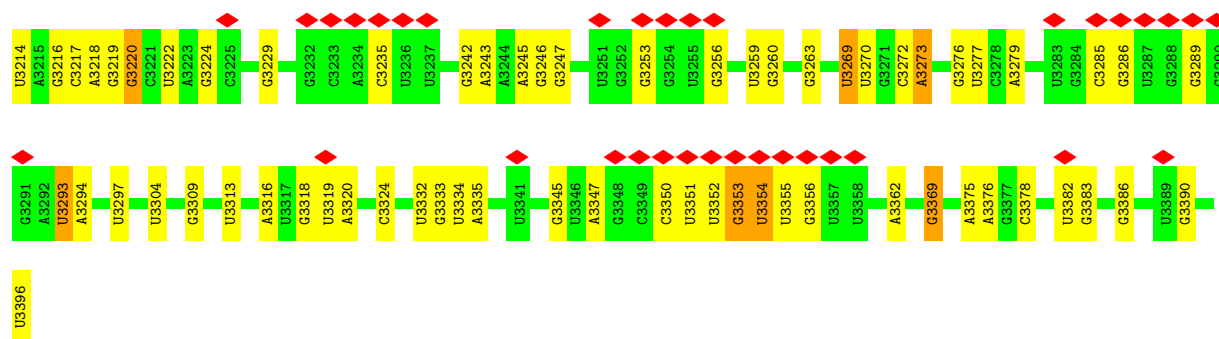


- Molecule 39: 25S ribosomal RNA

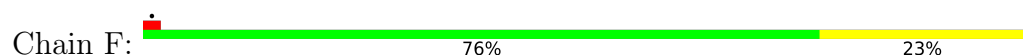








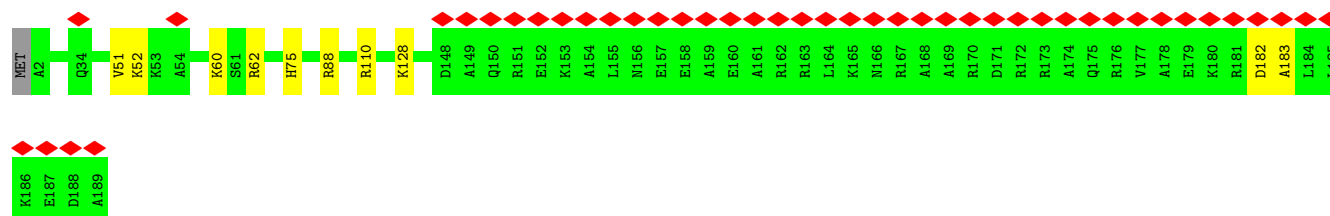
• Molecule 40: 5S ribosomal RNA



• Molecule 41: 5.8S ribosomal RNA



• Molecule 42: 60S ribosomal protein L19-A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153893	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.193	Depositor
Minimum map value	-0.115	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	345.24002, 345.24002, 345.24002	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TEL

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	b	0.49	0/1835	0.67	1/2479 (0.0%)
2	c	0.60	0/1018	0.60	0/1369
3	d	0.48	0/778	0.62	0/1034
4	e	0.47	0/1539	0.62	0/2073
5	f	0.59	0/555	0.59	0/738
6	g	0.67	0/696	0.76	0/923
7	h	0.39	0/1374	0.60	0/1842
8	I	0.55	0/979	0.58	0/1321
9	j	0.49	0/618	0.58	0/826
10	k	0.57	0/1568	0.71	0/2106
11	q	0.54	0/1004	0.58	0/1341
12	M	0.62	0/443	0.65	0/588
13	N	0.49	0/1068	0.56	0/1438
14	O	0.49	0/1118	0.65	0/1497
15	P	0.49	0/423	0.58	0/562
16	Q	0.53	0/860	0.61	0/1136
17	R	0.67	0/1757	0.68	0/2354
18	S	0.60	0/1204	0.70	0/1612
19	U	0.60	0/701	0.68	0/934
20	V	0.61	0/1585	0.63	0/2128
21	W	0.49	0/473	0.57	0/629
22	x	0.68	0/1948	0.67	0/2617
23	y	0.59	0/1443	0.62	0/1944
24	l	0.61	0/3146	0.69	0/4228
25	m	0.58	0/1465	0.67	0/1965
26	n	0.57	0/890	0.60	0/1196
27	o	0.50	0/1807	0.63	0/2425
28	p	0.59	0/2800	0.65	0/3790
29	r	0.62	0/1041	0.59	0/1394
30	s	0.55	0/1481	0.62	0/1990
31	t	0.43	0/2425	0.57	0/3271
32	u	0.57	1/1300 (0.1%)	0.64	0/1743

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	v	0.64	0/868	0.59	0/1168
34	w	0.38	0/812	0.56	0/1099
35	A	0.45	0/1260	0.53	0/1694
36	B	0.66	0/890	0.61	0/1189
37	C	0.59	0/1821	0.62	0/2451
38	D	0.53	0/978	0.68	3/1301 (0.2%)
39	E	0.51	0/75678	0.49	2/117987 (0.0%)
40	F	0.41	0/2883	0.41	0/4491
41	G	0.51	0/3745	0.46	0/5829
42	H	0.55	0/1538	0.64	0/2050
All	All	0.53	1/131815 (0.0%)	0.54	6/194752 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	b	0	1
3	d	0	1
4	e	0	1
9	j	0	1
10	k	0	1
16	Q	0	1
17	R	0	1
18	S	0	1
26	n	0	1
27	o	0	3
28	p	0	1
31	t	0	1
32	u	0	1
37	C	0	1
38	D	0	2
All	All	0	18

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	u	72	VAL	C-N	-5.13	1.31	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	D	92	LEU	N-CA-C	7.40	119.86	110.24
39	E	406	G	O4'-C1'-N9	5.36	116.24	108.20
38	D	91	ALA	CA-C-N	5.20	128.46	120.82
38	D	91	ALA	C-N-CA	5.20	128.46	120.82
39	E	2404	A	C5'-C4'-C3'	5.12	122.87	115.20
1	b	80	TYR	N-CA-C	-5.07	104.39	110.88

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	C	232	ARG	Peptide
38	D	83	LYS	Peptide
38	D	91	ALA	Peptide
16	Q	14	GLY	Peptide
17	R	93	LYS	Peptide
18	S	116	GLY	Peptide
1	b	156	ASP	Peptide
3	d	32	ALA	Peptide
4	e	22	SER	Peptide
9	j	34	ALA	Peptide
10	k	61	PRO	Peptide
26	n	6	ASP	Peptide
27	o	167	SER	Peptide
27	o	170	TRP	Peptide
27	o	171	GLY	Peptide
28	p	318	LEU	Peptide
31	t	258	LYS	Peptide
32	u	15	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b	1803	1876	1876	11	0
2	c	1003	1048	1048	14	0
3	d	771	849	849	3	0
4	e	1518	1587	1587	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	f	543	564	564	8	0
6	g	681	683	687	4	0
7	h	1353	1383	1383	8	0
8	I	964	1026	1025	12	0
9	j	612	682	682	4	0
10	k	1543	1608	1608	19	0
11	q	993	1081	1081	9	0
12	M	436	475	475	5	0
13	N	1053	1149	1149	13	0
14	O	1092	1155	1155	8	0
15	P	417	455	459	4	0
16	Q	847	915	918	7	0
17	R	1720	1779	1779	24	0
18	S	1173	1217	1215	12	0
19	U	694	737	738	7	0
20	V	1555	1660	1659	9	0
21	W	462	491	491	4	0
22	x	1914	1981	1981	21	0
23	y	1420	1437	1437	13	0
24	l	3075	3142	3142	34	0
25	m	1441	1544	1543	23	0
26	n	876	912	912	5	0
27	o	1770	1806	1808	14	0
28	p	2748	2859	2859	22	0
29	r	1020	1091	1090	7	0
30	s	1445	1487	1487	20	0
31	t	2375	2325	2325	16	0
32	u	1276	1323	1323	10	0
33	v	850	880	880	5	0
34	w	796	812	812	9	0
35	A	1239	1326	1326	12	0
36	B	880	941	945	5	0
37	C	1784	1862	1862	14	0
38	D	969	1078	1078	7	0
39	E	67609	33966	33976	263	0
40	F	2579	1304	1304	11	0
41	G	3352	1694	1695	20	0
42	H	1521	1617	1617	9	0
43	E	58	47	65	11	0
44	E	3	0	0	0	0
All	All	122233	87854	87895	556	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 3.

