



Full wwPDB EM Validation Report ⓘ

May 6, 2026 – 04:55 pm BST

PDB ID : 9TEX / pdb_00009tex
EMDB ID : EMD-55845
Title : Dal2 bound to the Escherichia coli 70S ribosome
Authors : Berger, M.J.; Safdari, H.A.; Wilson, D.N.
Deposited on : 2025-11-26
Resolution : 2.54 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:

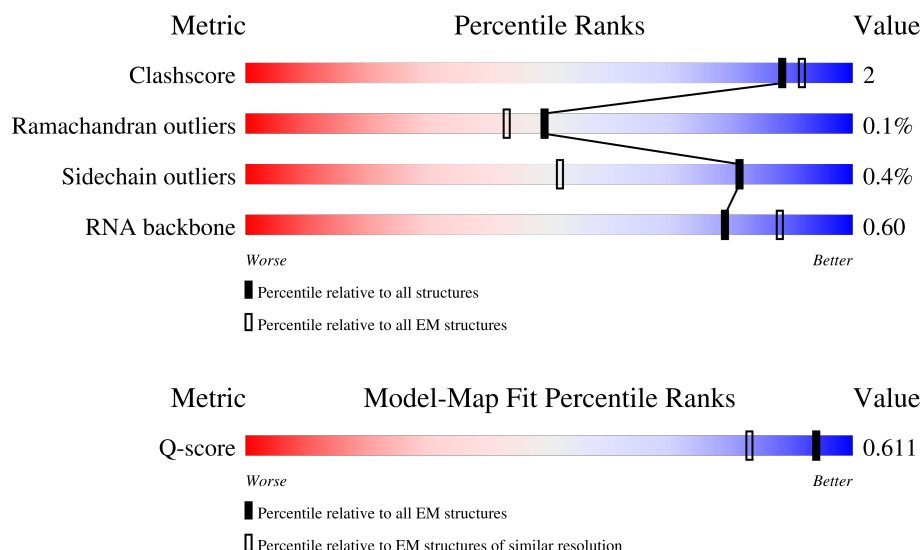
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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 2.54 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	7403 (2.04 - 3.04)

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	2904	 5% 78% 15% • 5%
2	A	1542	 7% 77% 20% • •
3	3	38	 8% 87% 13%

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Mol	Chain	Length	Quality of chain
4	4	70	
5	K	129	
6	L	124	
7	d	209	
8	l	136	
9	0	55	
10	1	46	
11	2	65	
12	B	241	
13	C	233	
14	D	206	
15	E	167	
16	F	135	
17	G	179	
18	H	130	
19	I	130	
20	J	103	
21	M	118	
22	N	101	
23	O	89	
24	P	82	
25	Q	84	
26	R	75	
27	S	92	
28	T	87	

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Mol	Chain	Length	Quality of chain
29	U	71	
30	X	6	
31	b	120	
32	c	273	
33	e	201	
34	f	179	
35	g	177	
36	h	149	
37	i	142	
38	j	123	
39	k	144	
40	m	127	
41	n	117	
42	o	115	
43	p	118	
44	q	103	
45	r	110	
46	s	100	
47	t	104	
48	u	94	
49	v	85	
50	w	78	
51	x	63	
52	y	59	
53	z	57	

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Mol	Chain	Length	Quality of chain
54	Z	77	<div><div><div></div><div></div><div></div></div><div>47%68%31%</div></div>
55	8	19	<div><div><div></div><div></div><div></div></div><div>16%58%11%32%</div></div>

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 139733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

- Molecule 2 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1519	Total	C	N	O	P	0	0
			32612	14552	5986	10555	1519		

- Molecule 3 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 4 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	59	Total	C	N	O	S	0	0
			472	293	89	84	6		

- Molecule 5 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	variant	UNP P0A7R9

- Molecule 6 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 8 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	82	MS6	MET	variant	UNP P0ADY7

- Molecule 9 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	0	49	Total	C	N	O	0	0
			405	261	74	70		

- Molecule 10 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 11 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 12 is a protein called 30S ribosomal protein S2.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 16 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 17 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	147	Total	C	N	O	S	0	0
			1164	728	222	210	4		

- Molecule 18 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 21 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 22 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 23 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 24 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 25 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	77	Total	C	N	O	S	0	0
			624	394	117	110	3		

- Molecule 26 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	R	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 27 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 28 is a protein called 30S ribosomal protein S20.

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

- Molecule 29 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 32 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 36 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 37 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 39 is a protein called 50S ribosomal protein L15.

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

- Molecule 40 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 42 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 43 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 44 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 47 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 48 is a protein called 50S ribosomal protein L25.

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

- Molecule 49 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	75	Total	C	N	O	S		
			569	353	113	102	1	0	0

- Molecule 50 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 51 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	62	Total	C	N	O	S		
			501	308	98	94	1	0	0

- Molecule 52 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	57	Total	C	N	O	S		
			444	278	86	78	2	0	0

- Molecule 53 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	z	56	Total	C	N	O	S		
			444	269	94	80	1	0	0

- Molecule 54 is a RNA chain called fMet-Initiator P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Z	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 55 is a protein called Dal2.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	8	13	Total	C	N	O	0	0
			115	76	22	17		

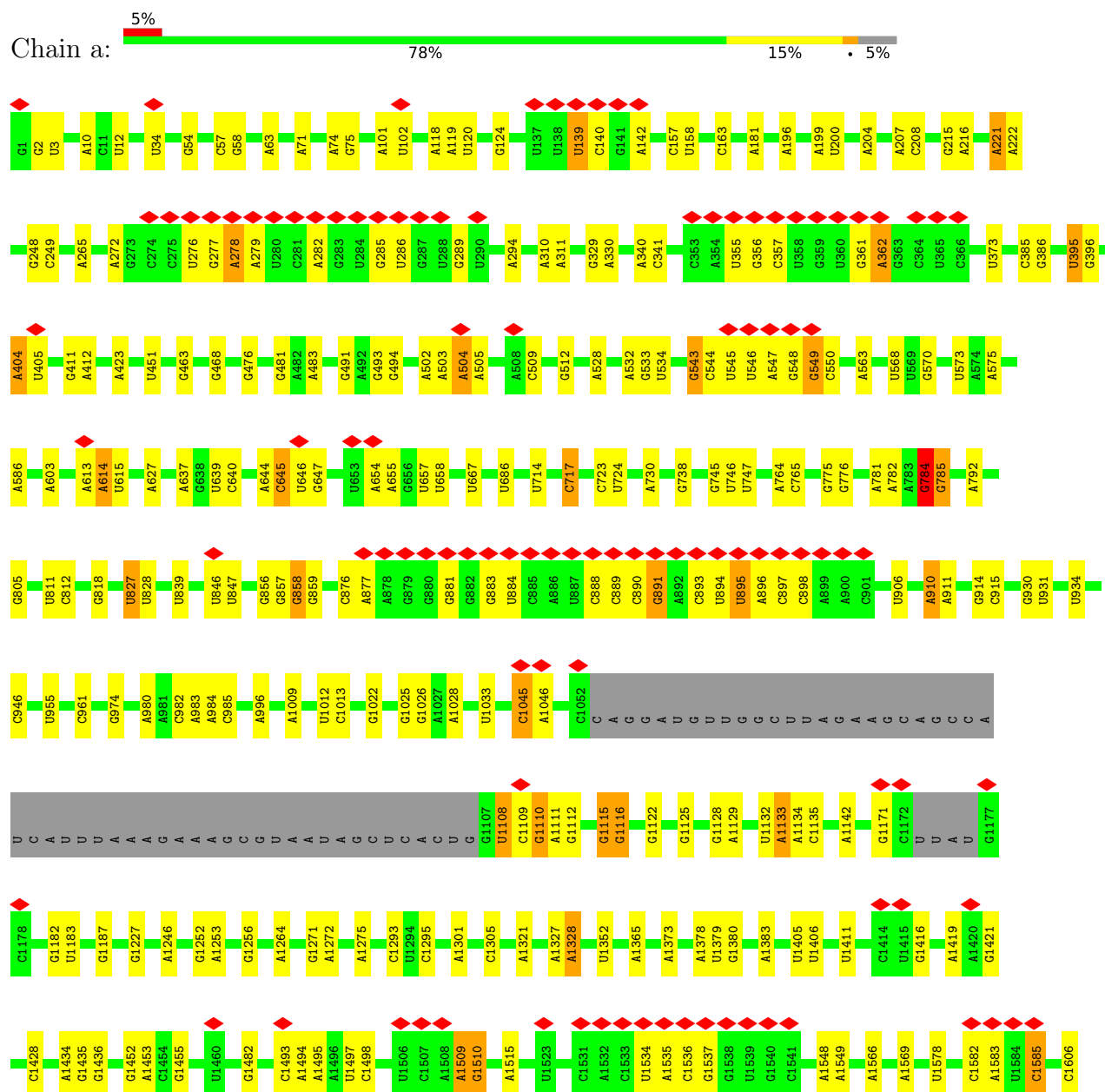
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

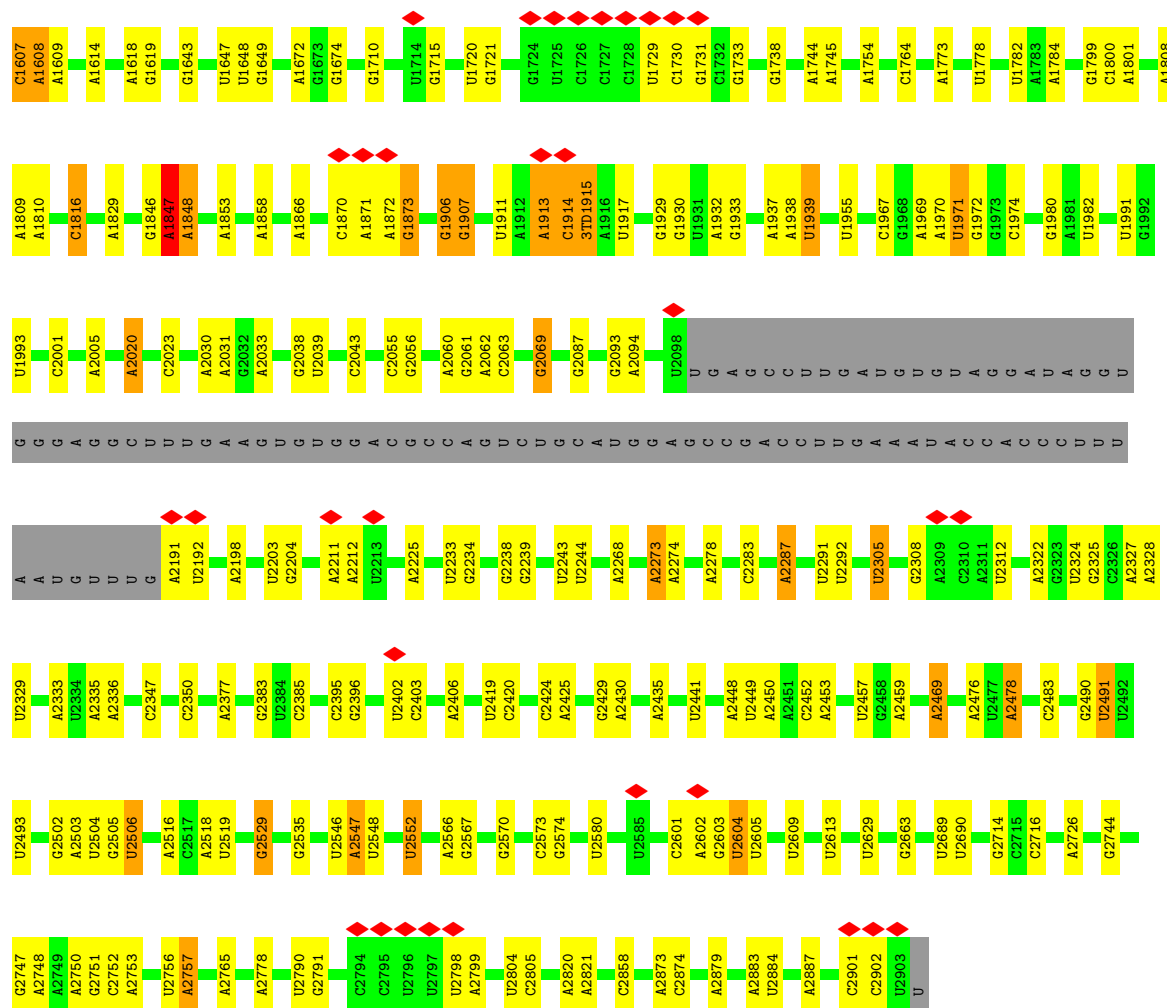
Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

3 Residue-property plots

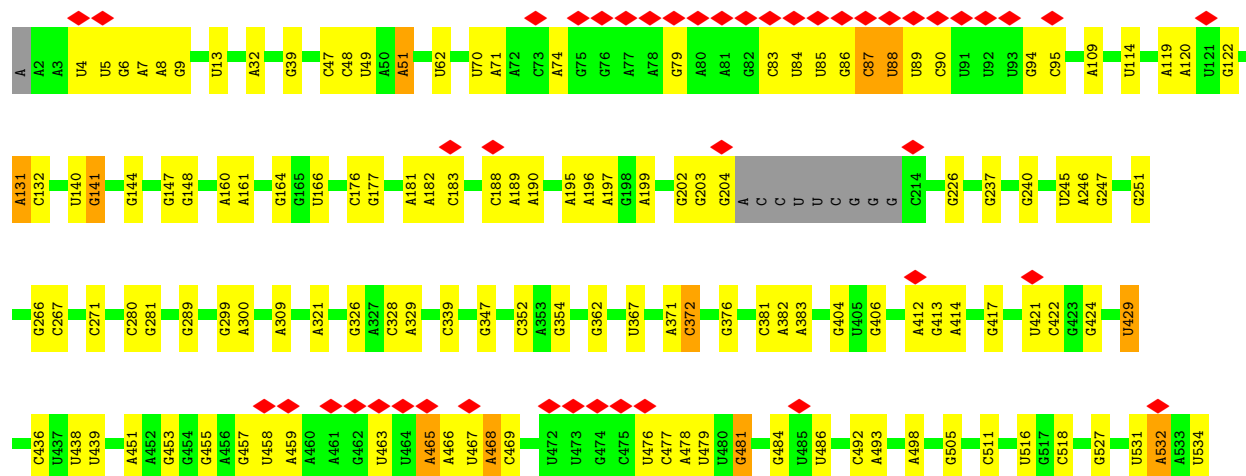
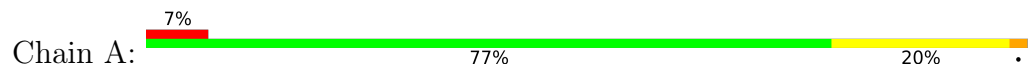
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