All (556) 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)
43:E:3401:TEL:H382	43:E:3401:TEL:C13	2.02	0.89
6:g:72:ARG:NH1	41:G:95:G:OP2	2.10	0.83
13:N:20:VAL:O	13:N:66:THR:OG1	1.98	0.82
39:E:3216:G:O2'	39:E:3220:G:OP2	1.97	0.81
25:m:92:ARG:NH1	39:E:784:A:O2'	2.14	0.81
43:E:3401:TEL:H112	43:E:3401:TEL:O18	1.81	0.80
16:Q:30:ALA:O	39:E:2767:U:O2'	2.00	0.80
17:R:93:LYS:O	39:E:289:A:O2'	1.98	0.80
19:U:46:THR:OG1	19:U:57:CYS:SG	2.39	0.79
35:A:46:ARG:NH2	39:E:3269:U:OP2	2.15	0.79
38:D:102:GLU:OE1	38:D:105:ARG:NH1	2.14	0.79
39:E:1779:C:N4	42:H:88:ARG:O	2.14	0.79
1:b:87:ALA:O	1:b:90:THR:OG1	2.01	0.78
8:I:31:THR:OG1	39:E:2523:A:OP1	1.99	0.78
39:E:221:A:O2'	39:E:223:U:OP2	2.01	0.78
28:p:10:SER:OG	28:p:13:GLY:O	2.01	0.78
23:y:126:ARG:NH1	23:y:140:GLU:OE2	2.17	0.78
39:E:1246:G:OP2	39:E:1263:A:O2'	2.02	0.77
25:m:8:LYS:NZ	39:E:971:G:OP1	2.18	0.77
30:s:109:ASP:OD1	30:s:113:ARG:NH1	2.17	0.77
39:E:533:A:N7	39:E:555:U:O2	2.18	0.77
11:q:2:ALA:N	39:E:212:G:OP2	2.18	0.77
2:c:12:ARG:NH1	39:E:3041:U:OP1	2.18	0.76
12:M:27:ILE:O	12:M:33:ASN:ND2	2.19	0.76
39:E:84:U:O2'	39:E:101:G:O6	2.04	0.76
39:E:907:G:N2	39:E:926:A:OP2	2.19	0.76
39:E:282:G:O2'	39:E:283:G:OP2	2.04	0.76
17:R:172:ARG:O	17:R:183:THR:OG1	2.03	0.76
14:O:33:SER:OG	14:O:35:SER:O	2.04	0.76
37:C:158:LYS:NZ	39:E:1104:G:OP2	2.19	0.75
25:m:181:SER:OG	39:E:2790:A:OP2	2.04	0.75
1:b:105:LYS:NZ	39:E:121:A:O2'	2.17	0.75
23:y:168:LEU:O	23:y:173:ARG:NH2	2.20	0.75
31:t:122:VAL:O	31:t:248:ARG:NH2	2.19	0.75
25:m:39:ARG:NH1	39:E:1348:U:OP1	2.20	0.75
29:r:81:ASP:O	29:r:84:THR:OG1	2.04	0.75
39:E:2872:A:O2'	39:E:2874:G:OP1	2.04	0.75
5:f:14:TYR:OH	24:l:375:GLU:OE2	2.05	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:124:ARG:NH1	39:E:3214:U:O4	2.20	0.75
3:d:28:TYR:OH	39:E:315:C:OP2	2.04	0.74
25:m:54:LEU:O	25:m:59:ARG:NH1	2.19	0.74
18:S:58:MET:SD	39:E:2786:G:N2	2.58	0.74
22:x:174:ARG:NH1	39:E:1793:C:O2	2.21	0.73
18:S:96:LYS:NZ	18:S:142:GLY:O	2.21	0.73
39:E:775:A:O2'	39:E:777:U:OP2	2.05	0.73
29:r:101:SER:OG	29:r:104:ASN:OD1	2.07	0.73
39:E:1714:A:N6	39:E:1730:G:O2'	2.21	0.73
39:E:2307:G:O2'	39:E:2310:U:OP2	2.05	0.73
32:u:4:SER:OG	39:E:2631:U:OP2	2.06	0.73
24:l:95:THR:OG1	24:l:98:GLY:O	2.06	0.72
35:A:31:ARG:NH2	35:A:81:ALA:O	2.22	0.72
34:w:34:ALA:O	34:w:38:ILE:HD12	1.89	0.72
17:R:192:LYS:O	17:R:196:THR:OG1	2.06	0.72
38:D:104:GLN:NE2	39:E:112:U:OP1	2.21	0.72
39:E:760:G:O2'	39:E:771:A:N6	2.21	0.72
10:k:64:LYS:O	10:k:67:ARG:NH1	2.23	0.72
24:l:345:ASN:OD1	24:l:347:SER:OG	2.08	0.71
27:o:210:ARG:NH1	27:o:211:GLU:OE2	2.23	0.71
39:E:1813:A:O2'	39:E:1817:G:N2	2.24	0.71
28:p:126:ILE:O	28:p:129:THR:OG1	2.09	0.71
21:W:36:ASP:OD1	39:E:2737:C:O2'	2.08	0.71
23:y:56:ARG:NH1	23:y:75:GLU:OE2	2.24	0.71
27:o:8:TYR:OH	27:o:97:ARG:O	2.07	0.71
39:E:2495:C:O2'	39:E:2496:C:OP1	2.09	0.71
39:E:1392:G:O2'	39:E:1418:A:N6	2.24	0.70
25:m:7:SER:OG	39:E:1103:A:O2'	2.07	0.70
39:E:2523:A:O2'	39:E:2524:A:O5'	2.07	0.70
25:m:123:THR:OG1	25:m:125:ASP:OD1	2.07	0.70
39:E:649:A:OP2	39:E:2868:U:O2'	2.07	0.70
39:E:1587:A:O2'	39:E:1588:A:O5'	2.06	0.70
4:e:44:THR:OG1	39:E:3186:A:N3	2.24	0.70
10:k:153:ASP:OD2	10:k:157:ARG:NH2	2.24	0.70
39:E:1572:U:O2'	39:E:1573:G:O4'	2.08	0.70
17:R:68:ARG:NH2	39:E:292:U:OP2	2.25	0.69
33:v:19:SER:OG	39:E:1330:A:OP1	2.10	0.69
11:q:16:ARG:NH1	39:E:216:G:OP1	2.26	0.69
1:b:50:VAL:HG12	8:I:30:ALA:HA	1.74	0.69
39:E:596:C:N3	39:E:608:A:O2'	2.25	0.69
41:G:39:G:O2'	41:G:105:A:N1	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:x:69:TYR:OH	39:E:2557:A:OP1	2.06	0.69
41:G:22:U:O2'	41:G:23:U:OP1	2.11	0.69
31:t:50:ARG:NH1	31:t:147:ASP:OD2	2.25	0.68
38:D:85:THR:HG22	38:D:88:LEU:HD12	1.73	0.68
31:t:41:LYS:NZ	32:u:32:LYS:O	2.21	0.68
4:e:113:GLU:OE2	4:e:115:ARG:NH2	2.26	0.68
13:N:94:TRP:O	13:N:97:SER:OG	2.09	0.68
39:E:532:A:N6	39:E:555:U:O2'	2.27	0.68
39:E:637:C:O2'	39:E:638:C:O5'	2.11	0.68
39:E:2842:U:OP1	39:E:2844:C:N4	2.26	0.67
39:E:1868:G:O2'	39:E:2118:C:O2'	2.07	0.67
39:E:1778:G:O2'	39:E:1780:G:OP2	2.11	0.67
37:C:88:ARG:NH2	37:C:91:GLY:O	2.27	0.67
8:I:39:LYS:NZ	39:E:14:U:OP1	2.27	0.67
22:x:70:ARG:NH2	39:E:1580:A:OP1	2.27	0.67
30:s:60:SER:OG	30:s:62:ASN:OD1	2.13	0.67
39:E:1064:A:OP2	39:E:1097:G:N2	2.27	0.67
17:R:62:TYR:OH	41:G:141:C:O3'	2.12	0.67
11:q:71:SER:N	11:q:81:GLN:O	2.28	0.66
37:C:110:ARG:NH2	39:E:1364:C:OP1	2.28	0.66
39:E:68:C:OP2	39:E:301:G:N2	2.28	0.66
39:E:1192:C:N4	39:E:1301:A:O2'	2.28	0.66
39:E:3070:A:OP1	42:H:62:ARG:NH2	2.27	0.66
39:E:2323:G:O2'	39:E:2325:G:OP2	2.12	0.66
30:s:26:ARG:NH2	32:u:150:THR:OG1	2.29	0.66
39:E:2208:A:O2'	39:E:2209:U:OP1	2.14	0.66
27:o:149:GLU:OE1	27:o:152:ARG:NH1	2.27	0.66
13:N:128:ARG:NH2	39:E:3214:U:OP2	2.29	0.65
18:S:3:SER:O	18:S:6:THR:OG1	2.10	0.65
24:l:287:LYS:O	24:l:293:ASN:ND2	2.28	0.65
15:P:100:TYR:O	39:E:2895:G:O2'	2.14	0.65
30:s:40:ARG:NH2	40:F:97:A:OP1	2.30	0.65
7:h:60:ARG:HH12	16:Q:103:ALA:HB1	1.60	0.65
24:l:14:LEU:O	39:E:3009:G:O2'	2.15	0.65
24:l:240:ARG:NH2	39:E:1907:C:O2	2.29	0.65
24:l:187:SER:O	24:l:190:GLU:N	2.29	0.65
23:y:25:SER:OG	39:E:1447:G:N7	2.28	0.65
32:u:101:CYS:SG	32:u:102:ARG:N	2.69	0.65
24:l:204:ALA:O	24:l:207:SER:OG	2.07	0.65
37:C:228:SER:O	37:C:232:ARG:NH2	2.30	0.65
8:I:107:VAL:HG12	8:I:108:LEU:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:E:1570:U:O2'	39:E:1572:U:O2	2.14	0.64
35:A:76:LEU:N	35:A:138:GLN:OE1	2.29	0.64
7:h:62:ASN:O	16:Q:103:ALA:HB2	1.97	0.64
24:l:124:LYS:NZ	39:E:3297:U:O4	2.31	0.64
39:E:1390:A:N6	39:E:1418:A:O2'	2.30	0.64
39:E:2185:G:O2'	39:E:2314:U:OP2	2.15	0.64
33:v:99:ARG:NH2	39:E:3175:U:O4	2.31	0.64
39:E:26:A:N3	39:E:328:U:O2'	2.31	0.64
39:E:1524:A:O2'	39:E:1526:U:OP2	2.10	0.63
39:E:2899:C:O2'	39:E:2901:G:OP2	2.13	0.63
10:k:128:ARG:NH2	38:D:109:ILE:O	2.31	0.63
28:p:82:THR:OG1	39:E:355:A:N1	2.25	0.63
30:s:43:TYR:OH	40:F:96:U:OP1	2.13	0.63
39:E:63:A:N3	39:E:78:U:O2'	2.31	0.63
22:x:93:LYS:NZ	39:E:2548:C:OP2	2.31	0.63
9:j:4:GLU:OE1	39:E:1746:U:O2'	2.15	0.63
27:o:192:ASP:OD2	39:E:1010:G:N2	2.31	0.63
17:R:73:ARG:NH1	39:E:33:G:OP1	2.31	0.63
39:E:1477:A:OP1	39:E:3075:G:O2'	2.14	0.63
7:h:133:ARG:NH2	7:h:153:LYS:O	2.32	0.62
31:t:12:TYR:OH	39:E:2688:U:OP1	2.17	0.62
17:R:114:ARG:NH1	17:R:151:ILE:O	2.32	0.62
4:e:36:LYS:NZ	4:e:152:GLU:OE2	2.32	0.62
35:A:60:ASP:OD1	35:A:62:THR:OG1	2.16	0.62
41:G:85:G:O2'	41:G:86:U:OP1	2.14	0.62
39:E:1719:G:OP1	42:H:110:ARG:NH2	2.33	0.62
2:c:14:SER:O	2:c:81:GLN:NE2	2.33	0.62
24:l:244:ARG:NH2	39:E:2948:C:OP1	2.33	0.62
4:e:49:ASN:OD1	4:e:52:LEU:N	2.32	0.61
12:M:45:ARG:NH2	39:E:1514:G:O2'	2.31	0.61
30:s:22:PRO:O	32:u:146:ASN:ND2	2.33	0.61
10:k:70:ARG:NH1	10:k:71:ALA:O	2.32	0.61
18:S:117:ARG:NH2	39:E:718:G:OP1	2.34	0.61
21:W:33:LYS:O	32:u:88:ARG:NH1	2.33	0.61
39:E:2711:C:O2'	39:E:2744:U:OP1	2.17	0.61
22:x:37:ARG:NH1	39:E:2526:C:OP1	2.34	0.61
39:E:3152:U:O3'	39:E:3293:U:O2'	2.18	0.60
16:Q:2:VAL:N	16:Q:90:HIS:O	2.35	0.60
39:E:637:C:O2'	39:E:638:C:O4'	2.19	0.60
39:E:3092:C:O2'	39:E:3094:A:OP2	2.15	0.60
36:B:58:ARG:NH2	39:E:1592:G:OP1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C:112:ASN:ND2	37:C:209:ASN:OD1	2.35	0.60
30:s:91:TYR:OH	30:s:93:GLU:OE2	2.08	0.60
33:v:16:TYR:OH	33:v:89:LEU:O	2.16	0.60
39:E:1307:G:O2'	39:E:1308:A:OP2	2.13	0.59
43:E:3401:TEL:H382	43:E:3401:TEL:O18	2.00	0.59
35:A:82:ARG:NH2	39:E:584:G:OP1	2.35	0.59
39:E:117:U:O2'	39:E:119:U:OP2	2.20	0.59
13:N:123:LEU:HD22	20:V:190:VAL:HG23	1.85	0.59
39:E:714:G:HO2'	39:E:753:C:HO2'	1.50	0.59
39:E:2712:U:HO2'	39:E:2743:A:HO2'	1.43	0.59
2:c:112:SER:O	2:c:132:ASN:ND2	2.35	0.59
5:f:34:SER:OG	39:E:3085:G:OP1	2.17	0.59
7:h:38:GLU:OE1	7:h:39:GLN:NE2	2.36	0.59
20:V:177:LYS:O	20:V:180:SER:OG	2.16	0.59
10:k:114:GLN:NE2	10:k:118:GLU:OE2	2.36	0.58
25:m:2:GLY:N	39:E:1333:C:OP1	2.37	0.58
35:A:51:ARG:O	35:A:72:ASN:ND2	2.36	0.58
36:B:88:ARG:NH2	39:E:2556:C:OP1	2.36	0.58
39:E:2393:G:O2'	39:E:2982:A:N6	2.35	0.58
30:s:50:LYS:NZ	40:F:76:A:N3	2.52	0.58
37:C:187:GLU:O	37:C:190:THR:O	2.22	0.58
10:k:76:THR:O	10:k:79:GLU:N	2.36	0.58
24:l:266:ARG:NH1	39:E:2392:C:O2'	2.36	0.58
31:t:218:ARG:NH1	31:t:221:GLU:OE2	2.37	0.58
39:E:2401:A:N1	43:E:3401:TEL:H573	2.19	0.58
39:E:3353:G:O2'	39:E:3354:U:O4'	2.15	0.58
9:j:2:ALA:N	9:j:51:LEU:O	2.37	0.58
11:q:3:LYS:HD2	11:q:8:VAL:HG13	1.84	0.58
18:S:21:ARG:NH1	39:E:640:U:OP1	2.36	0.58
39:E:2373:A:N3	39:E:2824:G:O2'	2.33	0.58
39:E:3375:A:O2'	39:E:3376:A:O5'	2.22	0.58
17:R:12:ARG:NH1	39:E:297:G:O6	2.37	0.57
18:S:77:LYS:O	18:S:80:THR:OG1	2.18	0.57
24:l:250:ALA:HB1	39:E:2947:G:N3	2.18	0.57
6:g:56:ARG:NH2	39:E:364:G:N7	2.52	0.57
39:E:1192:C:N4	39:E:1301:A:O3'	2.37	0.57
32:u:41:ASP:OD1	32:u:61:THR:OG1	2.15	0.57
39:E:831:G:O2'	39:E:1864:A:N3	2.36	0.57
24:l:12:GLY:O	39:E:3011:A:N6	2.38	0.57
30:s:155:ARG:NH1	30:s:171:PHE:O	2.38	0.57
39:E:1144:U:O2'	39:E:1145:G:OP2	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:83:ALA:O	39:E:1312:C:O2'	2.22	0.57
22:x:19:HIS:O	22:x:23:ARG:NH1	2.37	0.57
4:e:104:VAL:HG11	4:e:113:GLU:OE1	2.05	0.56
13:N:20:VAL:HG13	13:N:66:THR:OG1	2.05	0.56
13:N:113:THR:OG1	35:A:176:PHE:O	2.24	0.56
39:E:2523:A:HO2'	39:E:2524:A:P	2.28	0.56
19:U:22:LEU:HD23	22:x:180:LEU:HD12	1.88	0.56
1:b:84:ARG:NH1	41:G:156:U:OP2	2.38	0.56
39:E:542:G:O6	39:E:549:U:C4	2.59	0.56
24:l:250:ALA:HB1	39:E:2947:G:C2	2.40	0.56
39:E:1940:G:H21	39:E:3362:A:H8	1.53	0.56
23:y:141:SER:OG	39:E:2355:G:OP1	2.22	0.56
4:e:62:ARG:NH2	39:E:3115:C:OP1	2.38	0.56
25:m:38:ARG:NH1	39:E:1347:U:OP2	2.39	0.56
12:M:43:ASN:OD1	12:M:46:ARG:NH2	2.39	0.55
20:V:126:VAL:HG13	20:V:127:LEU:HD12	1.89	0.55
10:k:85:LEU:CD1	10:k:90:ALA:HB2	2.36	0.55
42:H:182:ASP:OD1	42:H:183:ALA:N	2.39	0.55
39:E:2445:A:O2'	39:E:2446:U:OP1	2.23	0.55
5:f:1:MET:N	24:l:71:GLU:OE2	2.32	0.55
39:E:707:U:OP1	39:E:780:A:O2'	2.15	0.55
39:E:1565:G:O2'	39:E:1566:A:OP1	2.24	0.55
13:N:21:VAL:HG12	13:N:65:LEU:HD23	1.87	0.55
27:o:98:ILE:HG23	27:o:122:HIS:HB2	1.89	0.55
7:h:99:THR:O	7:h:154:THR:OG1	2.22	0.55
39:E:3375:A:O2'	39:E:3376:A:O4'	2.25	0.55
41:G:125:U:O2'	41:G:126:A:OP1	2.24	0.55
23:y:59:PRO:HB2	23:y:61:ARG:HE	1.72	0.54
25:m:96:PHE:CZ	25:m:99:THR:HG21	2.41	0.54
10:k:180:ARG:NH2	39:E:2779:A:O2'	2.40	0.54
20:V:77:SER:OG	20:V:106:GLU:OE2	2.24	0.54
22:x:118:GLU:OE2	39:E:2177:G:N2	2.40	0.54
24:l:19:ARG:NH2	39:E:3045:G:OP1	2.39	0.54
6:g:68:LYS:NZ	41:G:57:C:OP2	2.40	0.54
6:g:25:ARG:NH2	39:E:360:G:OP1	2.39	0.54
24:l:160:VAL:HG13	24:l:183:LEU:HD11	1.88	0.54
39:E:1816:A:O2'	39:E:1817:G:N7	2.37	0.54
2:c:10:LYS:NZ	2:c:56:ASP:OD1	2.38	0.54
24:l:135:ALA:O	24:l:138:ALA:HB2	2.08	0.54
3:d:37:THR:HG22	17:R:5:LYS:NZ	2.23	0.54
16:Q:77:CYS:SG	16:Q:79:THR:HG22	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:o:37:LYS:HG3	27:o:40:ALA:HB2	1.89	0.54
30:s:77:VAL:HG11	30:s:106:LEU:CD1	2.38	0.54
4:e:80:THR:OG1	4:e:86:TYR:OH	2.15	0.53
17:R:162:ARG:O	39:E:29:C:O2'	2.25	0.53
31:t:50:ARG:NH2	40:F:6:C:O2'	2.41	0.53
31:t:221:GLU:O	40:F:50:U:O2'	2.26	0.53
17:R:41:ARG:NH1	39:E:9:U:OP1	2.41	0.53
29:r:99:ASN:O	39:E:1388:U:O2'	2.23	0.53
17:R:127:TYR:OH	39:E:1544:G:OP1	2.16	0.53
25:m:71:LEU:CD1	25:m:99:THR:HG22	2.39	0.53
28:p:73:ARG:NH2	39:E:2814:G:OP1	2.38	0.53
39:E:67:A:N6	39:E:271:C:O2'	2.39	0.53
13:N:126:GLN:OE1	39:E:3260:G:O2'	2.19	0.53
28:p:138:ARG:NH2	39:E:1383:G:O3'	2.42	0.53
39:E:3068:U:OP2	42:H:62:ARG:NH1	2.40	0.53
7:h:137:ARG:NH1	40:F:28:C:OP1	2.40	0.52
26:n:57:GLN:NE2	39:E:1474:A:O2'	2.41	0.52
28:p:341:SER:OG	39:E:514:G:N3	2.40	0.52
29:r:45:ARG:O	39:E:1145:G:O2'	2.23	0.52
39:E:691:A:N6	41:G:28:C:O2'	2.42	0.52
39:E:1940:G:OP1	42:H:75:HIS:ND1	2.40	0.52
14:O:55:LYS:N	39:E:2563:G:OP1	2.43	0.52
22:x:36:GLU:OE1	22:x:163:ARG:NH1	2.42	0.52
28:p:338:LYS:O	28:p:340:GLY:N	2.42	0.52
37:C:131:GLU:OE2	37:C:136:TYR:OH	2.12	0.52
39:E:1203:A:N3	39:E:2855:U:O2'	2.38	0.52
39:E:1724:U:OP2	42:H:128:LYS:NZ	2.41	0.52
16:Q:41:ARG:NH1	39:E:284:A:OP2	2.42	0.52
31:t:40:HIS:CE1	31:t:42:ALA:HB3	2.45	0.52
39:E:937:G:OP2	39:E:938:C:N4	2.40	0.52
32:u:13:TYR:OH	39:E:1050:U:OP2	2.15	0.52
39:E:2434:U:N3	39:E:2594:C:OP2	2.43	0.52
39:E:1314:C:O2'	39:E:1317:A:O2'	2.26	0.52
39:E:1831:U:O2'	41:G:114:G:OP1	2.19	0.51
19:U:2:ALA:N	39:E:853:G:O6	2.43	0.51
39:E:1481:A:O2'	39:E:1858:A:N3	2.44	0.51
39:E:2193:U:O2'	39:E:2313:A:OP2	2.22	0.51
23:y:47:TYR:O	23:y:51:VAL:HG23	2.11	0.51