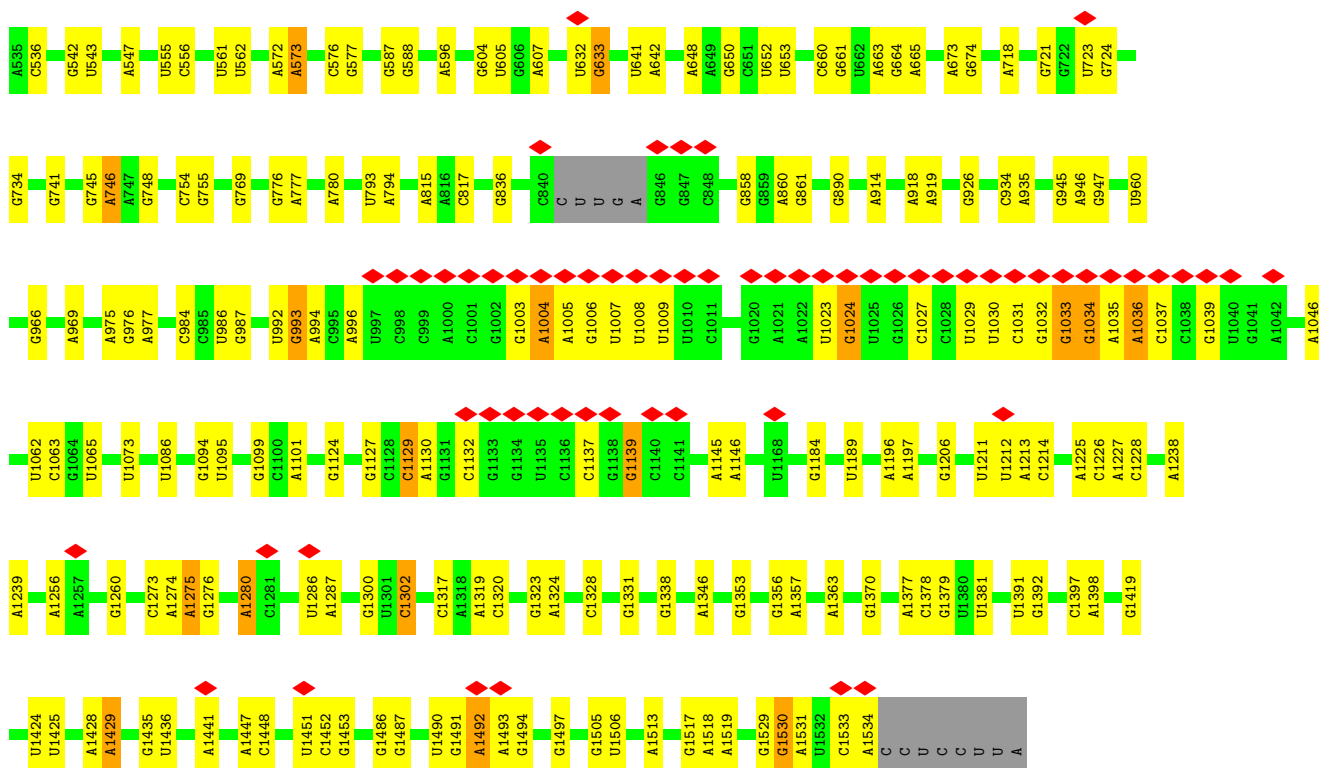
• Molecule 1: 23S rRNA



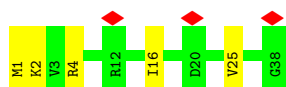
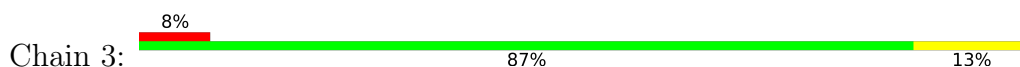


• Molecule 2: 16S rRNA

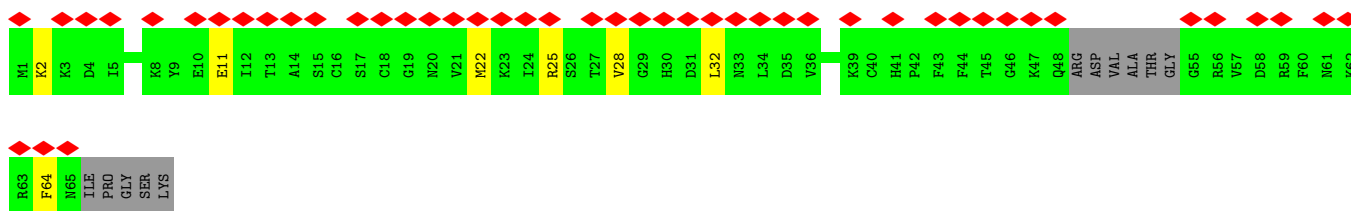
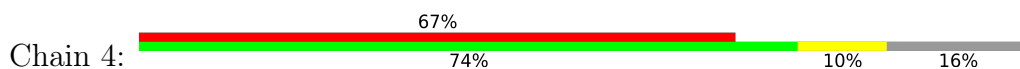




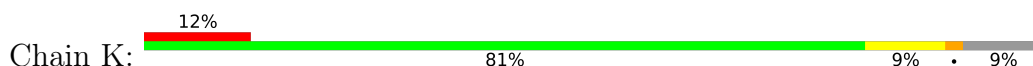
- Molecule 3: Large ribosomal subunit protein bL36A



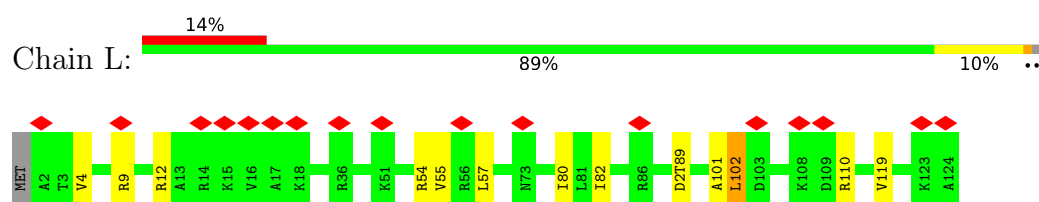
- Molecule 4: Large ribosomal subunit protein bL31A



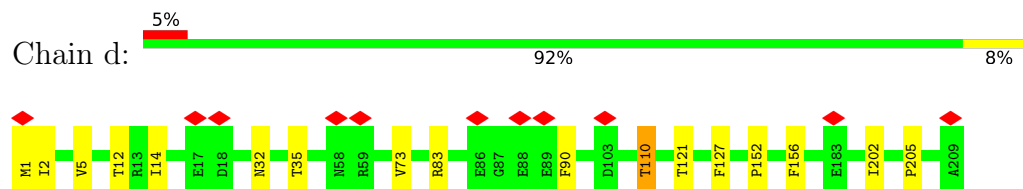
- Molecule 5: Small ribosomal subunit protein uS11



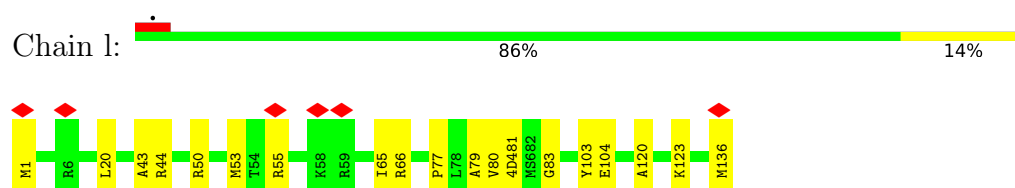
- Molecule 6: Small ribosomal subunit protein uS12



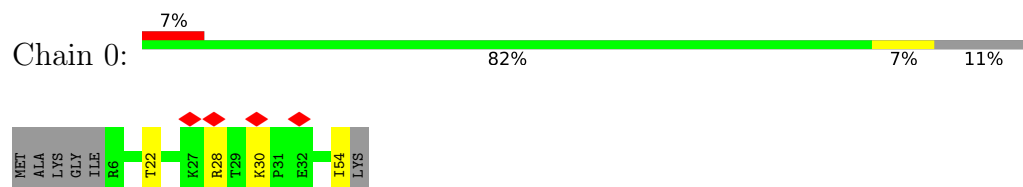
- Molecule 7: Large ribosomal subunit protein uL3



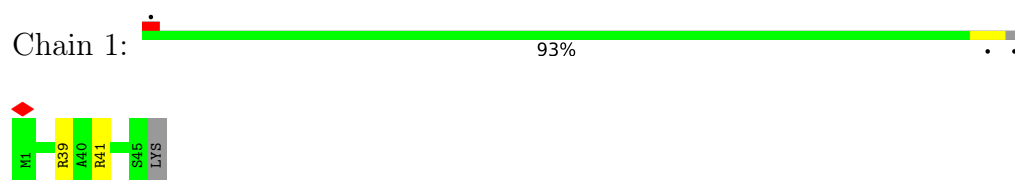
- Molecule 8: Large ribosomal subunit protein uL16



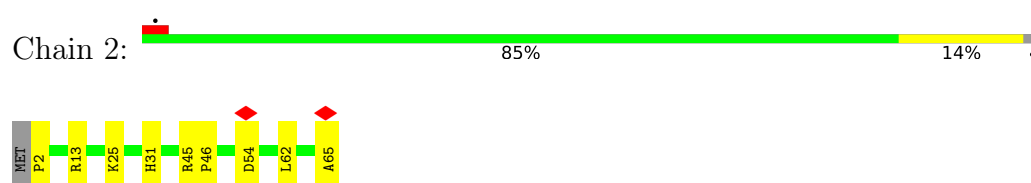
- Molecule 9: Large ribosomal subunit protein bL33



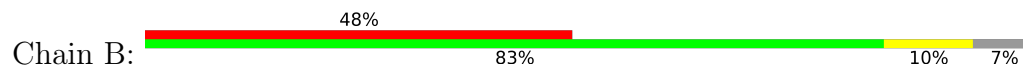
- Molecule 10: Large ribosomal subunit protein bL34

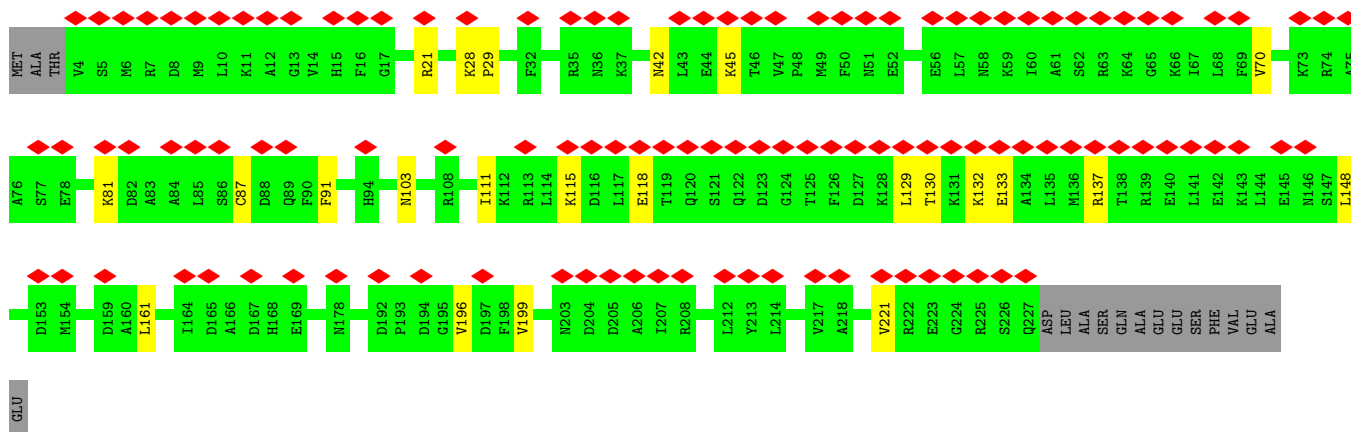


- Molecule 11: Large ribosomal subunit protein bL35

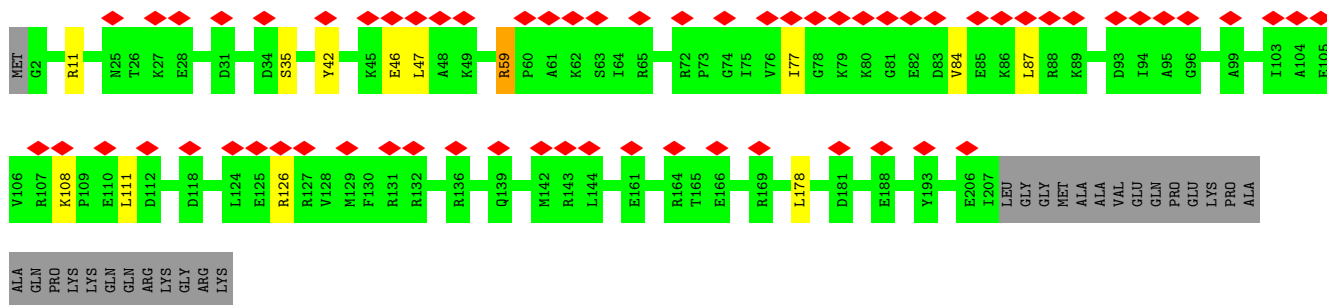
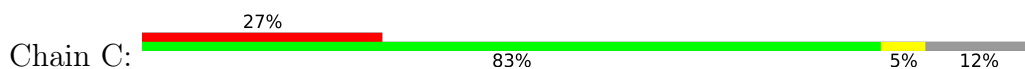