35:A:54:TYR:CE1	35:A:63:LEU:HD22	2.45	0.51
2:c:47:ASN:ND2	39:E:2880:U:OP1	2.40	0.51
26:n:5:LYS:O	26:n:77:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C:151:ARG:NE	37:C:244:ASN:OD1	2.40	0.51
25:m:148:GLU:OE2	25:m:151:ARG:NH2	2.44	0.51
39:E:1813:A:HO2'	39:E:1817:G:N2	2.09	0.51
17:R:30:TYR:O	17:R:65:ARG:NH1	2.44	0.51
22:x:129:ALA:HB3	22:x:132:ASN:OD1	2.10	0.51
28:p:77:VAL:O	28:p:86:GLY:N	2.40	0.51
39:E:1704:A:O2'	39:E:1705:U:O5'	2.24	0.51
21:W:18:ARG:NH1	39:E:952:A:OP1	2.44	0.51
39:E:542:G:O6	39:E:549:U:O4	2.29	0.51
43:E:3401:TEL:H382	43:E:3401:TEL:H3	1.93	0.51
5:f:48:ARG:NH1	39:E:2112:U:OP2	2.43	0.51
34:w:45:GLY:N	39:E:1687:U:O4	2.42	0.51
25:m:26:LEU:O	25:m:30:VAL:HG23	2.12	0.50
10:k:76:THR:OG1	10:k:101:ARG:NH1	2.45	0.50
27:o:3:ARG:NH2	27:o:98:ILE:HG22	2.26	0.50
39:E:2815:G:N7	39:E:2870:C:O2'	2.44	0.50
23:y:62:ARG:NH1	39:E:412:G:OP1	2.44	0.50
39:E:1551:C:O2'	39:E:2170:U:O2'	2.22	0.50
40:F:3:U:O2'	40:F:25:G:N3	2.44	0.50
14:O:64:LYS:NZ	39:E:1812:G:O6	2.45	0.50
20:V:59:ARG:NH1	39:E:1307:G:OP2	2.43	0.50
35:A:37:GLY:N	35:A:54:TYR:O	2.40	0.50
7:h:28:ASP:OD1	7:h:29:ARG:N	2.44	0.50
10:k:85:LEU:HD13	10:k:90:ALA:HB2	1.92	0.50
34:w:103:TYR:OH	39:E:1677:G:OP2	2.26	0.50
40:F:77:G:O2'	40:F:101:G:O6	2.28	0.50
2:c:44:SER:OG	39:E:2935:U:O4	2.30	0.50
2:c:88:ARG:HB3	24:l:72:VAL:HG12	1.93	0.50
15:P:79:GLU:O	15:P:81:SER:N	2.44	0.50
19:U:5:THR:OG1	39:E:837:A:OP1	2.22	0.50
39:E:1304:A:HO2'	39:E:2884:C:HO2'	1.59	0.50
39:E:2335:G:N2	39:E:2339:C:O2'	2.45	0.50
17:R:68:ARG:NH1	17:R:124:ASP:O	2.42	0.50
30:s:77:VAL:HG11	30:s:106:LEU:HD13	1.92	0.50
31:t:129:TYR:OH	31:t:175:HIS:O	2.23	0.49
22:x:149:ARG:HE	22:x:153:GLY:HA2	1.77	0.49
34:w:39:ASP:OD1	34:w:40:HIS:ND1	2.45	0.49
2:c:90:GLY:HA3	24:l:73:VAL:HG21	1.94	0.49
11:q:77:LYS:HE3	12:M:31:THR:HG23	1.95	0.49
17:R:54:LYS:NZ	39:E:114:A:OP1	2.45	0.49
28:p:67:THR:OG1	39:E:1436:U:O4	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:E:67:A:O2'	39:E:315:C:O2	2.31	0.49
39:E:2295:A:N3	39:E:2929:C:O2'	2.34	0.49
8:I:105:VAL:CG1	8:I:126:LEU:HD22	2.42	0.49
22:x:104:LEU:HA	22:x:107:VAL:HG22	1.93	0.49
31:t:93:THR:O	31:t:158:ARG:NH1	2.45	0.49
39:E:1003:A:N1	39:E:1049:C:O2'	2.43	0.49
25:m:98:LYS:O	25:m:99:THR:OG1	2.26	0.49
26:n:19:ARG:NH1	39:E:3324:C:OP1	2.42	0.49
39:E:1134:G:O2'	39:E:2642:A:N3	2.45	0.49
22:x:7:ASN:OD1	22:x:8:GLN:N	2.46	0.49
22:x:140:ASN:OD1	22:x:147:ARG:NH2	2.46	0.49
34:w:50:LEU:HD13	34:w:54:VAL:HG23	1.94	0.49
39:E:1285:G:O2'	39:E:1286:A:O4'	2.24	0.49
23:y:122:ALA:HB3	23:y:143:PRO:HB2	1.93	0.49
27:o:170:TRP:O	27:o:172:PHE:N	2.44	0.49
31:t:261:THR:OG1	31:t:262:LYS:N	2.45	0.49
39:E:2901:G:O2'	39:E:3024:A:N1	2.45	0.49
10:k:4:SER:O	18:S:44:ASN:ND2	2.42	0.49
19:U:60:CYS:SG	19:U:62:LYS:NZ	2.82	0.49
39:E:2810:C:OP2	39:E:2955:U:O2'	2.31	0.49
39:E:2991:A:O2'	39:E:3309:G:N7	2.46	0.49
1:b:48:ARG:NH2	39:E:2588:U:OP1	2.46	0.48
5:f:16:GLY:O	39:E:3050:U:O2'	2.27	0.48
30:s:137:ARG:NH1	39:E:1213:G:OP1	2.46	0.48
39:E:1093:A:O2'	39:E:1094:U:O4'	2.30	0.48
23:y:84:PRO:O	23:y:88:VAL:HG23	2.13	0.48
39:E:1713:G:N2	39:E:1731:A:OP2	2.46	0.48
10:k:89:TYR:O	10:k:92:THR:OG1	2.27	0.48
24:l:380:MET:O	39:E:3369:G:N1	2.47	0.48
40:F:72:A:O2'	40:F:74:C:OP1	2.09	0.48
37:C:185:ILE:O	37:C:189:ILE:HG22	2.14	0.48
24:l:256:HIS:O	39:E:2940:A:O2'	2.28	0.48
2:c:87:ARG:NE	2:c:121:GLU:OE2	2.47	0.48
25:m:141:ARG:NH1	39:E:743:C:N3	2.61	0.48
25:m:171:LYS:NZ	39:E:89:A:N7	2.62	0.48
38:D:7:TYR:OH	41:G:87:G:OP2	2.24	0.48
11:q:77:LYS:NZ	39:E:374:A:OP1	2.46	0.47
39:E:2247:G:O2'	39:E:2271:A:N1	2.42	0.47
39:E:2400:A:N1	43:E:3401:TEL:O48	2.48	0.47
43:E:3401:TEL:H3	43:E:3401:TEL:O20	2.15	0.47
2:c:104:ASN:OD1	2:c:108:GLU:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:E:2945:G:O2'	39:E:2948:C:OP2	2.27	0.47
21:W:35:VAL:O	21:W:40:ARG:NH2	2.47	0.47
28:p:29:PRO:O	28:p:124:SER:OG	2.30	0.47
39:E:2802:A:O2'	39:E:2803:A:O5'	2.29	0.47
14:O:22:LYS:NZ	14:O:132:SER:OG	2.47	0.47
24:l:162:VAL:HG21	24:l:181:ILE:HD12	1.97	0.47
42:H:51:VAL:HG22	42:H:52:LYS:H	1.79	0.47
33:v:56:SER:O	33:v:63:LYS:NZ	2.45	0.47
2:c:135:VAL:HG11	5:f:26:SER:OG	2.14	0.47
13:N:37:GLU:OE2	30:s:95:ARG:NH2	2.48	0.47
14:O:55:LYS:NZ	39:E:2564:G:OP2	2.28	0.47
22:x:36:GLU:O	22:x:92:LYS:N	2.47	0.47
39:E:1144:U:OP1	39:E:1367:G:O2'	2.31	0.47
39:E:2433:U:OP2	39:E:2434:U:O2'	2.24	0.47
43:E:3401:TEL:H381	43:E:3401:TEL:H221	1.97	0.47
35:A:35:VAL:O	35:A:38:THR:OG1	2.07	0.47
9:j:51:LEU:N	39:E:1613:A:OP1	2.47	0.47
25:m:125:ASP:OD1	25:m:126:GLN:N	2.47	0.47
27:o:173:THR:OG1	27:o:174:ASN:N	2.47	0.47
31:t:22:ARG:NH1	40:F:6:C:OP2	2.47	0.47
39:E:2560:C:N4	39:E:2575:G:OP2	2.48	0.47
26:n:41:LYS:NZ	26:n:47:ASP:OD1	2.44	0.47
25:m:152:HIS:ND1	25:m:162:ALA:O	2.41	0.46
22:x:9:ARG:NH1	39:E:912:G:N7	2.63	0.46
2:c:104:ASN:OD1	2:c:107:GLY:N	2.49	0.46
10:k:19:GLN:HA	10:k:22:VAL:HG23	1.98	0.46
27:o:115:ARG:NH2	39:E:2617:U:O2'	2.47	0.46
28:p:237:GLN:O	28:p:246:ARG:NH1	2.48	0.46
30:s:13:ARG:HE	30:s:51:VAL:HG12	1.81	0.46
34:w:50:LEU:HD13	34:w:54:VAL:CG2	2.44	0.46
39:E:845:G:O2'	39:E:847:A:N7	2.43	0.46
2:c:118:VAL:O	2:c:137:VAL:N	2.43	0.46
28:p:53:SER:OG	28:p:56:ALA:HB2	2.16	0.46
7:h:18:VAL:HG11	39:E:2682:C:O2'	2.16	0.46
17:R:63:ARG:NH2	17:R:131:GLU:OE2	2.45	0.46
24:l:232:ARG:NH1	24:l:266:ARG:O	2.47	0.46
8:I:90:ALA:O	8:I:120:LYS:NZ	2.48	0.46
13:N:23:ILE:O	13:N:30:GLY:N	2.44	0.46
15:P:114:LYS:NZ	39:E:2908:G:O2'	2.48	0.46
25:m:36:LEU:O	25:m:40:THR:OG1	2.17	0.46
39:E:1118:C:O2'	39:E:1154:A:N1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:E:3353:G:HO2'	39:E:3354:U:C1'	2.25	0.45
18:S:32:ARG:HD2	39:E:38:U:H4'	1.99	0.45
39:E:2901:G:N2	39:E:3030:G:O2'	2.49	0.45
18:S:42:ARG:NH2	39:E:2800:G:O6	2.41	0.45
22:x:230:VAL:HG21	39:E:2424:A:C2	2.51	0.45
28:p:48:GLN:NE2	39:E:336:A:N3	2.64	0.45
28:p:361:HIS:ND1	28:p:362:ASP:O	2.49	0.45
43:E:3401:TEL:C13	43:E:3401:TEL:C38	2.86	0.45
1:b:196:ALA:O	1:b:197:VAL:HG13	2.17	0.45
24:l:306:THR:HG21	24:l:316:GLU:OE1	2.17	0.45
38:D:63:ARG:NH2	38:D:79:ASP:O	2.50	0.45
17:R:14:LYS:HA	17:R:19:LEU:HD23	1.98	0.45
17:R:109:ARG:NH2	41:G:141:C:OP1	2.50	0.45
38:D:103:LYS:NZ	39:E:154:U:OP2	2.37	0.45
1:b:48:ARG:NH1	39:E:2587:U:O3'	2.50	0.45
19:U:22:LEU:HD23	22:x:180:LEU:CD1	2.47	0.45
39:E:1900:A:O2'	39:E:1906:G:N7	2.42	0.45
10:k:13:HIS:NE2	39:E:98:G:N7	2.63	0.44
11:q:70:ILE:HG23	11:q:80:VAL:HG22	1.99	0.44
25:m:64:VAL:HG22	25:m:96:PHE:CE1	2.52	0.44
27:o:156:TYR:OH	39:E:1206:G:OP1	2.20	0.44
37:C:191:VAL:HG23	37:C:191:VAL:O	2.17	0.44
39:E:155:G:N1	39:E:265:A:OP2	2.47	0.44
2:c:68:GLU:O	2:c:72:LYS:NZ	2.38	0.44
39:E:770:G:HO2'	39:E:771:A:H8	1.66	0.44
10:k:90:ALA:HB1	10:k:95:ILE:HB	1.98	0.44
23:y:108:ASP:N	23:y:152:GLU:OE2	2.42	0.44
24:l:46:PHE:HE2	24:l:81:THR:HG23	1.82	0.44
25:m:30:VAL:O	25:m:34:THR:HG23	2.17	0.44
29:r:82:LEU:HD11	29:r:112:ALA:HB2	1.99	0.44
34:w:33:TYR:OH	34:w:80:THR:OG1	2.10	0.44
36:B:8:ARG:NH2	39:E:1597:C:OP2	2.49	0.44
39:E:679:U:O2'	39:E:788:C:O2	2.36	0.44
29:r:96:ILE:HG21	29:r:105:ARG:HG2	2.00	0.44
39:E:436:A:OP2	39:E:621:A:N6	2.40	0.44
39:E:1693:C:O2'	39:E:1772:U:O3'	2.35	0.44
39:E:2838:A:N6	39:E:2850:G:O2'	2.48	0.44
41:G:126:A:O2'	41:G:129:C:N4	2.50	0.44
8:I:103:TYR:O	8:I:138:ARG:NH1	2.45	0.44
5:f:20:LEU:HD11	5:f:28:ILE:CG2	2.48	0.44
14:O:81:LEU:HD22	36:B:90:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:75:ALA:HB1	20:V:106:GLU:OE2	2.18	0.44
28:p:51:ALA:O	41:G:26:U:O2'	2.32	0.44
30:s:17:GLU:OE1	30:s:17:GLU:N	2.46	0.44
30:s:66:GLU:O	39:E:522:A:O2'	2.26	0.44
31:t:95:TRP:NE1	31:t:157:ALA:O	2.51	0.44
34:w:56:VAL:HG12	34:w:56:VAL:O	2.18	0.44
39:E:1624:G:O2'	39:E:1643:A:N1	2.40	0.44
11:q:13:ARG:NH1	41:G:25:G:N7	2.59	0.44
10:k:104:ARG:NH2	39:E:314:U:OP1	2.47	0.43
39:E:1055:A:N3	40:F:81:U:O2'	2.49	0.43
39:E:1303:A:O4'	39:E:2885:C:O2'	2.36	0.43
31:t:257:GLU:OE1	31:t:257:GLU:N	2.51	0.43
39:E:649:A:O2'	39:E:2870:C:OP1	2.34	0.43
39:E:2274:U:OP2	39:E:2311:G:N1	2.51	0.43
27:o:3:ARG:HH22	27:o:98:ILE:HG22	1.83	0.43
27:o:167:SER:OG	27:o:168:LYS:O	2.18	0.43
19:U:16:VAL:HG12	39:E:2320:A:H2	1.82	0.43
28:p:312:VAL:HG21	39:E:610:G:C8	2.53	0.43
11:q:13:ARG:NE	41:G:24:G:OP2	2.46	0.43
27:o:149:GLU:OE2	27:o:153:ARG:NH1	2.51	0.43
41:G:70:G:HO2'	41:G:71:A:P	2.42	0.43
12:M:9:ILE:HD12	12:M:51:ILE:HG23	2.00	0.43
20:V:189:ASP:OD1	20:V:190:VAL:N	2.51	0.43
30:s:35:VAL:HG22	37:C:233:GLU:OE1	2.18	0.43
18:S:98:THR:HG22	18:S:98:THR:O	2.18	0.43
32:u:120:LYS:NZ	39:E:1093:A:OP1	2.33	0.43
24:l:151:ILE:O	24:l:155:ALA:HB3	2.19	0.43
10:k:75:PHE:O	10:k:80:VAL:HG23	2.18	0.43
1:b:240:ASN:OD1	1:b:241:LYS:N	2.52	0.42
1:b:140:VAL:HG11	17:R:2:GLY:O	2.20	0.42
8:I:115:ARG:NH2	8:I:119:THR:OG1	2.50	0.42
25:m:66:ARG:NH2	39:E:785:G:OP1	2.49	0.42
30:s:108:GLN:NE2	39:E:1322:U:O2	2.43	0.42
24:l:297:SER:HA	24:l:300:ARG:HE	1.84	0.42
35:A:96:VAL:HG12	35:A:98:VAL:HG13	2.01	0.42
39:E:1179:A:O2'	39:E:1327:C:O2'	2.10	0.42
18:S:26:ARG:NH1	39:E:938:C:OP2	2.53	0.42
33:v:71:VAL:HG13	33:v:81:VAL:CG1	2.49	0.42
15:P:78:ILE:HG22	15:P:78:ILE:O	2.19	0.42
1:b:48:ARG:NH2	39:E:2586:G:O2'	2.45	0.42
20:V:19:LEU:O	20:V:23:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:l:113:GLU:HB3	24:l:176:ALA:HB2	2.01	0.42
37:C:33:ARG:NH2	39:E:595:G:OP1	2.51	0.42
3:d:37:THR:HG22	17:R:5:LYS:HZ1	1.82	0.42
28:p:195:ARG:NH1	39:E:340:C:OP2	2.43	0.42
39:E:2872:A:C8	43:E:3401:TEL:H572	2.55	0.42
5:f:27:LYS:NZ	5:f:28:ILE:O	2.53	0.42
8:I:105:VAL:HG11	8:I:126:LEU:HD22	2.01	0.42
28:p:203:ARG:NH2	28:p:226:GLU:OE1	2.52	0.42
39:E:763:G:O2'	39:E:764:U:OP1	2.27	0.42
4:e:5:GLN:NE2	4:e:7:GLU:OE1	2.51	0.42
4:e:41:ILE:HD11	4:e:67:ALA:HB1	2.02	0.42
23:y:41:LEU:HD12	23:y:150:VAL:HG11	2.02	0.42
23:y:47:TYR:OH	23:y:57:ALA:O	2.30	0.42
39:E:1671:C:OP1	42:H:60:LYS:NZ	2.53	0.42
39:E:2816:G:O2'	39:E:2869:U:OP2	2.34	0.42
14:O:36:HIS:O	14:O:38:PHE:N	2.49	0.41
37:C:236:ILE:O	37:C:240:VAL:HG23	2.20	0.41
39:E:1002:A:N1	39:E:1050:U:O2'	2.49	0.41
4:e:69:ARG:NH1	39:E:3114:A:OP1	2.52	0.41
41:G:69:U:H2'	41:G:70:G:O4'	2.20	0.41
25:m:71:LEU:HD12	25:m:99:THR:HG22	2.02	0.41
43:E:3401:TEL:H19	43:E:3401:TEL:H332	1.54	0.41
41:G:40:A:OP2	41:G:103:G:N1	2.45	0.41
8:I:121:LYS:NZ	39:E:1522:U:OP2	2.47	0.41
17:R:148:TYR:O	17:R:151:ILE:HG22	2.19	0.41
26:n:48:ASP:OD1	26:n:50:ARG:NE	2.53	0.41
17:R:72:LYS:NZ	39:E:2167:A:OP1	2.54	0.41
22:x:241:ARG:O	39:E:2240:G:N2	2.48	0.41
28:p:208:VAL:HG11	28:p:250:TRP:CZ3	2.55	0.41
39:E:1724:U:H1'	39:E:1725:C:C6	2.55	0.41
9:j:40:GLN:HE21	9:j:55:VAL:HG13	1.85	0.41
24:l:54:THR:OG1	24:l:360:ASP:O	2.38	0.41
36:B:36:LYS:NZ	39:E:1595:U:OP2	2.49	0.41
39:E:2746:A:H2'	39:E:2747:A:O4'	2.21	0.41
10:k:109:PHE:O	10:k:113:VAL:HG23	2.21	0.41
13:N:55:ARG:NH2	13:N:76:ALA:O	2.53	0.41
18:S:8:THR:HG21	39:E:662:U:OP1	2.21	0.41
22:x:116:VAL:HG13	22:x:126:LEU:HB2	2.03	0.41
24:l:92:TYR:HB2	24:l:157:VAL:HG13	2.03	0.41
28:p:257:LYS:O	28:p:261:VAL:HG23	2.21	0.41
29:r:15:LYS:NZ	39:E:426:G:OP1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:s:112:ALA:O	30:s:115:ARG:NH1	2.54	0.41
31:t:146:LEU:HD22	31:t:163:LEU:HD12	2.02	0.41
32:u:147:VAL:O	32:u:149:GLN:NE2	2.54	0.41
39:E:2680:A:O2'	39:E:2681:U:OP1	2.26	0.41
13:N:20:VAL:HG12	13:N:68:LEU:O	2.21	0.41
22:x:230:VAL:HG21	39:E:2424:A:N1	2.36	0.41
30:s:13:ARG:NH2	30:s:50:LYS:O	2.54	0.41
41:G:85:G:HO2'	41:G:86:U:P	2.38	0.41
1:b:161:GLU:OE2	17:R:26:ARG:NH1	2.48	0.40
16:Q:8:ARG:N	16:Q:22:GLN:OE1	2.54	0.40
31:t:261:THR:N	31:t:264:GLN:OE1	2.53	0.40
34:w:100:THR:HG23	34:w:100:THR:O	2.21	0.40
8:I:105:VAL:HG12	8:I:126:LEU:HD22	2.04	0.40
24:l:25:ILE:HG22	24:l:334:ARG:HH12	1.86	0.40
24:l:46:PHE:CE2	24:l:81:THR:HG23	2.56	0.40
24:l:284:ARG:HB3	24:l:323:MET:HB3	2.02	0.40
28:p:47:ARG:NH2	28:p:109:TRP:O	2.45	0.40
28:p:229:ASN:OD1	28:p:230:VAL:N	2.54	0.40
35:A:77:ARG:NH2	39:E:3273:A:OP2	2.54	0.40
8:I:68:THR:HG22	8:I:141:TYR:CD2	2.56	0.40
17:R:46:ASP:OD1	17:R:47:LYS:N	2.51	0.40
39:E:3177:G:O2'	39:E:3179:U:OP1	2.37	0.40
39:E:3332:U:H2'	39:E:3333:G:O4'	2.21	0.40
10:k:75:PHE:O	10:k:79:GLU:HB2	2.21	0.40
14:O:13:VAL:O	14:O:20:GLY:N	2.52	0.40
37:C:232:ARG:O	37:C:234:GLU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
39	E	3158/3396 (92%)	644 (20%)	70 (2%)
40	F	120/121 (99%)	17 (14%)	0
41	G	157/158 (99%)	37 (23%)	3 (1%)
All	All	3435/3675 (93%)	698 (20%)	73 (2%)