- Molecule 12: 30S ribosomal protein S2

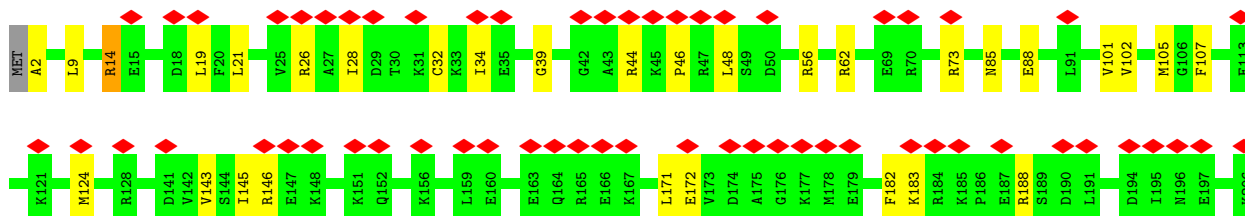
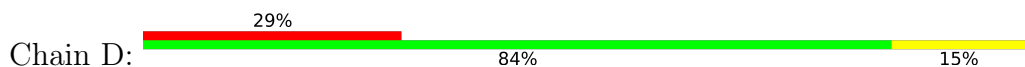




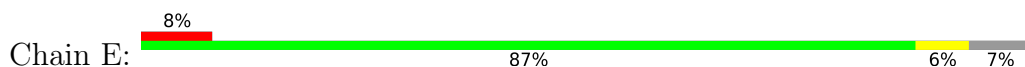
- Molecule 13: Small ribosomal subunit protein uS3



- Molecule 14: Small ribosomal subunit protein uS4

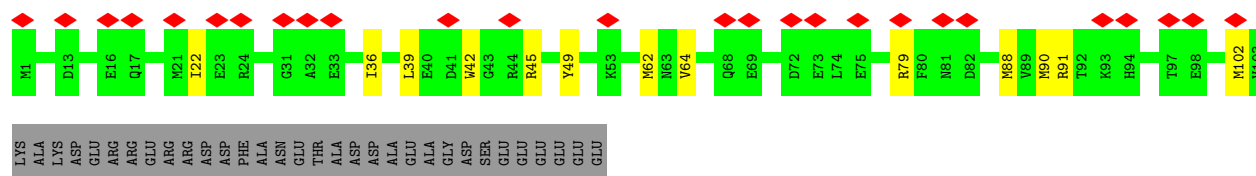


- Molecule 15: Small ribosomal subunit protein uS5



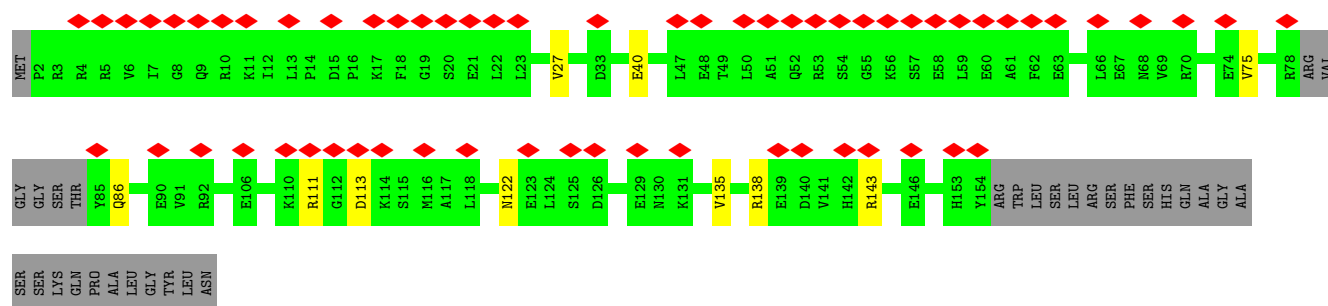
- Molecule 16: 30S ribosomal protein S6, fully modified isoform





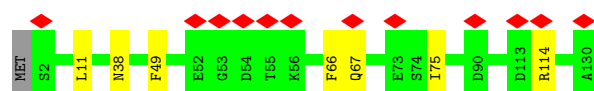
• Molecule 17: 30S ribosomal protein S7

Chain G:



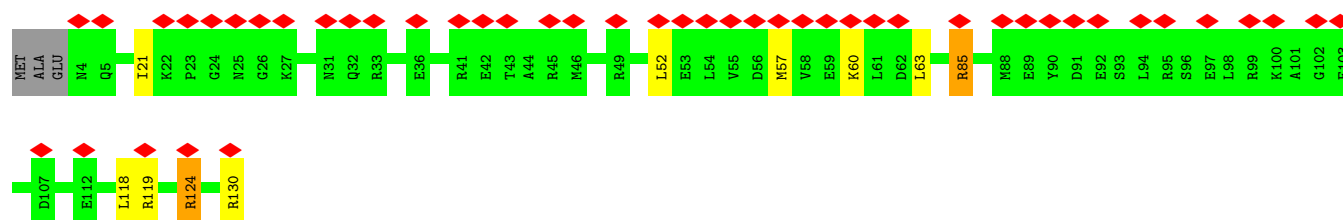
• Molecule 18: Small ribosomal subunit protein uS8

Chain H:



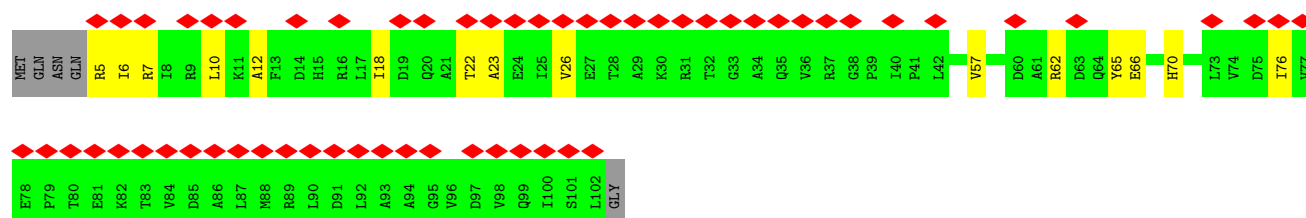
• Molecule 19: Small ribosomal subunit protein uS9

Chain I:

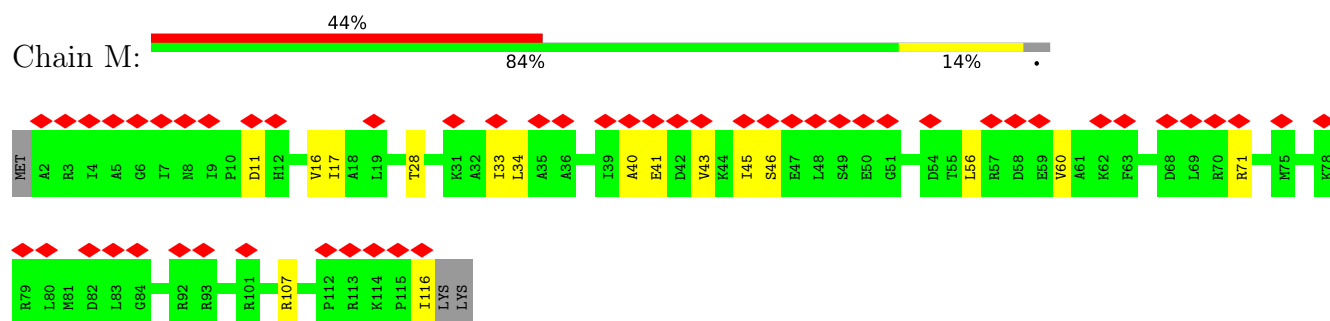


• Molecule 20: Small ribosomal subunit protein uS10

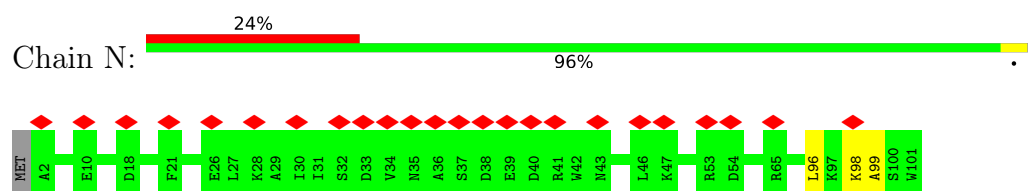
Chain J:



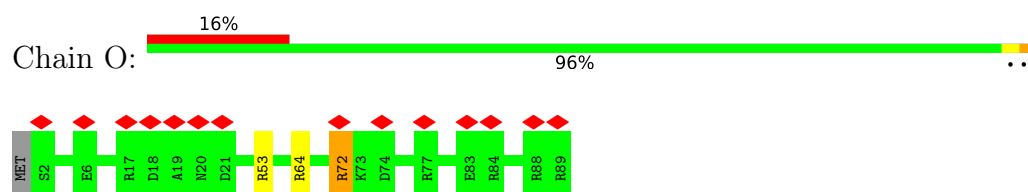
- Molecule 21: Small ribosomal subunit protein uS13



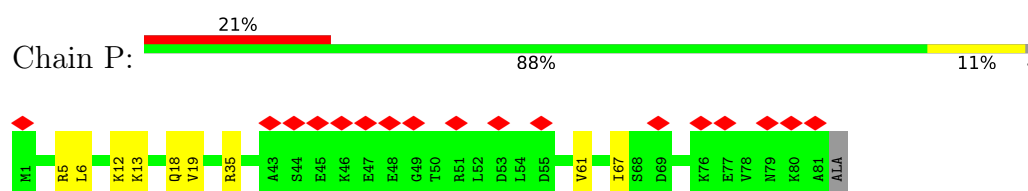
- Molecule 22: Small ribosomal subunit protein uS14



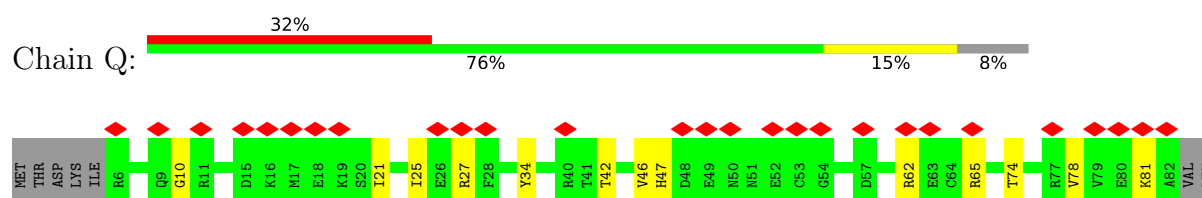
- Molecule 23: Small ribosomal subunit protein uS15



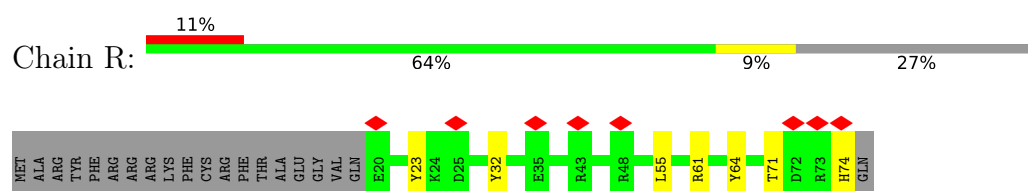
- Molecule 24: 30S ribosomal protein S16



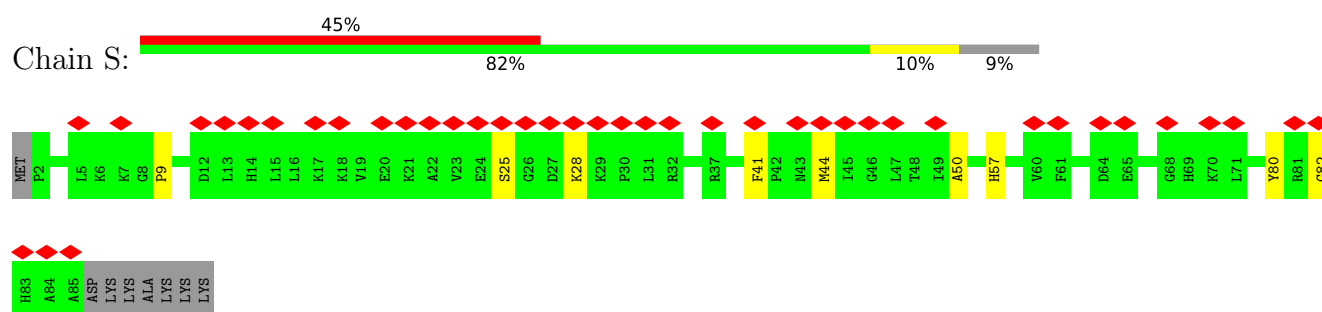
- Molecule 25: Small ribosomal subunit protein uS17



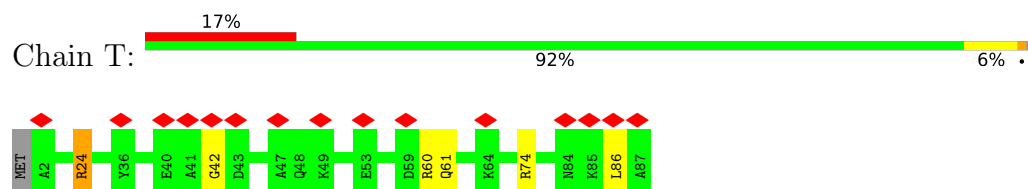
- Molecule 26: Small ribosomal subunit protein bS18



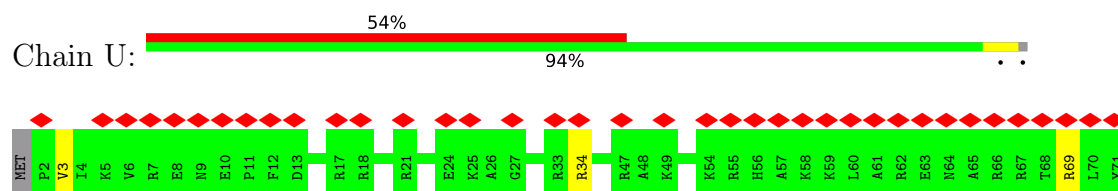
- Molecule 27: Small ribosomal subunit protein uS19



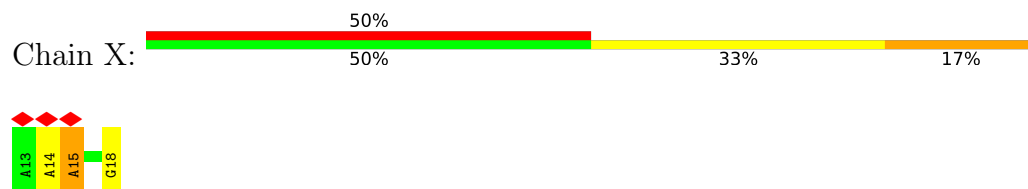
- Molecule 28: 30S ribosomal protein S20