All (698) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
39	E	11	A
39	E	13	A
39	E	14	U
39	E	30	G
39	E	40	A
39	E	41	G
39	E	43	A
39	E	45	A
39	E	49	A
39	E	59	G
39	E	60	A
39	E	65	A
39	E	66	A
39	E	73	C
39	E	86	G
39	E	87	U
39	E	92	G
39	E	111	C
39	E	115	A
39	E	116	A
39	E	118	U
39	E	119	U
39	E	122	A
39	E	128	G
39	E	134	U
39	E	135	C
39	E	147	U
39	E	148	G
39	E	154	U
39	E	155	G
39	E	156	G
39	E	157	A
39	E	164	A

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Mol	Chain	Res	Type
39	E	165	A
39	E	166	C
39	E	187	A
39	E	188	U
39	E	189	G
39	E	190	U
39	E	191	U
39	E	200	C
39	E	206	G
39	E	210	U
39	E	213	A
39	E	218	G
39	E	219	A
39	E	220	G
39	E	221	A
39	E	222	A
39	E	234	G
39	E	240	U
39	E	241	G
39	E	244	G
39	E	245	U
39	E	248	U
39	E	249	U
39	E	250	U
39	E	251	G
39	E	252	U
39	E	269	G
39	E	270	U
39	E	283	G
39	E	286	U
39	E	295	A
39	E	298	U
39	E	305	U
39	E	311	C
39	E	323	A
39	E	329	U
39	E	330	G
39	E	338	A
39	E	346	C
39	E	351	A
39	E	352	A
39	E	375	A