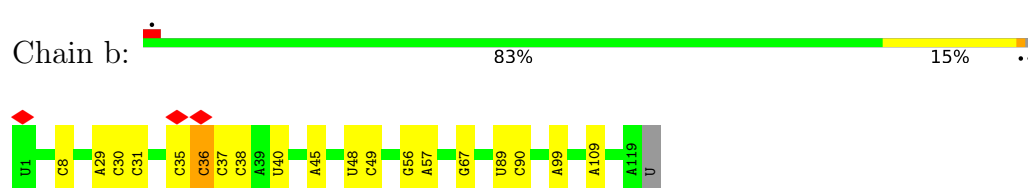
- Molecule 29: Small ribosomal subunit protein bS21



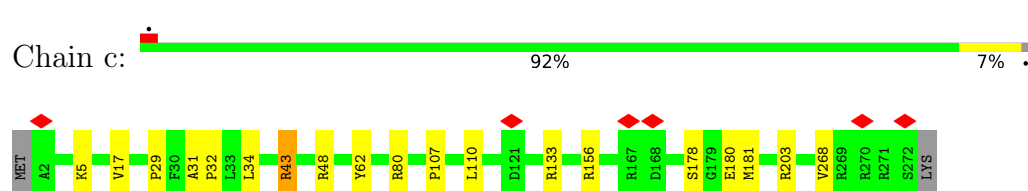
- Molecule 30: mRNA



- Molecule 31: 5S rRNA

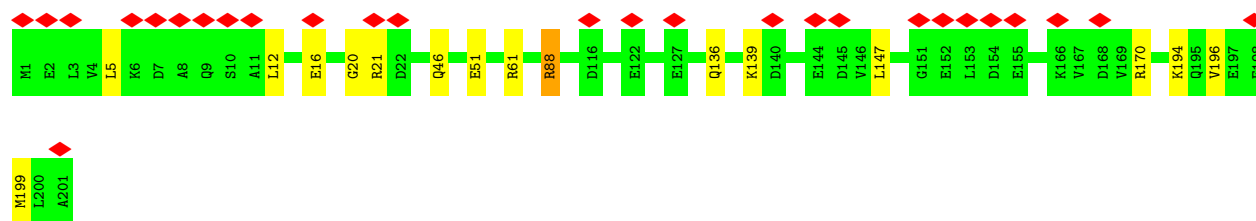


- Molecule 32: Large ribosomal subunit protein uL2

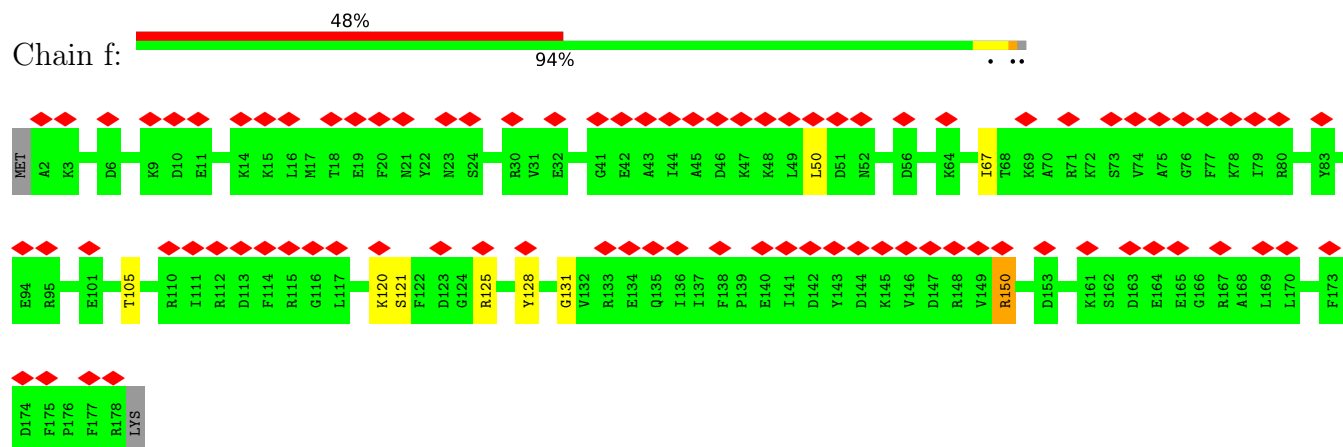


- Molecule 33: Large ribosomal subunit protein uL4

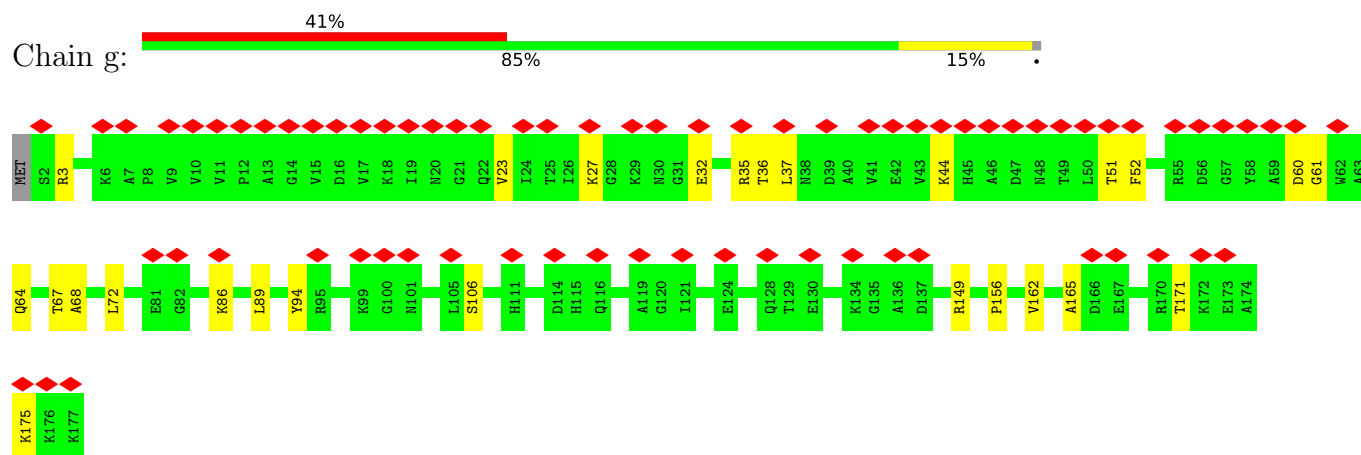




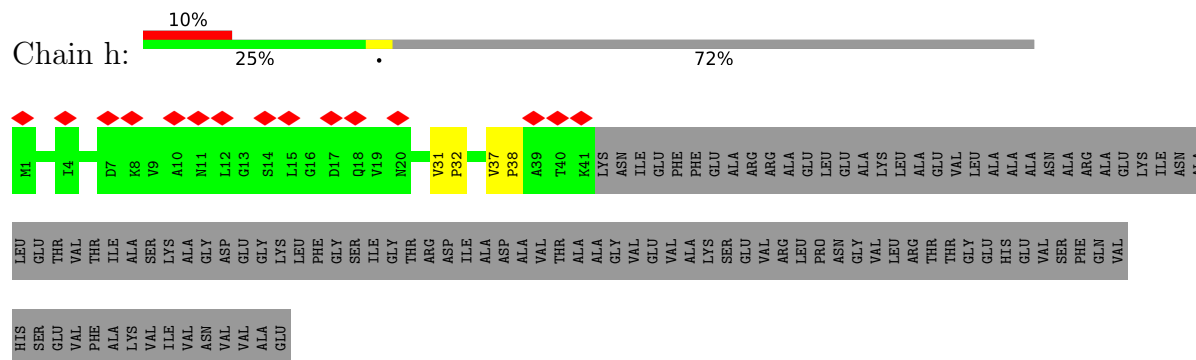
- Molecule 34: Large ribosomal subunit protein uL5



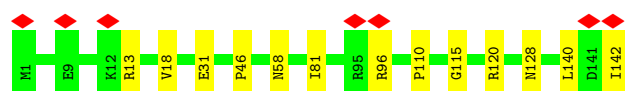
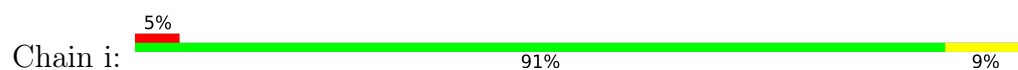
- Molecule 35: Large ribosomal subunit protein uL6



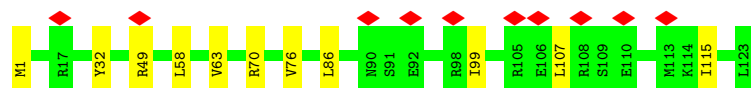
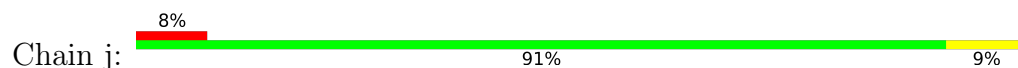
- Molecule 36: Large ribosomal subunit protein bL9



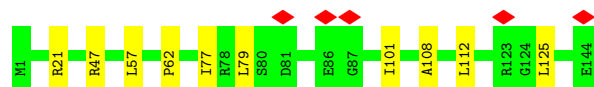
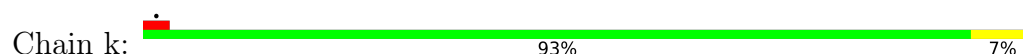
- Molecule 37: Large ribosomal subunit protein uL13



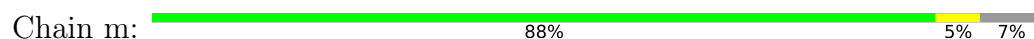
- Molecule 38: Large ribosomal subunit protein uL14



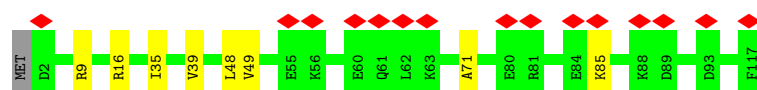
- Molecule 39: 50S ribosomal protein L15



- Molecule 40: Large ribosomal subunit protein bL17



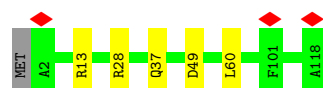
- Molecule 41: Large ribosomal subunit protein uL18



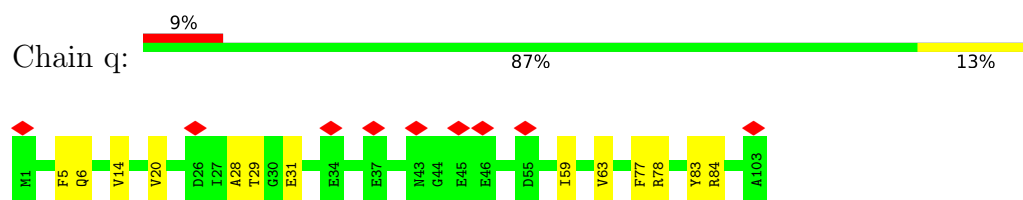
- Molecule 42: Large ribosomal subunit protein bL19



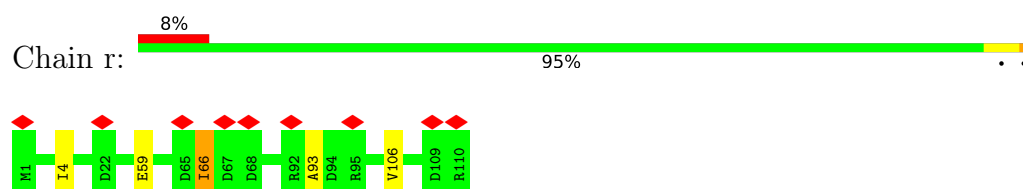
- Molecule 43: Large ribosomal subunit protein bL20



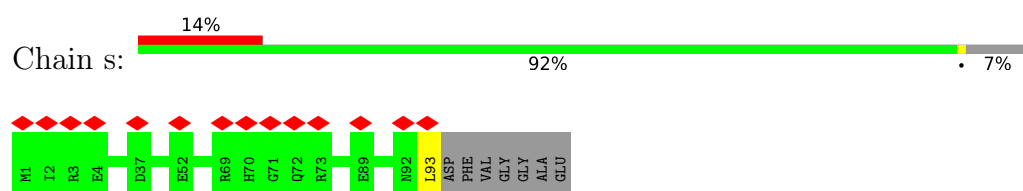
- Molecule 44: Large ribosomal subunit protein bL21



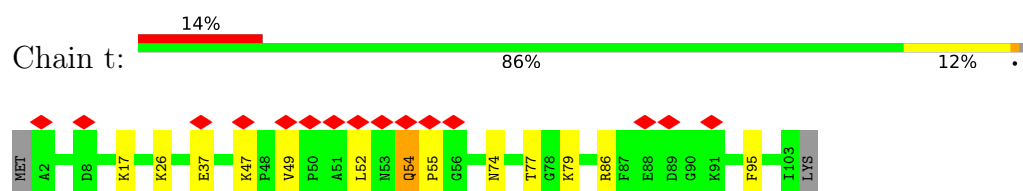
- Molecule 45: Large ribosomal subunit protein uL22



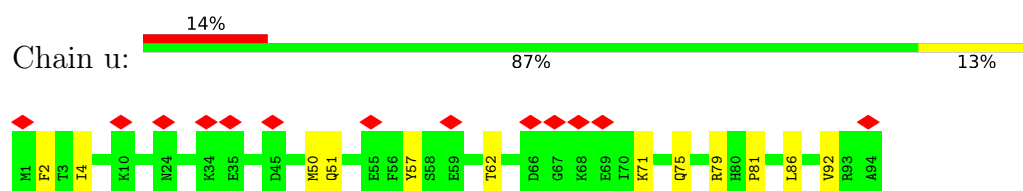
- Molecule 46: Large ribosomal subunit protein uL23



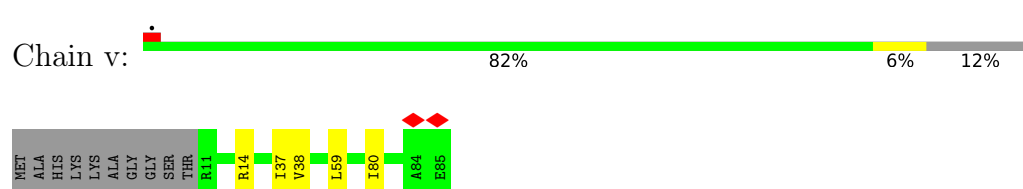
- Molecule 47: Large ribosomal subunit protein uL24



- Molecule 48: 50S ribosomal protein L25

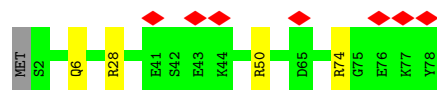


- Molecule 49: Large ribosomal subunit protein bL27

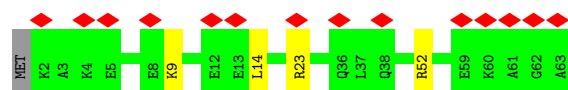


- Molecule 50: Large ribosomal subunit protein bL28

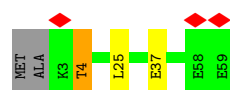
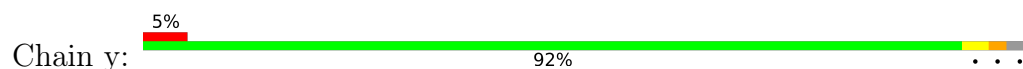




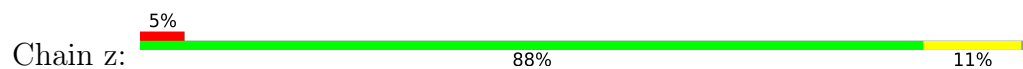
- Molecule 51: Large ribosomal subunit protein uL29



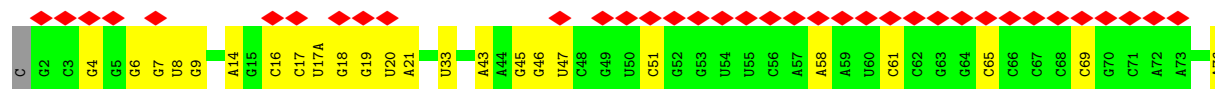
- Molecule 52: Large ribosomal subunit protein uL30



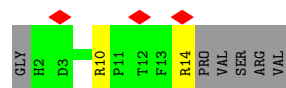
- Molecule 53: Large ribosomal subunit protein bL32



- Molecule 54: fMet-Initiator P-tRNA



- Molecule 55: Dal2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	334003	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.14	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	346.112, 346.112, 346.112	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, G7M, 5MU, OMG, MS6, D2T, 4D4, 6MZ, OMC, ZN, OMU, 5MC, MEQ, 2MG, 4OC, H2U, 1MG, 2MA, UR3, MA6, IAS, PSU

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	0.55	2/65651 (0.0%)	0.90	43/102413 (0.0%)
2	A	0.51	0/36236	0.85	8/56520 (0.0%)
3	3	0.62	0/303	0.78	0/397
4	4	0.58	0/480	0.90	0/638
5	K	0.85	1/884 (0.1%)	0.86	0/1191
6	L	0.57	0/960	0.80	0/1286
7	d	0.66	0/1576	0.85	0/2119
8	l	0.67	2/1073 (0.2%)	0.88	0/1433
9	0	0.57	0/412	0.87	0/549
10	1	0.80	0/370	0.90	0/487
11	2	0.78	0/513	0.90	0/676
12	B	0.55	0/1784	0.94	0/2403
13	C	0.55	0/1651	0.84	0/2225
14	D	0.53	0/1665	0.92	0/2227
15	E	0.60	0/1165	0.88	0/1568
16	F	0.53	0/858	0.87	0/1160
17	G	0.56	0/1179	0.92	0/1580
18	H	0.56	0/989	0.84	0/1326
19	I	0.55	0/1034	0.87	0/1375
20	J	0.59	0/796	0.87	0/1077
21	M	0.57	0/900	0.94	0/1204
22	N	0.55	0/817	0.91	0/1088
23	O	0.56	0/722	0.94	0/964
24	P	0.54	0/653	0.83	0/877
25	Q	0.54	0/633	0.80	0/849
26	R	0.57	0/462	0.90	0/621
27	S	0.60	0/685	0.88	0/922
28	T	0.55	0/676	0.95	0/895
29	U	0.57	0/597	0.95	0/792
30	X	0.59	0/147	0.89	0/227
31	b	0.51	0/2850	0.84	1/4444 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.70	0/2121	0.87	0/2852
33	e	0.65	0/1571	0.89	0/2113
34	f	0.54	0/1434	0.93	0/1926
35	g	0.57	0/1343	0.90	0/1816
36	h	0.56	0/306	0.92	0/413
37	i	0.64	0/1152	0.84	0/1551
38	j	0.61	0/955	0.87	0/1279
39	k	0.69	0/1062	0.85	0/1413
40	m	0.73	1/958 (0.1%)	0.92	1/1281 (0.1%)
41	n	0.58	0/902	0.88	0/1209
42	o	0.64	0/929	0.83	0/1242
43	p	0.72	0/960	0.91	0/1278
44	q	0.60	0/829	0.82	1/1107 (0.1%)
45	r	0.68	0/864	0.85	0/1156
46	s	0.58	0/744	0.81	0/994
47	t	0.56	0/787	0.86	0/1051
48	u	0.56	0/766	0.84	0/1025
49	v	0.67	0/576	0.82	0/762
50	w	0.67	0/635	0.86	0/848
51	x	0.51	0/502	0.97	0/667
52	y	0.58	0/448	0.89	1/598 (0.2%)
53	z	0.72	0/450	0.91	0/599
54	Z	0.56	0/1813	0.83	1/2825 (0.0%)
55	8	0.77	0/121	1.20	0/165
All	All	0.56	6/150949 (0.0%)	0.88	56/225703 (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	a	0	5
3	3	0	1
5	K	0	1
6	L	0	2
7	d	0	1
9	0	0	1
10	1	0	1
11	2	0	1
12	B	0	2
13	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	D	0	4
15	E	0	2
16	F	0	2
17	G	0	2
19	I	0	3
20	J	0	3
21	M	0	2
23	O	0	3
25	Q	0	3
26	R	0	1
28	T	0	3
29	U	0	2
32	c	0	4
33	e	0	3
34	f	0	2
35	g	0	1
37	i	0	3
38	j	0	1
39	k	0	1
41	n	0	1
42	o	0	2
43	p	0	2
44	q	0	1
48	u	0	1
49	v	0	1
50	w	0	2
51	x	0	2
53	z	0	1
55	8	0	2
All	All	0	78

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	120	GLY	C-N	17.33	1.56	1.33
8	l	79	ALA	C-N	-6.83	1.23	1.33
40	m	3	HIS	CG-CD2	-6.34	1.28	1.35
8	l	83	GLY	C-N	-5.66	1.25	1.33
1	a	2069	G7M	O3'-P	5.59	1.61	1.56
1	a	2552	OMU	O3'-P	5.23	1.61	1.56

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	2546	U	O3'-P-O5'	-8.39	91.41	104.00
1	a	2601	C	C4'-C3'-O3'	7.89	124.83	113.00
1	a	204	A	O3'-P-O5'	-7.44	92.85	104.00
1	a	781	A	O3'-P-O5'	-6.98	93.53	104.00
1	a	1373	A	O3'-P-O5'	-6.79	93.82	104.00
1	a	2493	U	O3'-P-O5'	-6.44	94.33	104.00
1	a	1672	A	O3'-P-O5'	-6.41	94.38	104.00
1	a	124	G	O3'-P-O5'	-6.41	94.38	104.00
2	A	1377	A	O3'-P-O5'	-6.24	94.64	104.00
2	A	652	U	O3'-P-O5'	-6.21	94.68	104.00
1	a	1025	G	O3'-P-O5'	6.01	113.01	104.00
1	a	2490	G	O3'-P-O5'	-5.99	95.02	104.00
1	a	504	A	C2'-C3'-O3'	5.96	118.43	109.50
1	a	2094	A	O3'-P-O5'	-5.95	95.08	104.00
1	a	528	A	O3'-P-O5'	-5.85	95.23	104.00
1	a	385	C	O3'-P-O5'	-5.80	95.30	104.00
2	A	455	G	O3'-P-O5'	-5.78	95.33	104.00
1	a	2519	U	O3'-P-O5'	-5.76	95.37	104.00
2	A	561	U	O3'-P-O5'	-5.74	95.39	104.00
1	a	1607	C	C2'-C3'-O3'	5.72	118.08	109.50
1	a	1293	C	O3'-P-O5'	-5.67	95.49	104.00
1	a	827	U	C2'-C3'-O3'	-5.66	105.21	113.70
1	a	2005	A	C2'-C3'-O3'	-5.63	105.26	113.70
1	a	2001	C	O3'-P-O5'	-5.62	95.57	104.00
1	a	1974	C	O3'-P-O5'	-5.62	95.57	104.00
1	a	1847	A	O3'-P-O5'	-5.58	95.64	104.00
1	a	1328	A	O3'-P-O5'	-5.55	95.67	104.00
2	A	246	A	O3'-P-O5'	-5.52	95.72	104.00
1	a	1606	C	O3'-P-O5'	-5.52	95.72	104.00
1	a	1133	A	O3'-P-O5'	-5.41	95.89	104.00
1	a	310	A	O3'-P-O5'	-5.34	95.99	104.00
1	a	1305	C	O3'-P-O5'	-5.34	96.00	104.00
1	a	2879	A	O3'-P-O5'	-5.29	96.06	104.00
44	q	6	GLN	CB-CA-C	5.28	118.47	109.75
1	a	1971	U	C4'-C3'-O3'	-5.27	105.10	113.00
1	a	784	G	O3'-P-O5'	-5.23	96.15	104.00
1	a	982	C	C2'-C3'-O3'	-5.20	105.90	113.70
1	a	1969	A	O3'-P-O5'	-5.17	96.25	104.00
1	a	2516	A	O3'-P-O5'	-5.17	96.25	104.00
54	Z	45	G	O3'-P-O5'	-5.15	96.28	104.00
1	a	1436	G	O3'-P-O5'	-5.15	96.28	104.00
1	a	856	G	O3'-P-O5'	-5.14	96.29	104.00
1	a	906	U	O3'-P-O5'	-5.14	96.30	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1643	G	O3'-P-O5'	-5.12	96.32	104.00
1	a	1810	A	O3'-P-O5'	-5.10	96.35	104.00
1	a	1866	A	O3'-P-O5'	-5.09	96.36	104.00
40	m	1	MET	CG-SD-CE	-5.09	89.70	100.90
1	a	54	G	O3'-P-O5'	-5.08	96.38	104.00
2	A	181	A	O3'-P-O5'	-5.06	96.41	104.00
1	a	404	A	C2'-C3'-O3'	5.05	117.07	109.50
1	a	1246	A	O3'-P-O5'	-5.05	96.43	104.00
1	a	1848	A	O3'-P-O5'	-5.04	96.44	104.00
52	y	4	THR	CA-CB-OG1	-5.03	102.06	109.60
31	b	8	C	O3'-P-O5'	-5.01	96.48	104.00
2	A	573	A	C4'-C3'-O3'	-5.01	105.49	113.00
2	A	780	A	O3'-P-O5'	-5.01	96.49	104.00

There are no chirality outliers.

All (78) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	0	28	ARG	Sidechain
10	1	41	ARG	Sidechain
11	2	13	ARG	Sidechain
3	3	4	ARG	Sidechain
55	8	10	ARG	Sidechain
55	8	14	ARG	Sidechain
12	B	137	ARG	Sidechain
12	B	21	ARG	Sidechain
13	C	11	ARG	Sidechain
13	C	126	ARG	Sidechain
13	C	59	ARG	Sidechain
14	D	14	ARG	Sidechain
14	D	26	ARG	Sidechain
14	D	62	ARG	Sidechain
14	D	73	ARG	Sidechain
15	E	112	ARG	Sidechain
15	E	69	ARG	Sidechain
16	F	45	ARG	Sidechain
16	F	79	ARG	Sidechain
17	G	111	ARG	Sidechain
17	G	143	ARG	Sidechain
19	I	119	ARG	Sidechain
19	I	124	ARG	Sidechain
19	I	85	ARG	Sidechain

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Mol	Chain	Res	Type	Group
20	J	5	ARG	Sidechain
20	J	62	ARG	Sidechain
20	J	7	ARG	Sidechain
5	K	118	HIS	Mainchain
6	L	54	ARG	Sidechain
6	L	9	ARG	Sidechain
21	M	107	ARG	Sidechain
21	M	71	ARG	Sidechain
23	O	53	ARG	Sidechain
23	O	64	ARG	Sidechain
23	O	72	ARG	Sidechain
25	Q	27	ARG	Sidechain
25	Q	62	ARG	Sidechain
25	Q	65	ARG	Sidechain
26	R	61	ARG	Sidechain
28	T	24	ARG	Sidechain
28	T	60	ARG	Sidechain
28	T	74	ARG	Sidechain
29	U	34	ARG	Sidechain
29	U	69	ARG	Sidechain
1	a	249	C	Sidechain
1	a	395	U	Sidechain
1	a	463	G	Sidechain
1	a	512	G	Sidechain
1	a	980	A	Sidechain
32	c	133	ARG	Sidechain
32	c	156	ARG	Sidechain
32	c	43	ARG	Sidechain
32	c	80	ARG	Sidechain
7	d	83	ARG	Sidechain
33	e	21	ARG	Sidechain
33	e	61	ARG	Sidechain
33	e	88	ARG	Sidechain
34	f	125	ARG	Sidechain
34	f	150	ARG	Sidechain
35	g	35	ARG	Sidechain
37	i	120	ARG	Sidechain
37	i	13	ARG	Sidechain
37	i	96	ARG	Sidechain
38	j	49	ARG	Sidechain
39	k	47	ARG	Sidechain
41	n	9	ARG	Sidechain

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Mol	Chain	Res	Type	Group
42	o	103	ARG	Sidechain
42	o	89	ARG	Sidechain
43	p	13	ARG	Sidechain
43	p	28	ARG	Sidechain
44	q	78	ARG	Sidechain
48	u	79	ARG	Sidechain
49	v	14	ARG	Sidechain
50	w	28	ARG	Sidechain
50	w	74	ARG	Sidechain
51	x	23	ARG	Sidechain
51	x	52	ARG	Sidechain
53	z	52	ARG	Sidechain

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	59130	0	29769	119	0
2	A	32612	0	16432	78	0
3	3	302	0	340	3	0
4	4	472	0	467	5	0
5	K	877	0	884	7	0
6	L	957	0	1017	7	0
7	d	1566	0	1618	15	0
8	l	1075	0	1146	15	0
9	0	405	0	437	4	0
10	1	367	0	405	1	0
11	2	504	0	572	5	0
12	B	1753	0	1780	12	0
13	C	1624	0	1696	6	0
14	D	1643	0	1707	19	0
15	E	1152	0	1196	10	0
16	F	839	0	833	7	0
17	G	1164	0	1213	5	0
18	H	979	0	1031	4	0
19	I	1022	0	1070	5	0
20	J	786	0	828	12	0
21	M	891	0	952	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	N	805	0	844	3	0
23	O	714	0	734	1	0
24	P	643	0	661	5	0
25	Q	624	0	658	7	0
26	R	455	0	478	5	0
27	S	668	0	693	5	0
28	T	670	0	719	3	0
29	U	589	0	629	1	0
30	X	131	0	66	1	0
31	b	2549	0	1291	6	0
32	c	2082	0	2154	10	0
33	e	1552	0	1619	8	0
34	f	1410	0	1444	4	0
35	g	1323	0	1371	17	0
36	h	303	0	327	2	0
37	i	1129	0	1162	11	0
38	j	946	0	1023	5	0
39	k	1053	0	1129	9	0
40	m	945	0	989	2	0
41	n	892	0	923	5	0
42	o	917	0	962	7	0
43	p	947	0	1019	3	0
44	q	816	0	839	6	0
45	r	857	0	922	3	0
46	s	738	0	807	0	0
47	t	779	0	831	9	0
48	u	753	0	780	9	0
49	v	569	0	581	3	0
50	w	625	0	652	1	0
51	x	501	0	531	2	0
52	y	444	0	483	2	0
53	z	444	0	458	4	0
54	Z	1623	0	825	1	0
55	8	115	0	113	0	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
All	All	139733	0	94110	440	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 2.