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Mol	Chain	Res	Type
39	E	376	G
39	E	385	A
39	E	390	G
39	E	398	A
39	E	399	A
39	E	401	U
39	E	402	A
39	E	403	C
39	E	421	G
39	E	422	A
39	E	429	U
39	E	440	A
39	E	495	G
39	E	521	A
39	E	532	A
39	E	535	G
39	E	544	C
39	E	545	U
39	E	546	C
39	E	547	G
39	E	548	G
39	E	550	A
39	E	555	U
39	E	557	A
39	E	559	A
39	E	569	A
39	E	578	A
39	E	579	G
39	E	592	A
39	E	597	G
39	E	608	A
39	E	609	G
39	E	611	A
39	E	612	U
39	E	620	U
39	E	621	A
39	E	634	C
39	E	636	C
39	E	637	C
39	E	649	A
39	E	660	A
39	E	667	C

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Mol	Chain	Res	Type
39	E	677	A
39	E	678	G
39	E	681	U
39	E	685	G
39	E	690	A
39	E	691	A
39	E	692	A
39	E	705	A
39	E	712	G
39	E	715	A
39	E	716	A
39	E	719	U
39	E	720	A
39	E	760	G
39	E	763	G
39	E	764	U
39	E	765	C
39	E	766	U
39	E	767	U
39	E	768	C
39	E	771	A
39	E	777	U
39	E	780	A
39	E	781	G
39	E	784	A
39	E	785	G
39	E	786	A
39	E	799	G
39	E	800	G
39	E	806	A
39	E	817	A
39	E	830	A
39	E	832	G
39	E	849	C
39	E	861	C
39	E	874	U
39	E	879	U
39	E	885	U
39	E	895	A
39	E	907	G
39	E	908	G
39	E	914	A

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Mol	Chain	Res	Type
39	E	916	G
39	E	917	A
39	E	923	C
39	E	926	A
39	E	934	G
39	E	937	G
39	E	939	U
39	E	944	C
39	E	959	C
39	E	960	U
39	E	974	G
39	E	977	C
39	E	980	A
39	E	981	U
39	E	991	G
39	E	994	G
39	E	1001	G
39	E	1010	G
39	E	1015	U
39	E	1016	C
39	E	1017	C
39	E	1018	G
39	E	1028	U
39	E	1029	G
39	E	1047	A
39	E	1049	C
39	E	1064	A
39	E	1065	A
39	E	1072	G
39	E	1075	A
39	E	1081	U
39	E	1082	U
39	E	1083	G
39	E	1087	G
39	E	1093	A
39	E	1096	U
39	E	1097	G
39	E	1098	A
39	E	1103	A
39	E	1104	G
39	E	1117	G
39	E	1131	G

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Mol	Chain	Res	Type
39	E	1144	U
39	E	1145	G
39	E	1153	A
39	E	1155	C
39	E	1159	A
39	E	1178	G
39	E	1180	A
39	E	1181	U
39	E	1186	G
39	E	1189	C
39	E	1191	U
39	E	1192	C
39	E	1197	A
39	E	1200	A
39	E	1201	C
39	E	1208	U
39	E	1217	A
39	E	1219	C
39	E	1221	A
39	E	1222	G
39	E	1225	A
39	E	1227	C
39	E	1230	G
39	E	1232	C
39	E	1235	U
39	E	1236	G
39	E	1237	G
39	E	1238	C
39	E	1239	C
39	E	1241	U
39	E	1242	G
39	E	1244	A
39	E	1245	A
39	E	1246	G
39	E	1248	C
39	E	1251	A
39	E	1252	A
39	E	1253	U
39	E	1254	C
39	E	1257	C
39	E	1258	U
39	E	1259	A

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Mol	Chain	Res	Type
39	E	1260	A
39	E	1262	G
39	E	1263	A
39	E	1264	G
39	E	1265	U
39	E	1266	G
39	E	1267	U
39	E	1268	G
39	E	1270	A
39	E	1271	A
39	E	1272	C
39	E	1273	A
39	E	1274	A
39	E	1276	U
39	E	1281	G
39	E	1282	G
39	E	1286	A
39	E	1294	A
39	E	1304	A
39	E	1305	U
39	E	1306	G
39	E	1307	G
39	E	1308	A
39	E	1309	U
39	E	1313	G
39	E	1316	C
39	E	1325	U
39	E	1330	A
39	E	1348	U
39	E	1350	A
39	E	1351	U
39	E	1355	A
39	E	1356	U
39	E	1357	G
39	E	1386	A
39	E	1392	G
39	E	1399	A
39	E	1400	G
39	E	1408	G
39	E	1418	A
39	E	1419	A
39	E	1421	G

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Mol	Chain	Res	Type
39	E	1431	G
39	E	1434	G
39	E	1437	C
39	E	1446	A
39	E	1450	G
39	E	1455	U
39	E	1456	A
39	E	1475	A
39	E	1482	A
39	E	1483	G
39	E	1488	G
39	E	1496	C
39	E	1503	A
39	E	1508	C
39	E	1523	U
39	E	1536	G
39	E	1554	U
39	E	1555	U
39	E	1556	C
39	E	1557	A
39	E	1559	A
39	E	1560	G
39	E	1563	C
39	E	1566	A
39	E	1567	U
39	E	1568	U
39	E	1569	U
39	E	1570	U
39	E	1571	A
39	E	1572	U
39	E	1576	G
39	E	1578	C
39	E	1580	A
39	E	1581	C
39	E	1582	C
39	E	1583	A
39	E	1587	A
39	E	1588	A
39	E	1589	A
39	E	1590	G
39	E	1593	A
39	E	1605	A

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Mol	Chain	Res	Type
39	E	1620	U
39	E	1629	U
39	E	1630	U
39	E	1631	C
39	E	1642	A
39	E	1643	A
39	E	1645	U
39	E	1646	G
39	E	1657	C
39	E	1658	G
39	E	1683	A
39	E	1696	A
39	E	1702	U
39	E	1704	A
39	E	1718	G
39	E	1724	U
39	E	1725	C
39	E	1730	G
39	E	1741	A
39	E	1750	A
39	E	1751	G
39	E	1752	A
39	E	1762	C
39	E	1763	U
39	E	1765	U
39	E	1770	G
39	E	1780	G
39	E	1797	A
39	E	1798	A
39	E	1813	A
39	E	1815	U
39	E	1816	A
39	E	1817	G
39	E	1818	U
39	E	1819	U
39	E	1820	U
39	E	1821	U
39	E	1839	A
39	E	1840	U
39	E	1841	A
39	E	1846	C
39	E	1849	C

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Mol	Chain	Res	Type
39	E	1850	A
39	E	1866	C
39	E	1868	G
39	E	1879	A
39	E	1880	U
39	E	1886	A
39	E	1893	A
39	E	1901	A
39	E	1906	G
39	E	1953	G
39	E	1954	G
39	E	1955	U
39	E	2100	A
39	E	2102	U
39	E	2111	G
39	E	2112	U
39	E	2113	A
39	E	2114	C
39	E	2121	G
39	E	2122	G
39	E	2131	A
39	E	2138	A
39	E	2139	A
39	E	2140	U
39	E	2144	A
39	E	2158	A
39	E	2164	A
39	E	2169	G
39	E	2170	U
39	E	2179	C
39	E	2188	A
39	E	2192	C
39	E	2205	U
39	E	2206	G
39	E	2209	U
39	E	2210	G
39	E	2225	U
39	E	2249	G
39	E	2256	A
39	E	2257	C
39	E	2272	G
39	E	2273	G

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Mol	Chain	Res	Type
39	E	2274	U
39	E	2281	A
39	E	2283	G
39	E	2284	C
39	E	2307	G
39	E	2310	U
39	E	2313	A
39	E	2314	U
39	E	2315	G
39	E	2334	U
39	E	2335	G
39	E	2336	U
39	E	2340	U
39	E	2373	A
39	E	2374	C
39	E	2375	G
39	E	2388	U
39	E	2391	G
39	E	2393	G
39	E	2394	G
39	E	2395	G
39	E	2397	A
39	E	2398	A
39	E	2402	A
39	E	2403	G
39	E	2404	A
39	E	2405	C
39	E	2411	U
39	E	2419	A
39	E	2435	G
39	E	2439	A
39	E	2443	A
39	E	2446	U
39	E	2451	G
39	E	2496	C
39	E	2501	U
39	E	2502	A
39	E	2503	G
39	E	2507	C
39	E	2513	U
39	E	2514	U
39	E	2515	A

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Mol	Chain	Res	Type
39	E	2522	G
39	E	2523	A
39	E	2524	A
39	E	2525	G
39	E	2531	C
39	E	2533	G
39	E	2537	U
39	E	2538	U
39	E	2540	A
39	E	2541	U
39	E	2542	U
39	E	2546	C
39	E	2549	G
39	E	2552	C
39	E	2554	A
39	E	2555	G
39	E	2559	U
39	E	2560	C
39	E	2571	U
39	E	2572	C
39	E	2573	G
39	E	2585	G
39	E	2593	A
39	E	2594	C
39	E	2606	G
39	E	2607	G
39	E	2621	G
39	E	2626	A
39	E	2627	C
39	E	2629	U
39	E	2651	G
39	E	2652	U
39	E	2656	A
39	E	2666	C
39	E	2674	A
39	E	2677	G
39	E	2679	A
39	E	2680	A
39	E	2681	U
39	E	2689	A
39	E	2691	A
39	E	2694	A

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Mol	Chain	Res	Type
39	E	2703	A
39	E	2704	A
39	E	2714	G
39	E	2728	G
39	E	2729	U
39	E	2740	A
39	E	2752	U
39	E	2753	G
39	E	2762	A
39	E	2772	C
39	E	2773	C
39	E	2777	G
39	E	2796	G
39	E	2800	G
39	E	2801	A
39	E	2802	A
39	E	2803	A
39	E	2804	A
39	E	2810	C
39	E	2814	G
39	E	2817	A
39	E	2833	A
39	E	2834	G
39	E	2842	U
39	E	2844	C
39	E	2845	A
39	E	2867	C
39	E	2870	C
39	E	2872	A
39	E	2874	G
39	E	2875	U
39	E	2887	A
39	E	2888	U
39	E	2889	C
39	E	2898	G
39	E	2914	G
39	E	2917	G
39	E	2922	G
39	E	2923	U
39	E	2933	A
39	E	2935	U
39	E	2936	A

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Mol	Chain	Res	Type
39	E	2938	G
39	E	2941	A
39	E	2942	C
39	E	2947	G
39	E	2951	G
39	E	2954	U
39	E	2968	G
39	E	2971	A
39	E	2972	G
39	E	2977	G
39	E	2978	U
39	E	2983	C
39	E	2990	G
39	E	2996	U
39	E	2997	G
39	E	3004	C
39	E	3011	A
39	E	3012	A
39	E	3022	G
39	E	3023	U
39	E	3040	A
39	E	3049	A
39	E	3056	U
39	E	3057	U
39	E	3058	U
39	E	3059	G
39	E	3078	U
39	E	3086	A
39	E	3092	C
39	E	3117	C
39	E	3122	A
39	E	3130	A
39	E	3131	U
39	E	3142	A
39	E	3143	C
39	E	3152	U
39	E	3153	U
39	E	3154	C
39	E	3156	U
39	E	3157	U
39	E	3158	G
39	E	3170	A

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Mol	Chain	Res	Type
39	E	3172	A
39	E	3174	A
39	E	3175	U
39	E	3176	G
39	E	3179	U
39	E	3181	C
39	E	3186	A
39	E	3187	A
39	E	3197	G
39	E	3206	C
39	E	3207	U
39	E	3208	G
39	E	3209	A
39	E	3210	A
39	E	3212	C
39	E	3217	C
39	E	3218	A
39	E	3219	G
39	E	3220	G
39	E	3222	U
39	E	3224	G
39	E	3229	G
39	E	3235	C
39	E	3242	G
39	E	3243	A
39	E	3245	A
39	E	3246	G
39	E	3247	G
39	E	3253	G
39	E	3256	G
39	E	3259	U
39	E	3263	G
39	E	3270	U
39	E	3272	C
39	E	3273	A
39	E	3276	G
39	E	3277	U
39	E	3279	A
39	E	3285	C
39	E	3286	G
39	E	3289	G
39	E	3294	A

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Mol	Chain	Res	Type
39	E	3304	U
39	E	3313	U
39	E	3316	A
39	E	3318	G
39	E	3319	U
39	E	3320	A
39	E	3334	U
39	E	3335	A
39	E	3345	G
39	E	3347	A
39	E	3351	U
39	E	3352	U
39	E	3353	G
39	E	3354	U
39	E	3355	U
39	E	3356	G
39	E	3369	G
39	E	3378	C
39	E	3382	U
39	E	3383	G
39	E	3386	G
39	E	3390	G
39	E	3396	U
40	F	11	A
40	F	22	A
40	F	38	U
40	F	42	A
40	F	48	U
40	F	49	G
40	F	54	U
40	F	55	A
40	F	65	G
40	F	73	C
40	F	76	A
40	F	78	U
40	F	87	G
40	F	91	G
40	F	102	A
40	F	112	G
40	F	121	U
41	G	17	A
41	G	21	C

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Mol	Chain	Res	Type
41	G	22	U
41	G	23	U
41	G	24	G
41	G	25	G
41	G	34	U
41	G	35	C
41	G	49	G
41	G	51	G
41	G	52	A
41	G	53	A
41	G	59	A
41	G	60	U
41	G	62	C
41	G	63	G
41	G	81	U
41	G	82	U
41	G	83	C
41	G	84	C
41	G	85	G
41	G	86	U
41	G	87	G
41	G	90	U
41	G	91	C
41	G	95	G
41	G	97	A
41	G	104	A
41	G	106	C
41	G	112	U
41	G	113	U
41	G	125	U
41	G	126	A
41	G	144	G
41	G	148	G
41	G	151	C
41	G	152	G

All (73) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
39	E	86	G
39	E	154	U
39	E	155	G