All (440) 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)
15:E:154:ALA:HA	15:E:164:ILE:HD11	1.38	1.06
14:D:28:ILE:HG12	14:D:34:ILE:HD11	1.41	0.99
35:g:52:PHE:CZ	35:g:72:LEU:HD12	2.04	0.92
13:C:77:ILE:HA	13:C:84:VAL:HG23	1.57	0.85
37:i:18:VAL:HG21	37:i:142:ILE:HD12	1.59	0.85
35:g:52:PHE:CE1	35:g:72:LEU:HD12	2.14	0.82
1:a:2757:A:N1	35:g:67:THR:HG21	1.93	0.82
1:a:2420:C:H5'	9:0:54:ILE:HD11	1.63	0.81
15:E:154:ALA:HA	15:E:164:ILE:CD1	2.11	0.79
17:G:75:VAL:HG11	17:G:86:GLN:HB3	1.65	0.79
8:l:1:MET:HE1	8:l:44:ARG:N	1.98	0.78
6:L:4:VAL:HG13	25:Q:34:TYR:HB3	1.68	0.75
1:a:2420:C:C5'	9:0:54:ILE:HD11	2.18	0.73
17:G:75:VAL:CG1	17:G:86:GLN:HB3	2.20	0.72
35:g:89:LEU:CD2	35:g:162:VAL:HG22	2.20	0.70
15:E:154:ALA:HB2	15:E:164:ILE:HD12	1.75	0.69
5:K:111:THR:HG23	29:U:3:VAL:HG22	1.73	0.68
15:E:154:ALA:CA	15:E:164:ILE:HD11	2.20	0.68
1:a:568:U:H1'	1:a:2030:6MZ:H9C1	1.75	0.68
18:H:38:ASN:OD1	18:H:49:PHE:CZ	2.48	0.67
15:E:154:ALA:CA	15:E:164:ILE:CD1	2.73	0.67
27:S:25:SER:HB2	27:S:28:LYS:HE3	1.76	0.67
41:n:48:LEU:O	41:n:85:LYS:NZ	2.25	0.66
2:A:664:G:H22	2:A:741:G:H1	1.43	0.66
35:g:52:PHE:HZ	35:g:72:LEU:HD12	1.60	0.66
20:J:12:ALA:HB3	20:J:18:ILE:HG13	1.77	0.66
32:c:29:PRO:HG2	32:c:34:LEU:HD11	1.78	0.65
20:J:12:ALA:HB3	20:J:18:ILE:CG1	2.27	0.65
20:J:18:ILE:HD12	20:J:70:HIS:HB2	1.79	0.64
37:i:31:GLU:CG	37:i:142:ILE:HG23	2.28	0.63
35:g:23:VAL:HG22	35:g:36:THR:HG22	1.81	0.63
1:a:12:U:H2'	1:a:12:U:O2	1.98	0.63
13:C:77:ILE:HA	13:C:84:VAL:CG2	2.27	0.62
6:L:55:VAL:HG21	6:L:80:ILE:HD11	1.82	0.62
1:a:548:G:H2'	1:a:549:G:H1'	1.82	0.62
14:D:28:ILE:CG1	14:D:34:ILE:HD11	2.24	0.62
8:l:77:PRO:HG2	8:l:80:VAL:HG21	1.81	0.61
1:a:1872:A:H3'	1:a:1873:G:O4'	2.00	0.61
48:u:4:ILE:HG12	48:u:50:MET:HE1	1.82	0.61
1:a:139:U:H5''	1:a:140:C:H5	1.64	0.61
14:D:48:LEU:HD21	14:D:56:ARG:HG3	1.82	0.61
8:l:20:LEU:HD13	48:u:81:PRO:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:87:CYS:SG	12:B:221:VAL:HB	2.42	0.60
14:D:172:GLU:HG3	14:D:183:LYS:HD2	1.83	0.60
33:e:5:LEU:HD11	33:e:12:LEU:HB2	1.83	0.59
2:A:203:G:O2'	2:A:465:A:N1	2.35	0.59
2:A:1302:C:C5	21:M:17:ILE:HG13	2.38	0.59
28:T:24:ARG:HB3	28:T:61:GLN:HE22	1.67	0.59
1:a:894:U:H2'	1:a:895:U:O4'	2.02	0.59
2:A:237:G:OP1	25:Q:42:THR:HG22	2.03	0.59
14:D:32:CYS:SG	14:D:34:ILE:HD13	2.43	0.59
48:u:62:THR:HG22	48:u:71:LYS:CD	2.33	0.58
2:A:1073:U:O2'	12:B:103:ASN:ND2	2.37	0.58
35:g:27:LYS:HG3	35:g:32:GLU:HG2	1.85	0.58
1:a:930:G:H1'	52:y:25:LEU:HD11	1.84	0.58
19:I:52:LEU:HD11	19:I:63:LEU:HD11	1.87	0.57
8:l:1:MET:HE1	8:l:44:ARG:CA	2.33	0.57
13:C:35:SER:OG	13:C:59:ARG:NH2	2.37	0.56
31:b:36:C:N4	31:b:49:C:O2	2.38	0.56
32:c:107:PRO:HD2	32:c:110:LEU:HD22	1.88	0.56
2:A:769:G:H4'	2:A:1513:A:H4'	1.87	0.56
2:A:1033:G:H3'	2:A:1034:G:H8	1.71	0.56
1:a:1252:G:H1	43:p:37:GLN:HE21	1.52	0.56
1:a:2020:A:H5'	53:z:9:THR:CG2	2.35	0.56
8:l:53:MET:HE1	8:l:103:TYR:CD2	2.41	0.55
1:a:2305:U:H5''	34:f:131:GLY:HA3	1.87	0.55
2:A:532:A:N6	2:A:1206:G:O2'	2.39	0.55
1:a:543:G:H8	1:a:543:G:H5''	1.72	0.55
1:a:2328:A:H2'	1:a:2329:U:C6	2.42	0.55
11:2:54:ASP:HB3	39:k:57:LEU:HD22	1.87	0.55
1:a:1434:A:H2'	1:a:1435:G:C8	2.42	0.55
4:4:28:VAL:HG21	4:4:32:LEU:HD21	1.87	0.55
2:A:79:G:H1	2:A:90:C:H42	1.55	0.55
20:J:6:ILE:HB	20:J:76:ILE:HB	1.89	0.55
12:B:42:ASN:HD22	12:B:45:LYS:HG2	1.72	0.55
6:L:110:ARG:HB3	6:L:119:VAL:HG21	1.88	0.55
8:l:53:MET:HG3	8:l:120:ALA:HB2	1.89	0.55
52:y:4:THR:OG1	52:y:37:GLU:HG2	2.07	0.55
16:F:88:MET:HE3	26:R:64:TYR:CD2	2.41	0.54
7:d:14:ILE:HA	42:o:12:GLN:HE22	1.72	0.54
44:q:28:ALA:HB3	44:q:31:GLU:HG3	1.90	0.54
1:a:2506:U:H2'	1:a:2506:U:O2	2.08	0.54
39:k:77:ILE:HD13	39:k:108:ALA:HB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2:G:H2'	1:a:3:U:C6	2.43	0.53
1:a:276:U:H2'	1:a:277:G:C8	2.42	0.53
2:A:1273:C:H2'	2:A:1274:A:O4'	2.08	0.53
7:d:156:PHE:CE1	37:i:81:ILE:HD13	2.43	0.53
2:A:673:A:H2'	2:A:674:G:C8	2.44	0.53
51:x:9:LYS:HB2	51:x:14:LEU:HD12	1.90	0.53
12:B:70:VAL:HG21	12:B:161:LEU:HD11	1.90	0.53
8:l:1:MET:HE1	8:l:43:ALA:C	2.32	0.53
20:J:12:ALA:HB3	20:J:18:ILE:HD11	1.90	0.53
47:t:74:ASN:HD22	47:t:77:THR:HG23	1.73	0.53
1:a:2757:A:N1	35:g:67:THR:CG2	2.70	0.53
2:A:429:U:H3'	14:D:9:LEU:HD12	1.90	0.52
1:a:1509:A:O2'	1:a:1510:G:H8	1.91	0.52
2:A:451:A:H61	2:A:481:G:H5'	1.74	0.52
35:g:156:PRO:O	35:g:171:THR:HA	2.09	0.52
38:j:70:ARG:HG2	38:j:76:VAL:HG22	1.91	0.52
48:u:75:GLN:HB2	48:u:92:VAL:HG23	1.90	0.52
20:J:12:ALA:HB3	20:J:18:ILE:CD1	2.39	0.52
1:a:1187:G:H5''	44:q:83:TYR:CE1	2.45	0.52
7:d:35:THR:HG22	7:d:73:VAL:HG21	1.91	0.52
47:t:26:LYS:HD3	47:t:37:GLU:HB3	1.91	0.52
4:4:22:MET:HE1	34:f:105:THR:HG21	1.91	0.51
39:k:77:ILE:CD1	39:k:108:ALA:HB1	2.41	0.51
12:B:70:VAL:CG2	12:B:161:LEU:HD11	2.40	0.51
38:j:1:MET:HE3	38:j:32:TYR:CZ	2.45	0.51
42:o:100:LEU:HD11	42:o:110:ILE:HD11	1.92	0.51
2:A:1328:C:H5''	21:M:28:THR:HG21	1.93	0.51
44:q:5:PHE:HB3	44:q:59:ILE:HD12	1.93	0.51
1:a:355:U:H2'	1:a:356:G:H8	1.75	0.51
3:3:16:ILE:HD13	3:3:25:VAL:HG22	1.92	0.51
5:K:67:ALA:HB2	5:K:96:THR:HG23	1.93	0.50
2:A:382:A:H2'	2:A:383:A:C8	2.47	0.50
26:R:32:TYR:HB3	26:R:55:LEU:HD21	1.93	0.50
51:x:9:LYS:HB2	51:x:14:LEU:CD1	2.41	0.50
2:A:404:G:N7	14:D:2:ALA:HB3	2.26	0.50
2:A:188:C:H2'	2:A:189:A:O4'	2.11	0.50
33:e:46:GLN:O	33:e:88:ARG:NH1	2.44	0.50
2:A:1391:U:H2'	2:A:1392:G:C8	2.46	0.50
14:D:32:CYS:SG	14:D:34:ILE:CD1	2.99	0.50
21:M:11:ASP:HB3	21:M:46:SER:HB3	1.94	0.50
31:b:29:A:H2'	31:b:30:C:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:i:140:LEU:HD23	37:i:142:ILE:HD11	1.93	0.50
37:i:140:LEU:HG	37:i:142:ILE:HG13	1.94	0.50
2:A:1228:C:H1'	21:M:116:ILE:HD11	1.94	0.50
13:C:42:TYR:CZ	13:C:46:GLU:HG3	2.46	0.50
11:2:62:LEU:HB3	11:2:65:ALA:HB2	1.93	0.50
30:X:14:A:H2'	30:X:15:A:H5'	1.93	0.50
32:c:5:LYS:HD2	32:c:17:VAL:HG22	1.94	0.50
15:E:154:ALA:CB	15:E:164:ILE:HD12	2.41	0.49
1:a:277:G:H1'	1:a:278:A:C5	2.47	0.49
1:a:493:G:H2'	1:a:494:G:O4'	2.12	0.49
2:A:946:A:H2'	2:A:947:G:C8	2.47	0.49
2:A:1023:U:H2'	2:A:1024:G:C8	2.47	0.49
25:Q:78:VAL:HG11	25:Q:81:LYS:HE3	1.94	0.49
2:A:718:A:H5'	5:K:119:IAS:C	2.43	0.49
14:D:171:LEU:HD23	14:D:182:PHE:HA	1.95	0.49
1:a:1799:G:O2'	32:c:180:GLU:OE2	2.25	0.49
2:A:1004:A:H2'	2:A:1005:A:O4'	2.12	0.49
1:a:1853:A:N1	1:a:2087:G:H1'	2.28	0.49
2:A:1356:G:H2'	2:A:1357:A:C8	2.48	0.49
15:E:56:VAL:N	15:E:57:PRO:HD2	2.28	0.49
48:u:51:GLN:HG2	48:u:86:LEU:HD11	1.94	0.49
1:a:1906:G:H2'	1:a:1907:G:H5''	1.95	0.48
40:m:24:MET:HE1	40:m:40:LYS:HD3	1.95	0.48
8:l:66:ARG:NH1	8:l:104:GLU:OE2	2.46	0.48
33:e:12:LEU:HD11	33:e:194:LYS:HE3	1.95	0.48
1:a:549:G:H2'	1:a:550:C:C6	2.48	0.48
1:a:644:A:H2'	1:a:645:C:O4'	2.13	0.48
7:d:12:THR:CG2	42:o:5:ILE:HG23	2.43	0.48
1:a:468:G:N7	10:l:39:ARG:NH2	2.53	0.48
1:a:2327:A:H2'	1:a:2328:A:C8	2.49	0.48
1:a:2491:U:H5''	1:a:2570:G:H5''	1.95	0.48
1:a:811:U:H2'	39:k:21:ARG:HA	1.96	0.48
8:l:136:MET:HE2	48:u:57:TYR:CD1	2.49	0.48
13:C:47:LEU:HD21	13:C:87:LEU:HD11	1.96	0.48
1:a:876:C:H2'	1:a:877:A:O4'	2.13	0.48
27:S:50:ALA:HB1	27:S:57:HIS:HB3	1.96	0.48
1:a:1799:G:N7	32:c:178:SER:OG	2.44	0.47
19:I:57:MET:HA	19:I:60:LYS:HD3	1.95	0.47
37:i:110:PRO:O	37:i:115:GLY:HA3	2.13	0.47
1:a:57:C:H2'	1:a:58:G:O4'	2.14	0.47
1:a:888:C:H2'	1:a:889:C:O4'	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1720:U:H2'	1:a:1721:G:O4'	2.14	0.47
2:A:87:C:H2'	2:A:88:U:C6	2.50	0.47
12:B:129:LEU:HB3	12:B:133:GLU:HB2	1.95	0.47
12:B:130:THR:O	12:B:132:LYS:N	2.46	0.47
4:4:2:LYS:HE3	31:b:40:U:H2'	1.97	0.47
11:2:45:ARG:N	11:2:46:PRO:HD2	2.29	0.47
49:v:38:VAL:HG12	49:v:59:LEU:HB2	1.96	0.47
1:a:1115:G:O2'	1:a:1116:G:O5'	2.25	0.47
1:a:1614:A:C2	45:r:93:ALA:HB2	2.49	0.47
1:a:1778:U:H2'	1:a:1784:A:N6	2.29	0.47
6:L:101:ALA:O	6:L:102:LEU:C	2.57	0.47
48:u:2:PHE:HB3	48:u:50:MET:HE3	1.96	0.47
1:a:1028:A:N6	1:a:1125:G:H2'	2.30	0.47
1:a:2901:C:H2'	1:a:2902:C:C6	2.50	0.47
39:k:77:ILE:HD11	39:k:101:ILE:HG21	1.96	0.47
41:n:49:VAL:HG13	41:n:85:LYS:HD2	1.96	0.47
41:n:49:VAL:CG1	41:n:85:LYS:HD2	2.44	0.47
1:a:1108:U:H2'	1:a:1109:C:C6	2.50	0.47
1:a:2419:U:H4'	9:0:22:THR:HG21	1.96	0.47
2:A:542:G:H5'	14:D:39:GLY:HA3	1.96	0.47
4:4:11:GLU:HA	4:4:25:ARG:HA	1.96	0.47
33:e:147:LEU:HD11	33:e:170:ARG:HG3	1.96	0.47
48:u:62:THR:HG22	48:u:71:LYS:HD3	1.97	0.47
1:a:221:A:N1	1:a:265:A:O2'	2.47	0.47
1:a:2469:A:H4'	8:l:55:ARG:HD2	1.97	0.47
38:j:63:VAL:HG12	38:j:107:LEU:HD11	1.96	0.47
2:A:492:C:H2'	2:A:493:A:C8	2.50	0.47
17:G:113:ASP:OD2	17:G:122:ASN:ND2	2.48	0.46
39:k:77:ILE:HD12	39:k:77:ILE:N	2.30	0.46
14:D:102:VAL:HG13	14:D:107:PHE:HB2	1.98	0.46
14:D:105:MET:HE1	14:D:143:VAL:HB	1.97	0.46
44:q:29:THR:O	44:q:63:VAL:O	2.33	0.46
14:D:28:ILE:HG23	14:D:34:ILE:HG13	1.96	0.46
24:P:61:VAL:HG21	24:P:67:ILE:HD11	1.97	0.46
28:T:42:GLY:HA2	28:T:86:LEU:HD11	1.98	0.46
2:A:945:G:C2	2:A:946:A:C8	3.03	0.46
2:A:1086:U:H3	2:A:1099:G:H22	1.64	0.46
7:d:5:VAL:H	7:d:32:ASN:ND2	2.13	0.46
1:a:890:C:H3'	1:a:891:G:O4'	2.16	0.46
1:a:1109:C:H2'	1:a:1110:G:C4	2.51	0.46
2:A:1127:G:H5'	2:A:1280:A:O2'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:G:27:VAL:HG11	17:G:40:GLU:HG3	1.98	0.46
1:a:2452:C:H2'	1:a:2453:A:C8	2.51	0.46
49:v:37:ILE:HG21	49:v:80:ILE:HG21	1.98	0.46
1:a:1264:A:H5'	53:z:8:PRO:HG2	1.98	0.46
1:a:1932:A:H2'	1:a:1933:G:O4'	2.16	0.46
2:A:160:A:H2'	2:A:161:A:O4'	2.16	0.46
4:4:64:PHE:CG	27:S:9:PRO:HD3	2.51	0.45
1:a:1939:5MU:OP1	1:a:2604:PSU:O2'	2.34	0.45
1:a:2478:A:OP2	3:3:2:LYS:NZ	2.49	0.45
5:K:35:THR:HG22	5:K:41:ALA:HA	1.98	0.45
5:K:118:HIS:HE1	26:R:71:THR:CG2	2.30	0.45
8:l:136:MET:HE2	48:u:57:TYR:HD1	1.80	0.45
33:e:196:VAL:HA	33:e:199:MET:HE2	1.99	0.45
1:a:1548:A:H2'	1:a:1549:A:C8	2.52	0.45
27:S:80:TYR:CZ	27:S:82:GLY:HA2	2.52	0.45
2:A:376:G:H5''	24:P:5:ARG:HB2	1.99	0.45
41:n:39:VAL:HB	41:n:49:VAL:HG22	1.98	0.45
1:a:723:C:H2'	1:a:724:U:O4'	2.16	0.45
1:a:2243:U:H2'	1:a:2244:U:C6	2.52	0.45
1:a:2483:C:N3	8:l:123:LYS:NZ	2.57	0.45
2:A:140:U:H2'	2:A:141:G:O4'	2.16	0.45
34:f:121:SER:HB2	34:f:128:TYR:CE1	2.52	0.45
20:J:18:ILE:CD1	20:J:70:HIS:HB2	2.44	0.45
39:k:108:ALA:HB3	39:k:125:LEU:HD22	1.99	0.45
2:A:371:A:H2'	2:A:372:C:O4'	2.17	0.45
7:d:1:MET:HB3	7:d:205:PRO:HG2	1.98	0.45
8:l:1:MET:HE1	8:l:44:ARG:HA	1.98	0.45
16:F:22:ILE:HG21	16:F:39:LEU:HD21	1.99	0.45
25:Q:21:ILE:HG13	25:Q:46:VAL:HB	1.98	0.45
2:A:604:G:H2'	2:A:605:U:O4'	2.16	0.45
14:D:85:ASN:HB3	14:D:88:GLU:HG2	1.98	0.45
11:2:25:LYS:HB3	39:k:62:PRO:HG2	1.98	0.45
44:q:77:PHE:HD1	44:q:84:ARG:HD3	1.82	0.45
1:a:483:A:H5''	47:t:47:LYS:HD2	1.99	0.44
1:a:2552:OMU:H6	1:a:2552:OMU:O5'	2.16	0.44
2:A:986:U:H2'	2:A:987:G:O4'	2.18	0.44
15:E:88:VAL:HG22	15:E:93:ARG:HG2	1.99	0.44
1:a:2756:U:H1'	1:a:2757:A:H5''	1.99	0.44
1:a:1434:A:H2'	1:a:1435:G:H8	1.81	0.44
1:a:1980:G:O2'	1:a:1982:U:OP2	2.34	0.44
1:a:2287:A:OP1	9:0:30:LYS:NZ	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2747:G:O2'	35:g:67:THR:HG22	2.18	0.44
2:A:505:G:H5'	2:A:534:U:H2'	1.99	0.44
32:c:203:ARG:HH21	32:c:203:ARG:HG3	1.83	0.44