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Mol	Chain	Res	Type
39	E	269	G
39	E	282	G
39	E	374	A
39	E	547	G
39	E	677	A
39	E	763	G
39	E	764	U
39	E	767	U
39	E	770	G
39	E	916	G
39	E	925	A
39	E	979	U
39	E	993	G
39	E	1064	A
39	E	1103	A
39	E	1144	U
39	E	1196	C
39	E	1199	C
39	E	1307	G
39	E	1355	A
39	E	1554	U
39	E	1558	A
39	E	1565	G
39	E	1580	A
39	E	1587	A
39	E	1695	U
39	E	1751	G
39	E	1820	U
39	E	1840	U
39	E	1900	A
39	E	2101	C
39	E	2112	U
39	E	2178	A
39	E	2208	A
39	E	2273	G
39	E	2283	G
39	E	2404	A
39	E	2434	U
39	E	2445	A
39	E	2495	C
39	E	2500	A
39	E	2501	U

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Mol	Chain	Res	Type
39	E	2513	U
39	E	2523	A
39	E	2541	U
39	E	2593	A
39	E	2665	U
39	E	2680	A
39	E	2728	G
39	E	2816	G
39	E	2950	G
39	E	3022	G
39	E	3055	U
39	E	3056	U
39	E	3057	U
39	E	3121	U
39	E	3156	U
39	E	3173	G
39	E	3175	U
39	E	3185	U
39	E	3219	G
39	E	3269	U
39	E	3293	U
39	E	3350	C
39	E	3352	U
39	E	3353	G
39	E	3382	U
41	G	16	G
41	G	85	G
41	G	125	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
43	TEL	E	3401	-	60,62,62	1.37	6 (10%)	78,92,92	1.94	17 (21%)

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
43	TEL	E	3401	-	1/1/19/19	16/73/108/108	0/4/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	E	3401	TEL	O5-C10	5.71	1.44	1.35
43	E	3401	TEL	O9-C15	4.85	1.45	1.34
43	E	3401	TEL	C40-N41	-3.62	1.34	1.38
43	E	3401	TEL	O5-C2	-2.93	1.43	1.47
43	E	3401	TEL	C36-N31	-2.70	1.33	1.37
43	E	3401	TEL	O9-C4	-2.06	1.43	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	E	3401	TEL	O9-C15-C21	9.34	120.15	110.93
43	E	3401	TEL	C17-C11-N6	-4.98	105.71	113.25
43	E	3401	TEL	N31-C37-N41	-4.01	109.15	112.35
43	E	3401	TEL	C4-O9-C15	-3.68	111.78	118.20
43	E	3401	TEL	C28-C24-C19	-3.48	110.43	116.10
43	E	3401	TEL	C36-N31-C37	3.18	108.27	106.71
43	E	3401	TEL	C43-C40-N41	3.08	126.72	122.45
43	E	3401	TEL	O9-C15-O20	-2.84	118.82	123.95
43	E	3401	TEL	O20-C15-C21	-2.79	121.03	124.65
43	E	3401	TEL	C8-C4-C2	-2.67	111.55	115.23
43	E	3401	TEL	C56-N52-C47	2.56	121.33	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	E	3401	TEL	C43-C40-C36	-2.53	125.78	129.65
43	E	3401	TEL	C1-C2-C3	-2.40	111.91	116.36
43	E	3401	TEL	C24-C19-C13	-2.38	109.33	113.32
43	E	3401	TEL	C55-C50-C54	-2.35	109.71	113.27
43	E	3401	TEL	C43-C47-N52	-2.17	120.27	123.50
43	E	3401	TEL	C42-O39-C34	-2.08	112.72	116.26

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
43	E	3401	TEL	C21

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	E	3401	TEL	O9-C4-C8-C14
43	E	3401	TEL	C23-C19-C24-C28
43	E	3401	TEL	C21-C15-O9-C4
43	E	3401	TEL	C2-C4-C8-C14
43	E	3401	TEL	C17-C22-C27-N31
43	E	3401	TEL	O20-C15-O9-C4
43	E	3401	TEL	N41-C40-C43-C47
43	E	3401	TEL	O20-C15-C21-C25
43	E	3401	TEL	O9-C15-C21-C25
43	E	3401	TEL	C36-C40-C43-C46
43	E	3401	TEL	N6-C3-C7-C12
43	E	3401	TEL	N41-C40-C43-C46
43	E	3401	TEL	C36-C40-C43-C47
43	E	3401	TEL	C13-C19-C24-C28
43	E	3401	TEL	C34-C28-O32-C38
43	E	3401	TEL	O32-C28-C34-C30

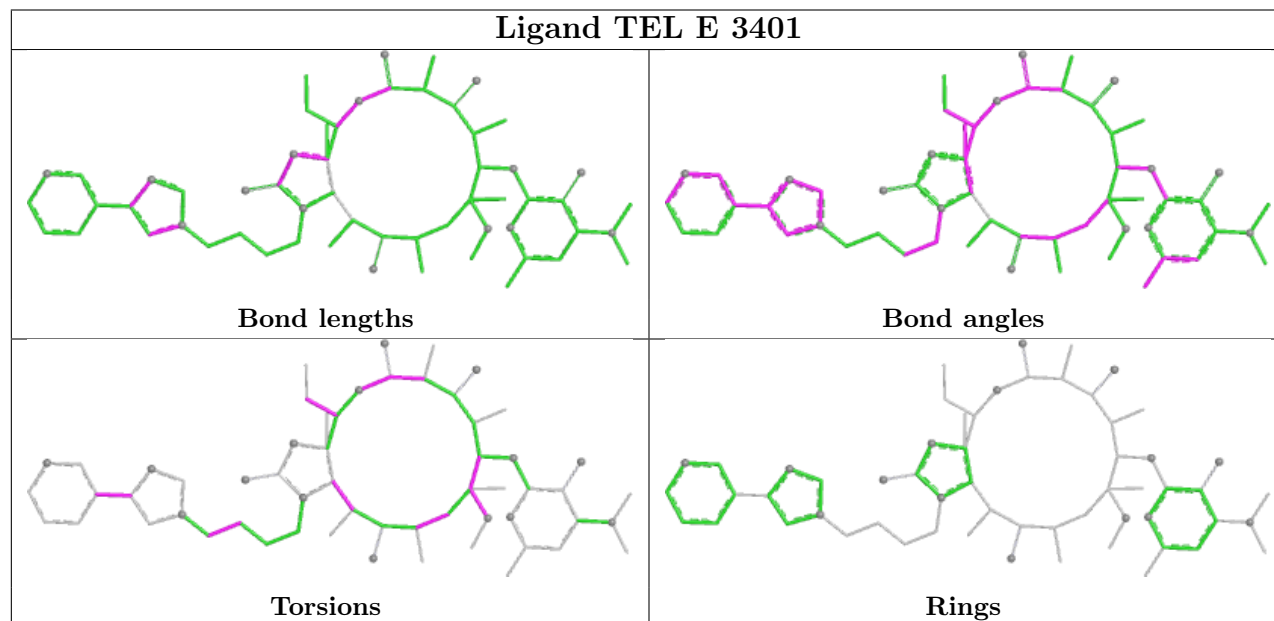
There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	E	3401	TEL	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

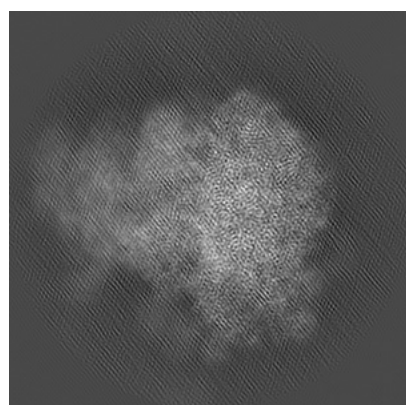
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11951. These allow visual inspection of the internal detail of the map and identification of artifacts.

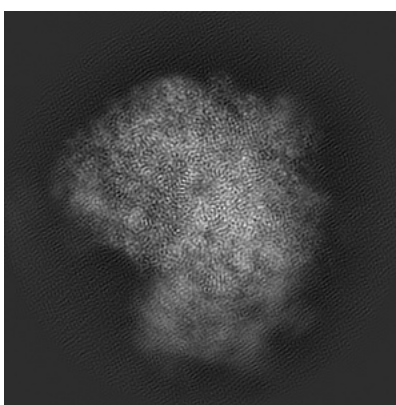
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

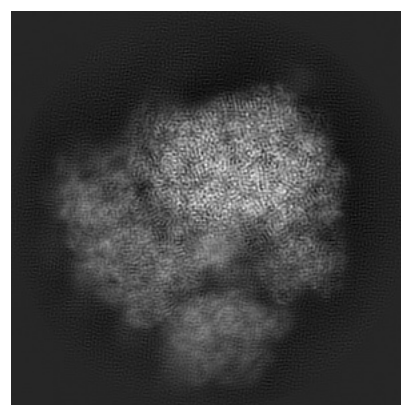
6.1.1 Primary map



X



Y

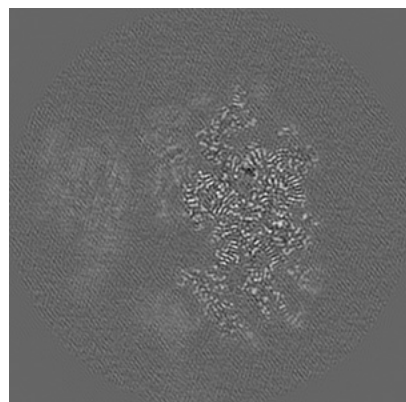


Z

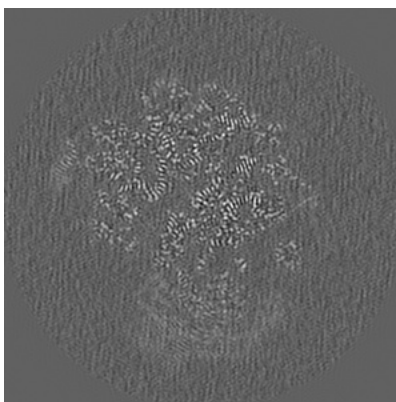
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

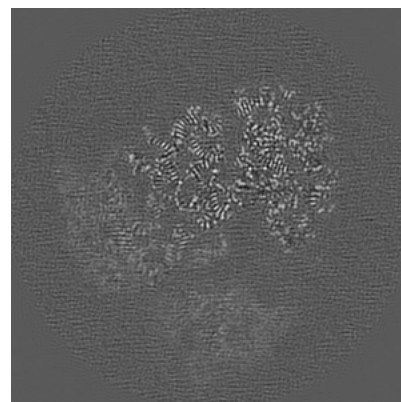
6.2.1 Primary map



X Index: 210



Y Index: 210

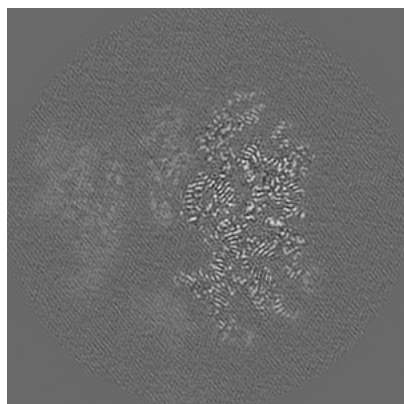


Z Index: 210

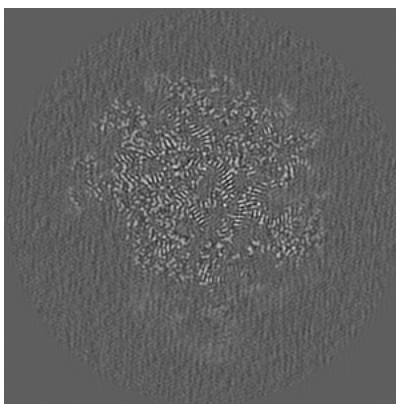
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

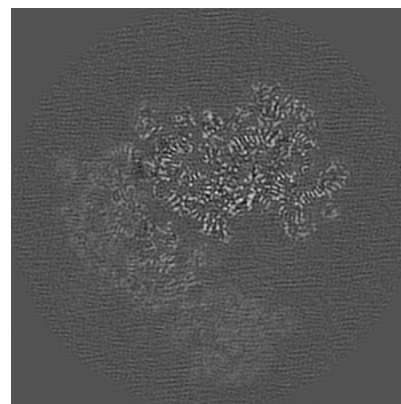
6.3.1 Primary map



X Index: 205



Y Index: 251

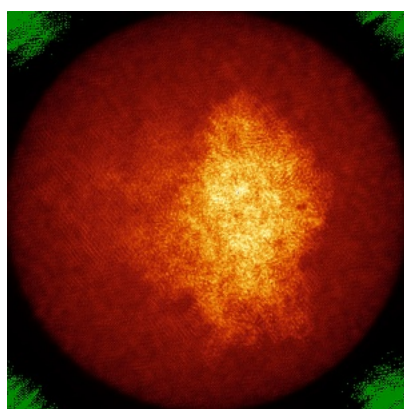


Z Index: 223

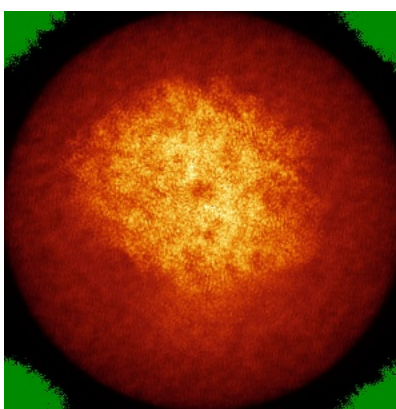
The images above show the largest variance slices of the map in three orthogonal directions.