1:a:2233:U:H2'	1:a:2234:G:C8	2.52	0.44
2:A:147:G:H2'	2:A:148:G:C8	2.52	0.44
19:I:21:ILE:HG12	19:I:63:LEU:HD22	2.00	0.44
45:r:59:GLU:OE1	45:r:66:ILE:HB	2.18	0.44
1:a:395:U:O2'	1:a:396:G:N7	2.48	0.44
2:A:476:U:H2'	2:A:477:C:C6	2.53	0.44
2:A:1036:A:H2'	2:A:1037:C:O4'	2.18	0.44
16:F:90:MET:HE1	26:R:23:TYR:CZ	2.53	0.44
34:f:50:LEU:HD11	34:f:67:ILE:HD12	1.98	0.44
1:a:570:G:H2'	1:a:2030:6MZ:N7	2.33	0.44
1:a:639:U:H2'	1:a:640:C:C6	2.52	0.44
1:a:1915:3TD:H6	1:a:1915:3TD:O5'	2.18	0.44
8:l:50:ARG:HD3	8:l:65:ILE:HD11	2.00	0.44
21:M:11:ASP:HA	21:M:45:ILE:HB	2.00	0.44
37:i:31:GLU:HB3	37:i:142:ILE:CG2	2.48	0.44
1:a:1582:C:H2'	1:a:1583:A:O4'	2.17	0.44
2:A:176:C:H2'	2:A:177:G:N3	2.33	0.44
1:a:2529:G:H4'	35:g:175:LYS:HB2	2.00	0.43
2:A:89:U:H2'	2:A:90:C:C6	2.53	0.43
47:t:74:ASN:ND2	47:t:77:THR:HG23	2.32	0.43
1:a:476:G:H4'	1:a:502:A:N1	2.33	0.43
1:a:910:A:H2'	1:a:911:A:C8	2.52	0.43
2:A:381:C:H2'	2:A:382:A:O4'	2.18	0.43
16:F:42:TRP:CD2	16:F:102:MET:HG2	2.52	0.43
17:G:135:VAL:HG13	17:G:138:ARG:NH2	2.33	0.43
20:J:65:TYR:HB3	22:N:96:LEU:HD11	2.00	0.43
33:e:136:GLN:HA	33:e:139:LYS:HE3	2.00	0.43
50:w:6:GLN:HE21	50:w:50:ARG:H	1.65	0.43
1:a:534:U:O2'	43:p:49:ASP:OD2	2.21	0.43
1:a:2038:G:H2'	1:a:2039:U:O4'	2.18	0.43
12:B:81:LYS:HG3	12:B:91:PHE:CZ	2.54	0.43
16:F:49:TYR:HB3	26:R:74:HIS:CD2	2.54	0.43
37:i:46:PRO:HD3	43:p:60:LEU:HD13	2.01	0.43
47:t:86:ARG:HG3	47:t:95:PHE:CD1	2.52	0.43
1:a:1710:G:H4'	1:a:2858:C:O2	2.19	0.43
2:A:754:C:OP1	23:O:72:ARG:NH2	2.51	0.43
15:E:164:ILE:O	18:H:114:ARG:NH2	2.52	0.43
16:F:36:ILE:HD13	16:F:64:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:207:A:H2'	1:a:208:C:O4'	2.19	0.43
2:A:1323:G:H2'	2:A:1324:A:C8	2.53	0.43
6:L:4:VAL:CG1	25:Q:34:TYR:HB3	2.44	0.43
21:M:16:VAL:CG2	21:M:41:GLU:HB3	2.48	0.43
2:A:195:A:H2'	2:A:196:A:C8	2.54	0.43
2:A:1032:G:C5	2:A:1033:G:H1'	2.53	0.43
7:d:5:VAL:H	7:d:32:ASN:HD21	1.67	0.43
21:M:33:ILE:HD13	21:M:60:VAL:HG22	2.01	0.43
25:Q:47:HIS:HB3	25:Q:74:THR:HG22	1.99	0.43
32:c:43:ARG:HA	32:c:48:ARG:O	2.19	0.43
42:o:34:GLU:O	42:o:37:LYS:HG2	2.18	0.43
2:A:632:U:H3'	2:A:633:G:H5'	2.01	0.43
5:K:23:ILE:HG12	5:K:96:THR:HG21	2.01	0.43
6:L:57:LEU:HD21	6:L:82:ILE:HD13	2.01	0.43
7:d:152:PRO:HG3	7:d:156:PHE:CZ	2.54	0.43
18:H:11:LEU:HD22	18:H:75:ILE:HD11	1.99	0.43
3:3:1:MET:HE2	3:3:1:MET:HB2	1.98	0.42
21:M:34:LEU:HD23	21:M:56:LEU:HD21	1.99	0.42
38:j:99:ILE:HG12	38:j:115:ILE:HG23	2.01	0.42
1:a:279:A:H1'	1:a:362:A:O2'	2.18	0.42
1:a:373:U:O2'	1:a:423:A:H1'	2.19	0.42
1:a:667:U:O2	11:2:2:PRO:HD2	2.19	0.42
1:a:2063:C:O2	1:a:2450:A:N1	2.52	0.42
2:A:1428:A:H2'	2:A:1429:A:O4'	2.18	0.42
12:B:196:VAL:HB	12:B:199:VAL:HG22	2.01	0.42
14:D:107:PHE:HB3	14:D:145:ILE:HD11	2.00	0.42
21:M:16:VAL:HG22	21:M:34:LEU:HD12	2.01	0.42
31:b:30:C:H2'	31:b:31:C:H5'	2.01	0.42
39:k:79:LEU:HD12	39:k:112:LEU:HD12	2.01	0.42
1:a:613:A:H2'	1:a:614:A:O4'	2.20	0.42
1:a:857:G:H2'	1:a:858:G:O4'	2.18	0.42
1:a:1378:A:O2'	1:a:1380:G:N7	2.52	0.42
1:a:2273:A:H2'	1:a:2274:A:C8	2.54	0.42
7:d:1:MET:HE2	7:d:205:PRO:HG2	1.99	0.42
37:i:31:GLU:HB3	37:i:142:ILE:HG23	2.00	0.42
1:a:1913:A:C2	2:A:1492:A:H2'	2.54	0.42
14:D:124:MET:HG3	14:D:146:ARG:HG2	2.00	0.42
19:I:118:LEU:HD22	19:I:124:ARG:HG2	2.01	0.42
20:J:10:LEU:HD12	20:J:22:THR:HG22	2.01	0.42
44:q:14:VAL:HG11	44:q:20:VAL:HG21	2.01	0.42
1:a:1494:A:H2'	1:a:1495:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:131:A:H2'	2:A:132:C:C6	2.55	0.42
12:B:28:LYS:N	12:B:29:PRO:CD	2.83	0.42
35:g:94:TYR:HA	35:g:106:SER:O	2.19	0.42
38:j:58:LEU:HD11	38:j:86:LEU:HD13	2.00	0.42
1:a:1275:A:N1	1:a:1295:C:O2'	2.49	0.42
1:a:1607:C:H4'	1:a:1608:A:O5'	2.20	0.42
2:A:309:A:O2'	2:A:607:A:N1	2.46	0.42
2:A:404:G:O2'	2:A:498:A:N1	2.50	0.42
12:B:111:ILE:HD13	12:B:148:LEU:HB3	2.02	0.42
24:P:18:GLN:OE1	24:P:35:ARG:NE	2.52	0.42
47:t:54:GLN:N	47:t:55:PRO:HD2	2.33	0.42
47:t:86:ARG:HG3	47:t:95:PHE:CE1	2.55	0.42
1:a:657:U:H2'	1:a:658:U:C6	2.55	0.42
1:a:1182:G:H2'	1:a:1183:U:O4'	2.20	0.42
1:a:2751:G:H2'	1:a:2751:G:N3	2.34	0.42
2:A:918:A:H2'	2:A:919:A:O4'	2.19	0.42
20:J:12:ALA:N	20:J:18:ILE:HD11	2.35	0.42
49:v:59:LEU:HD12	49:v:80:ILE:HD12	2.00	0.42
2:A:543:U:OP1	14:D:14:ARG:HD2	2.19	0.42
14:D:101:VAL:HG12	14:D:105:MET:HE2	2.02	0.42
18:H:66:PHE:CD2	18:H:67:GLN:HG2	2.55	0.42
27:S:41:PHE:HB2	27:S:44:MET:HE3	2.02	0.42
35:g:44:LYS:HB2	35:g:51:THR:HB	2.01	0.42
32:c:181:MET:HB3	32:c:268:VAL:HB	2.01	0.42
1:a:2547:A:H2'	1:a:2548:U:C6	2.55	0.42
7:d:110:THR:HG23	7:d:202:ILE:HB	2.02	0.42
35:g:86:LYS:HG3	35:g:165:ALA:HB3	2.02	0.42
2:A:1530:G:H2'	2:A:1531:A:C8	2.55	0.41
12:B:115:LYS:O	12:B:118:GLU:HG2	2.20	0.41
15:E:115:LEU:HD13	15:E:123:VAL:HG11	2.02	0.41
20:J:23:ALA:HA	20:J:26:VAL:HG22	2.02	0.41
31:b:48:U:H2'	31:b:49:C:C6	2.55	0.41
1:a:1583:A:H4'	1:a:1585:C:C4	2.55	0.41
35:g:60:ASP:HB3	35:g:64:GLN:HG2	2.03	0.41
1:a:340:A:H2'	1:a:341:C:O4'	2.19	0.41
1:a:2395:C:H2'	1:a:2396:G:O4'	2.19	0.41
7:d:2:ILE:CD1	7:d:90:PHE:CZ	3.03	0.41
7:d:121:THR:HB	7:d:127:PHE:CD2	2.55	0.41
35:g:37:LEU:HD13	35:g:68:ALA:HB1	2.02	0.41
1:a:157:C:H2'	1:a:158:U:O4'	2.21	0.41
2:A:189:A:H2'	2:A:190:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:19:LEU:HB2	14:D:21:LEU:HG	2.02	0.41
2:A:299:G:H2'	2:A:300:A:C8	2.56	0.41
2:A:1129:C:H2'	2:A:1139:G:N7	2.35	0.41
19:I:130:ARG:NH1	54:Z:33:U:OP2	2.47	0.41
24:P:12:LYS:HG2	24:P:13:LYS:HG2	2.02	0.41
37:i:31:GLU:HG2	37:i:142:ILE:HG23	2.03	0.41
1:a:1754:A:O3'	42:o:103:ARG:NH2	2.53	0.41
1:a:2469:A:H4'	8:l:55:ARG:CD	2.50	0.41
1:a:2804:U:H2'	1:a:2805:C:C6	2.56	0.41
2:A:51:A:N7	2:A:114:U:O2'	2.52	0.41
2:A:745:G:O2'	2:A:746:A:H5'	2.21	0.41
5:K:85:MET:HE3	5:K:113:VAL:HG11	2.03	0.41
24:P:6:LEU:CD2	24:P:19:VAL:HG22	2.50	0.41
1:a:1045:C:O2	1:a:1045:C:O4'	2.38	0.41
2:A:555:U:H2'	2:A:556:C:C6	2.56	0.41
2:A:1029:U:O2'	2:A:1032:G:N1	2.49	0.41
7:d:2:ILE:HD13	7:d:90:PHE:CZ	2.56	0.41
35:g:149:ARG:HA	35:g:162:VAL:HB	2.02	0.41
45:r:4:ILE:HG12	45:r:106:VAL:HG22	2.02	0.41
2:A:466:A:H2'	2:A:468:A:C8	2.55	0.41
2:A:993:G:H2'	2:A:993:G:N3	2.36	0.41
20:J:66:GLU:HB3	22:N:99:ALA:HB2	2.02	0.41
32:c:31:ALA:N	32:c:32:PRO:CD	2.84	0.41
47:t:77:THR:HB	47:t:79:LYS:HE3	2.02	0.41
2:A:1062:U:H2'	2:A:1063:C:C6	2.56	0.41
2:A:1189:U:OP1	22:N:98:LYS:NZ	2.54	0.41
2:A:1275:A:H2'	2:A:1276:G:O4'	2.21	0.41
2:A:1435:G:H2'	2:A:1436:U:C6	2.56	0.41
13:C:108:LYS:HD3	13:C:111:LEU:HD12	2.03	0.41
21:M:40:ALA:HB3	21:M:43:VAL:HG23	2.03	0.41
28:T:24:ARG:HB3	28:T:61:GLN:NE2	2.35	0.41
36:h:37:VAL:HG22	36:h:38:PRO:HD2	2.02	0.41
41:n:35:ILE:HG21	41:n:71:ALA:HA	2.03	0.41
53:z:43:ILE:HG22	53:z:49:TYR:HB2	2.03	0.41
1:a:547:A:H4'	1:a:548:G:O4'	2.21	0.41
1:a:1327:A:H2'	1:a:1328:A:O4'	2.21	0.41
1:a:1405:U:H2'	1:a:1406:U:C6	2.55	0.41
1:a:2291:U:H2'	1:a:2292:U:C6	2.56	0.41
1:a:2887:A:N3	53:z:27:SER:OG	2.50	0.41
2:A:49:U:O2	2:A:362:G:H1'	2.20	0.41
31:b:36:C:H5''	31:b:38:C:H41	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:784:G:H5'	1:a:785:G:OP1	2.22	0.40
1:a:1846:G:C6	1:a:1847:A:C6	3.09	0.40
1:a:2491:U:H5''	1:a:2570:G:C5'	2.51	0.40
2:A:663:A:H5'	2:A:836:G:OP1	2.20	0.40
2:A:860:A:H2'	2:A:861:G:O4'	2.21	0.40
2:A:1424:U:H2'	2:A:1425:U:O4'	2.22	0.40
7:d:12:THR:HG21	42:o:5:ILE:HG23	2.03	0.40
33:e:51:GLU:OE1	33:e:88:ARG:NH1	2.47	0.40
47:t:49:VAL:HB	47:t:52:LEU:O	2.21	0.40
1:a:543:G:H5''	1:a:543:G:C8	2.56	0.40
1:a:2191:A:H2'	1:a:2192:U:C6	2.57	0.40
2:A:109:A:C6	2:A:326:G:C6	3.09	0.40
40:m:55:ALA:HA	40:m:80:PHE:CE2	2.56	0.40
1:a:818:G:H5'	1:a:839:U:OP1	2.22	0.40
1:a:1744:A:H3'	1:a:1745:A:H8	1.86	0.40
1:a:1816:C:H3'	32:c:62:TYR:CE1	2.56	0.40
2:A:562:U:H1'	6:L:12:ARG:HB3	2.04	0.40
2:A:1486:G:H2'	2:A:1487:G:O4'	2.21	0.40
7:d:14:ILE:HA	42:o:12:GLN:NE2	2.36	0.40
16:F:91:ARG:HG3	16:F:91:ARG:HH11	1.86	0.40
36:h:31:VAL:HB	36:h:32:PRO:HD3	2.04	0.40
1:a:714:U:H1'	1:a:717:C:H5	1.87	0.40
2:A:660:C:H2'	2:A:661:G:O4'	2.22	0.40
2:A:1490:U:H2'	2:A:1491:G:O4'	2.20	0.40
25:Q:10:GLY:HA3	25:Q:25:ILE:HD13	2.03	0.40
33:e:16:GLU:O	33:e:20:GLY:N	2.52	0.40
37:i:58:ASN:HD21	37:i:128:ASN:HD22	1.69	0.40
1:a:1914:C:H2'	1:a:1915:3TD:H6	2.04	0.40
1:a:2752:C:H2'	1:a:2753:A:O4'	2.21	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	3	36/38 (95%)	36 (100%)	0	0	100	100
4	4	55/70 (79%)	53 (96%)	2 (4%)	0	100	100
5	K	113/129 (88%)	110 (97%)	2 (2%)	1 (1%)	14	20
6	L	120/124 (97%)	115 (96%)	4 (3%)	1 (1%)	16	22
7	d	206/209 (99%)	201 (98%)	5 (2%)	0	100	100
8	l	132/136 (97%)	130 (98%)	2 (2%)	0	100	100
9	0	47/55 (86%)	47 (100%)	0	0	100	100
10	1	43/46 (94%)	43 (100%)	0	0	100	100
11	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
12	B	222/241 (92%)	219 (99%)	3 (1%)	0	100	100
13	C	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
14	D	203/206 (98%)	202 (100%)	0	1 (0%)	24	34
15	E	154/167 (92%)	153 (99%)	1 (1%)	0	100	100
16	F	101/135 (75%)	101 (100%)	0	0	100	100
17	G	143/179 (80%)	137 (96%)	6 (4%)	0	100	100
18	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
19	I	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
20	J	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	12	17
21	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
22	N	98/101 (97%)	98 (100%)	0	0	100	100
23	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
24	P	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
25	Q	75/84 (89%)	72 (96%)	3 (4%)	0	100	100
26	R	53/75 (71%)	53 (100%)	0	0	100	100
27	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
28	T	84/87 (97%)	84 (100%)	0	0	100	100
29	U	68/71 (96%)	68 (100%)	0	0	100	100
32	c	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
33	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
34	f	175/179 (98%)	173 (99%)	2 (1%)	0	100	100
35	g	174/177 (98%)	170 (98%)	3 (2%)	1 (1%)	21	29
36	h	39/149 (26%)	37 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	i	140/142 (99%)	140 (100%)	0	0	100	100
38	j	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
39	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
40	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
41	n	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
42	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
43	p	115/118 (98%)	115 (100%)	0	0	100	100
44	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
45	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
46	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
47	t	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
48	u	92/94 (98%)	92 (100%)	0	0	100	100
49	v	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
50	w	75/78 (96%)	75 (100%)	0	0	100	100
51	x	60/63 (95%)	60 (100%)	0	0	100	100
52	y	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
53	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
55	8	11/19 (58%)	10 (91%)	1 (9%)	0	100	100
All	All	5463/5932 (92%)	5362 (98%)	96 (2%)	5 (0%)	49	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	L	102	LEU
20	J	57	VAL
5	K	17	SER
14	D	46	PRO
35	g	61	GLY