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

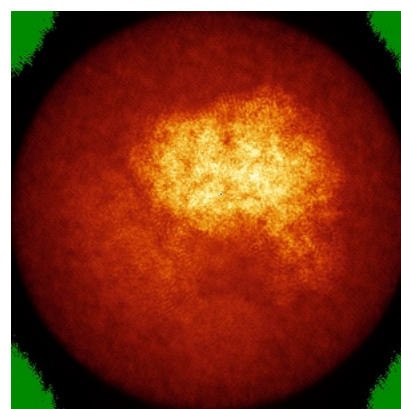
6.4.1 Primary map



X



Y

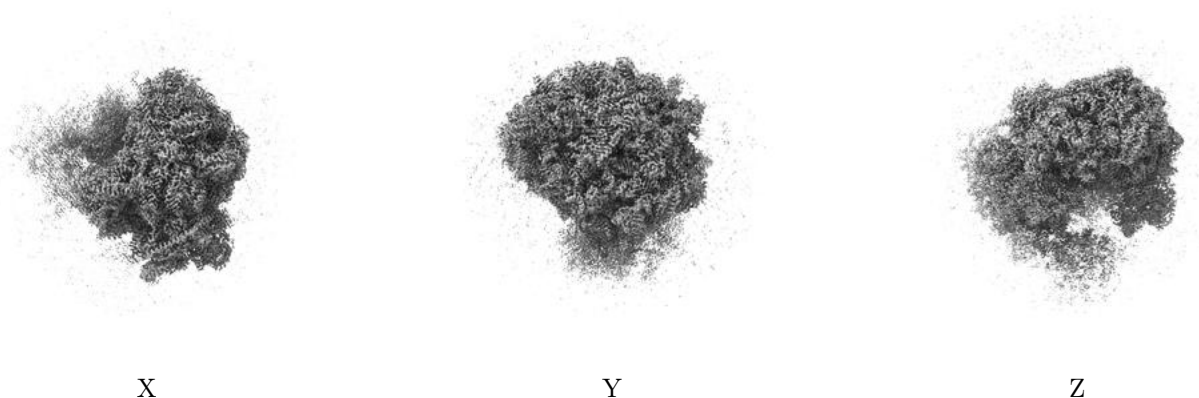


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

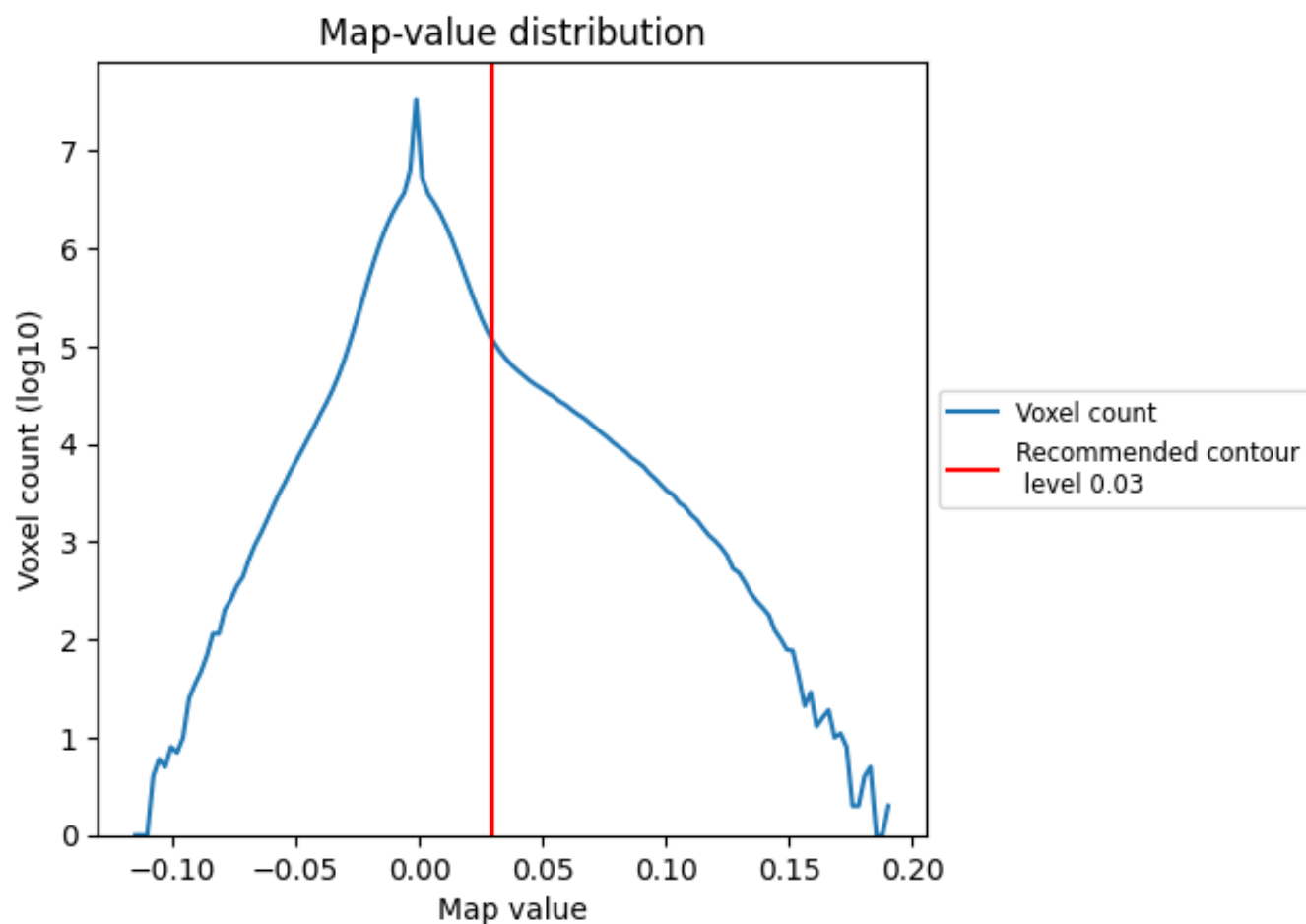
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

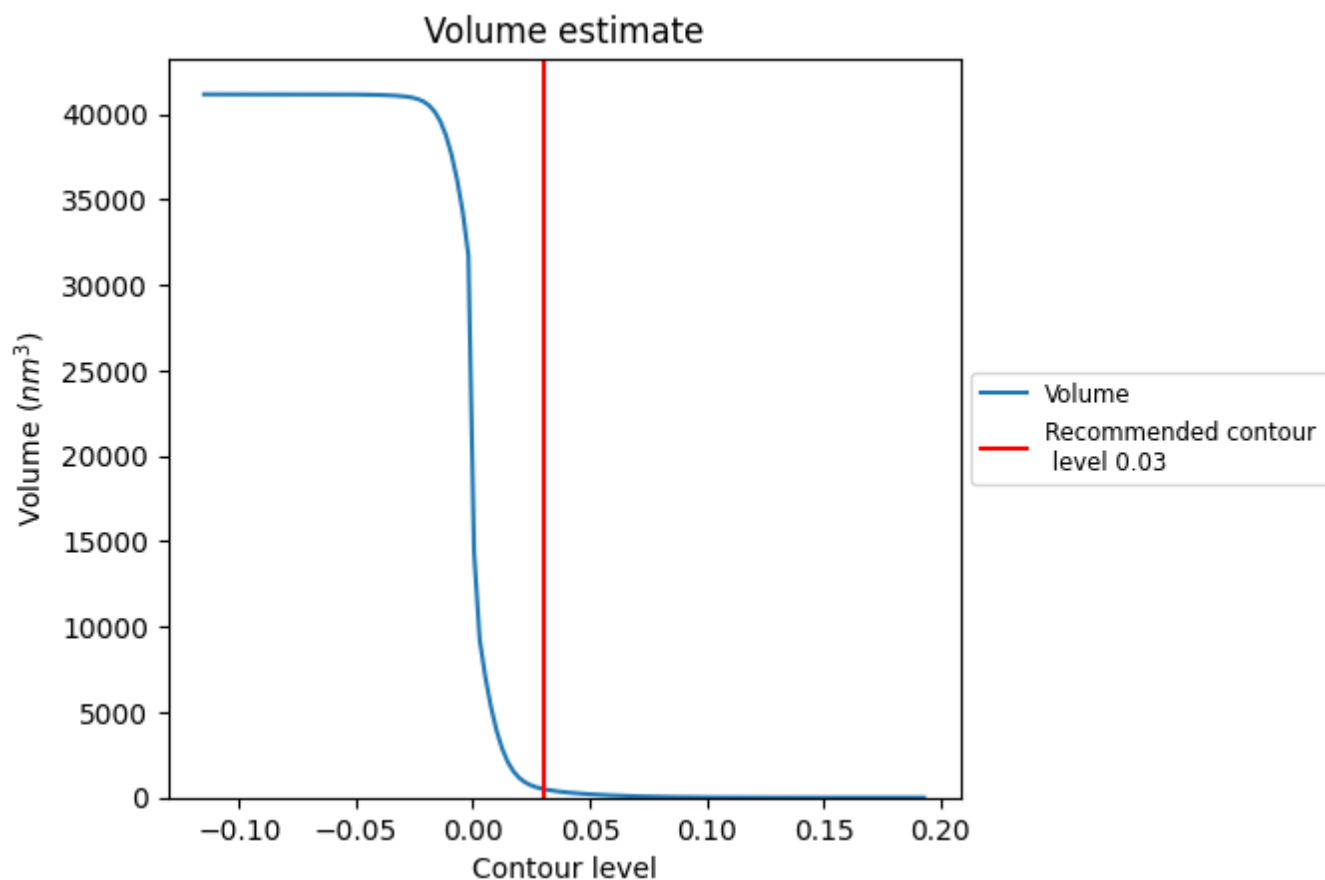
This section contains the results of statistical analysis of the map.

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.

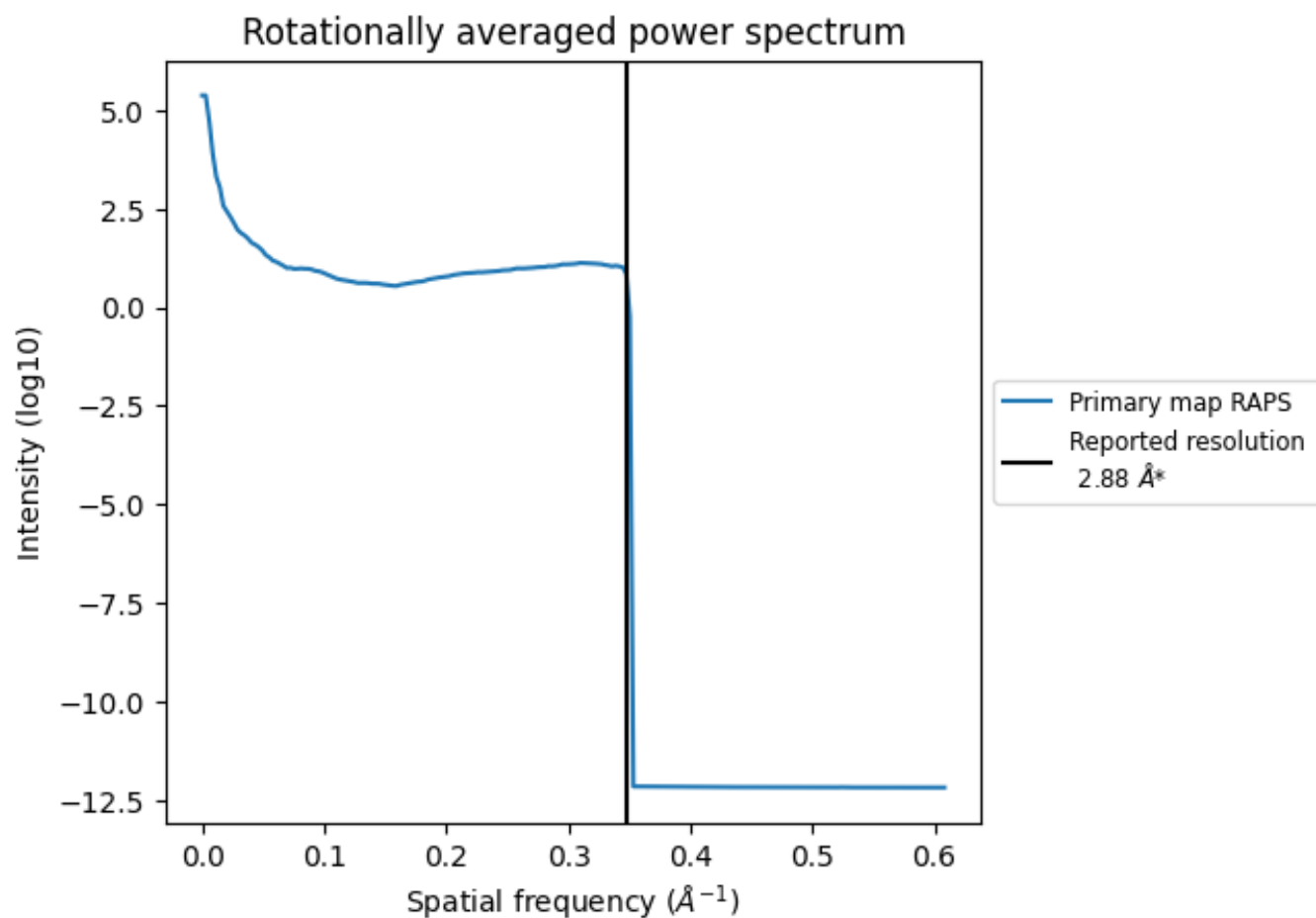
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 506 nm^3 ; this corresponds to an approximate mass of 457 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 ⓘ

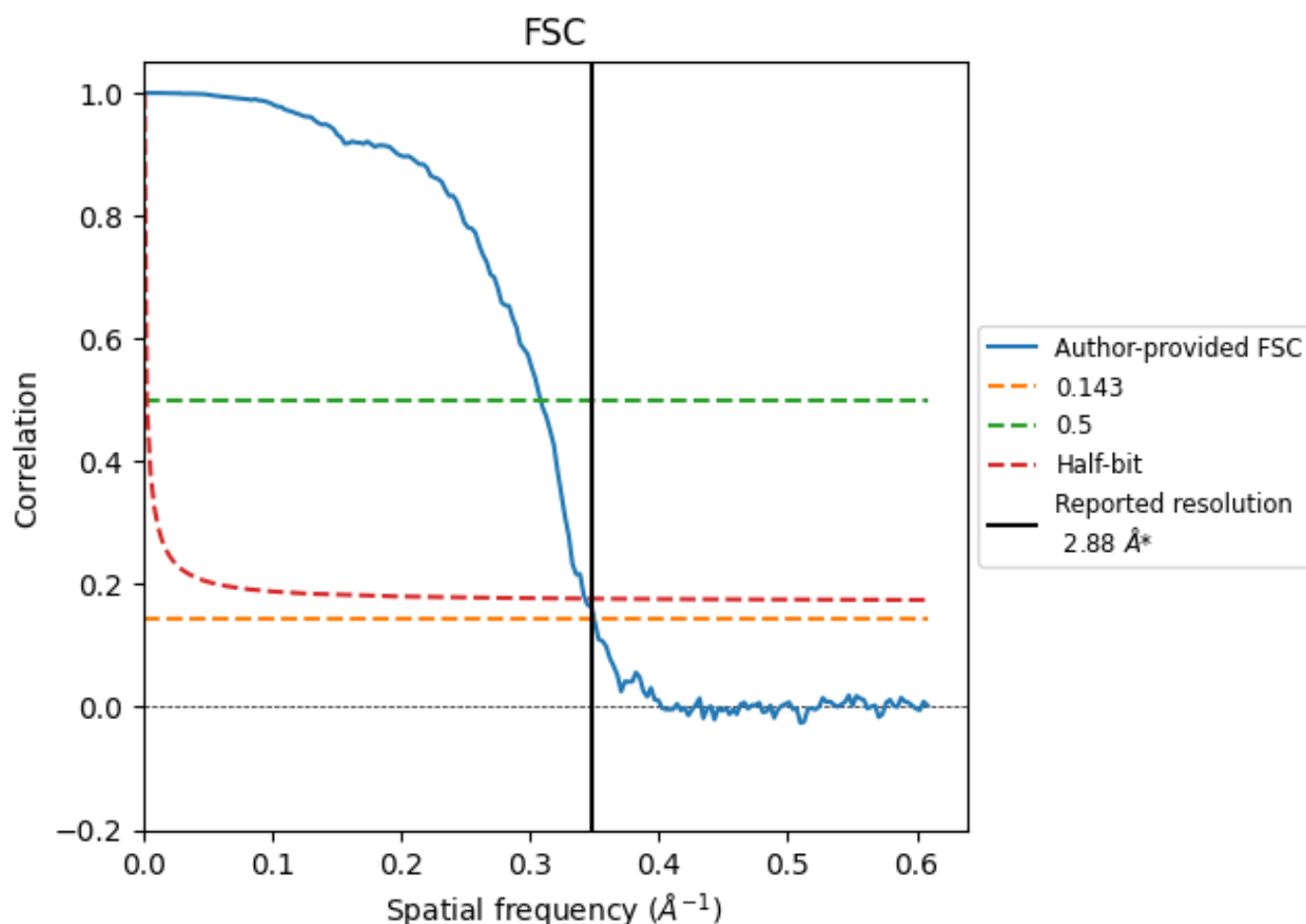


*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

8.2 Resolution estimates [i](#)

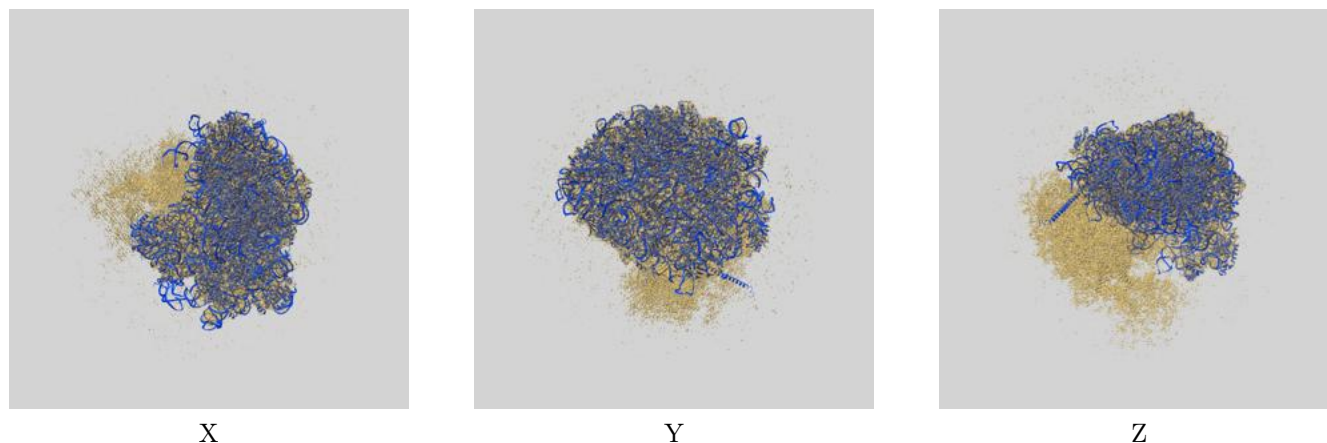
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.86	3.24	2.92
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

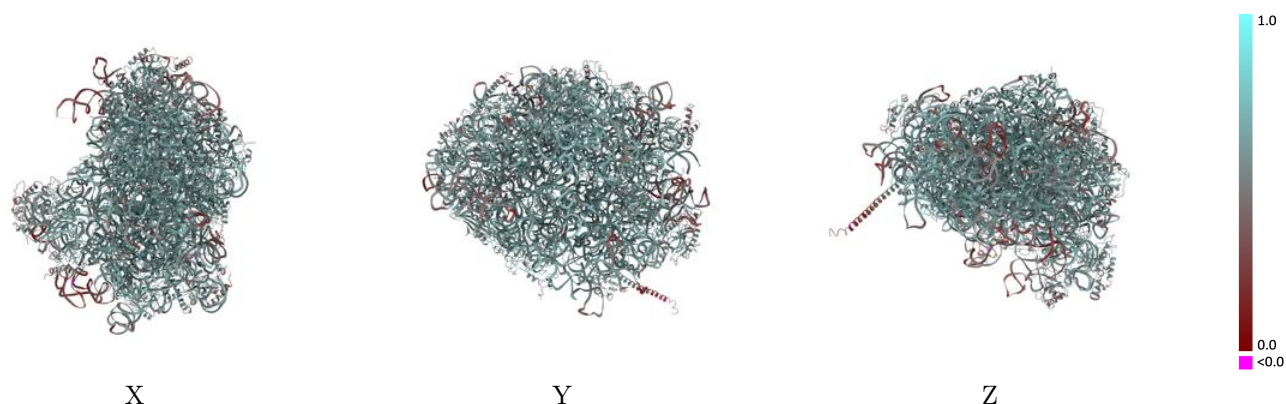
This section contains information regarding the fit between EMDB map EMD-11951 and PDB model 7AZY. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



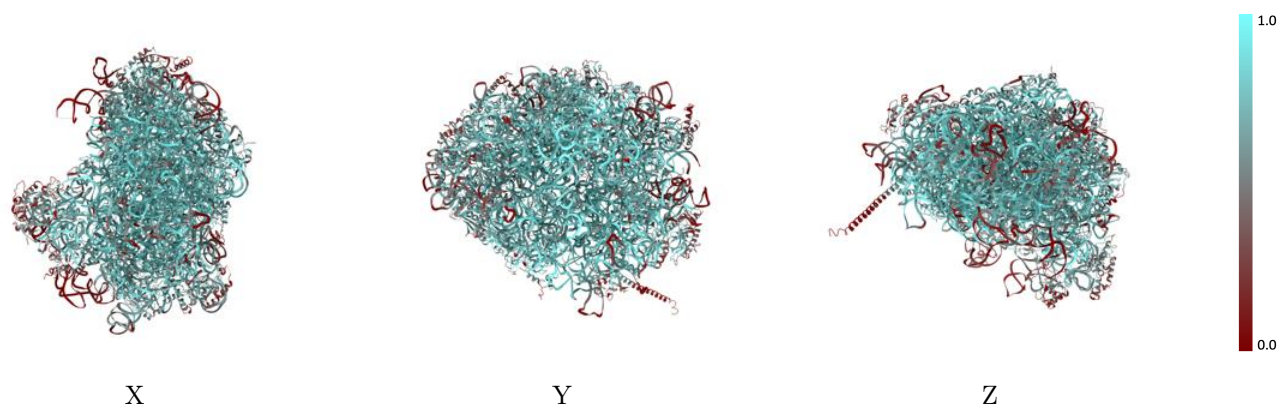
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



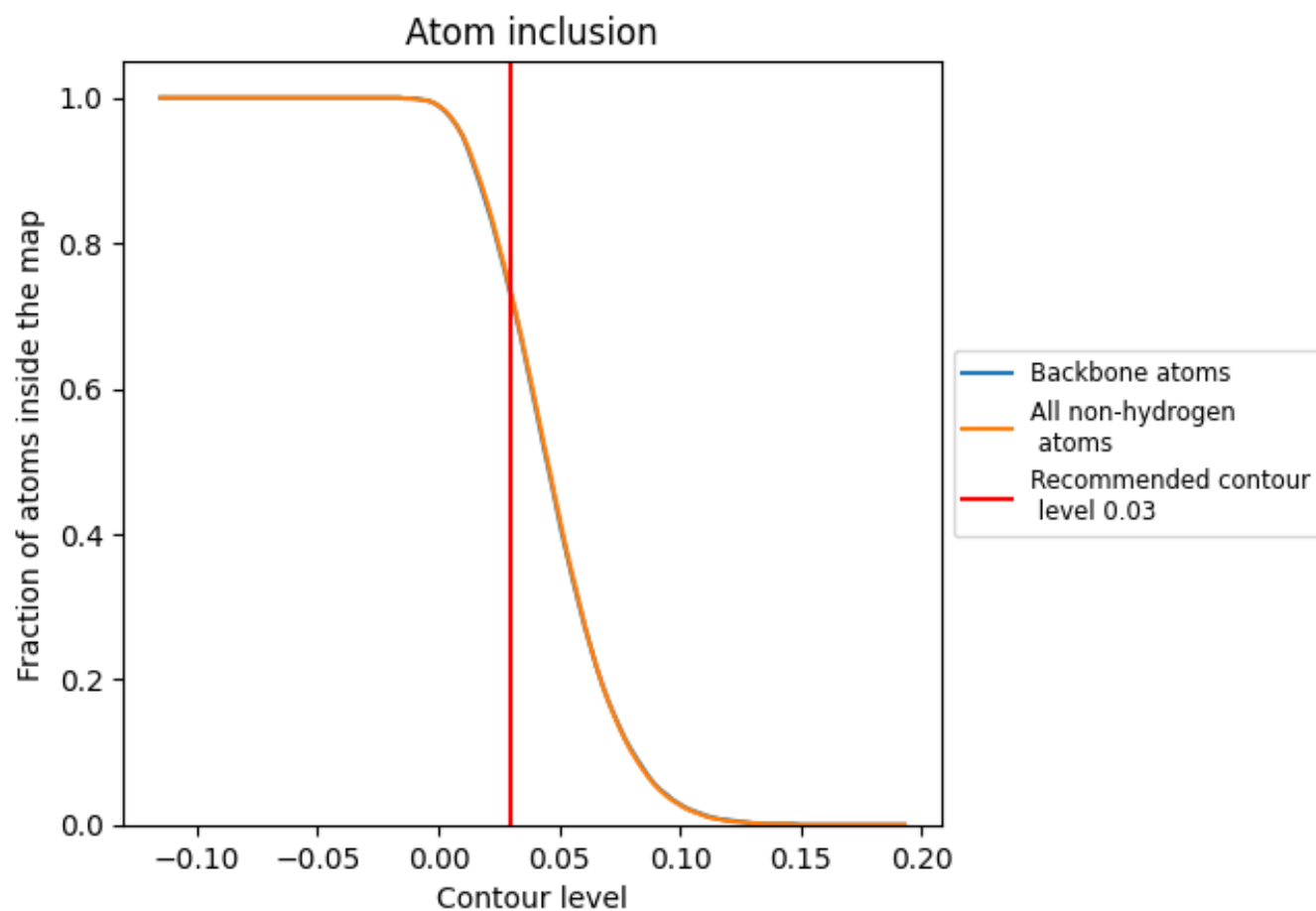
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 73% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7320	 0.5800
A	 0.5210	 0.5350
B	 0.7190	 0.5820
C	 0.7260	 0.5930
D	 0.6500	 0.5650
E	 0.7740	 0.5850
F	 0.7660	 0.5930
G	 0.8390	 0.6130
H	 0.5920	 0.5250
I	 0.7110	 0.5830
M	 0.7470	 0.5970
N	 0.6290	 0.5610
O	 0.5740	 0.5440
P	 0.6600	 0.5730
Q	 0.6260	 0.5710
R	 0.8120	 0.6110
S	 0.7490	 0.5970
U	 0.7060	 0.5900
V	 0.7400	 0.5990
W	 0.5840	 0.5330
b	 0.5620	 0.5290
c	 0.7250	 0.6010
d	 0.5690	 0.5320
e	 0.6070	 0.5660
f	 0.6890	 0.5710
g	 0.8180	 0.6080
h	 0.3750	 0.4820
j	 0.4560	 0.5110
k	 0.6700	 0.5740
l	 0.7520	 0.5950
m	 0.7400	 0.5970
n	 0.6750	 0.5720
o	 0.5850	 0.5350
p	 0.6980	 0.5810
q	 0.6930	 0.5750



Continued on next page...

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Chain	Atom inclusion	Q-score
r	 0.7480	 0.6060
s	 0.7090	 0.5840
t	 0.4800	 0.5300
u	 0.6990	 0.5770
v	 0.7790	 0.6200
w	 0.4400	 0.5160
x	 0.7920	 0.6130
y	 0.7030	 0.5760