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	3	34/34 (100%)	34 (100%)	0	100	100
4	4	54/62 (87%)	54 (100%)	0	100	100
5	K	89/98 (91%)	88 (99%)	1 (1%)	65	79
6	L	102/103 (99%)	102 (100%)	0	100	100
7	d	163/163 (100%)	162 (99%)	1 (1%)	78	87
8	l	107/107 (100%)	107 (100%)	0	100	100
9	0	45/49 (92%)	45 (100%)	0	100	100
10	1	37/38 (97%)	37 (100%)	0	100	100
11	2	51/52 (98%)	50 (98%)	1 (2%)	48	67
12	B	186/199 (94%)	186 (100%)	0	100	100
13	C	170/190 (90%)	169 (99%)	1 (1%)	78	87
14	D	172/173 (99%)	170 (99%)	2 (1%)	63	78
15	E	119/126 (94%)	119 (100%)	0	100	100
16	F	90/116 (78%)	89 (99%)	1 (1%)	65	79
17	G	122/147 (83%)	122 (100%)	0	100	100
18	H	104/105 (99%)	104 (100%)	0	100	100
19	I	105/107 (98%)	104 (99%)	1 (1%)	68	80
20	J	86/90 (96%)	86 (100%)	0	100	100
21	M	93/96 (97%)	93 (100%)	0	100	100
22	N	83/84 (99%)	83 (100%)	0	100	100
23	O	76/77 (99%)	76 (100%)	0	100	100
24	P	65/65 (100%)	65 (100%)	0	100	100
25	Q	71/78 (91%)	71 (100%)	0	100	100
26	R	48/65 (74%)	48 (100%)	0	100	100
27	S	72/79 (91%)	72 (100%)	0	100	100
28	T	65/66 (98%)	65 (100%)	0	100	100
29	U	60/61 (98%)	60 (100%)	0	100	100
32	c	216/218 (99%)	216 (100%)	0	100	100
33	e	165/165 (100%)	165 (100%)	0	100	100
34	f	148/150 (99%)	146 (99%)	2 (1%)	59	75
35	g	137/138 (99%)	136 (99%)	1 (1%)	76	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	h	32/114 (28%)	32 (100%)	0	100	100
37	i	116/116 (100%)	116 (100%)	0	100	100
38	j	104/104 (100%)	104 (100%)	0	100	100
39	k	103/103 (100%)	103 (100%)	0	100	100
40	m	98/103 (95%)	98 (100%)	0	100	100
41	n	86/87 (99%)	85 (99%)	1 (1%)	63	78
42	o	99/100 (99%)	99 (100%)	0	100	100
43	p	89/90 (99%)	89 (100%)	0	100	100
44	q	84/84 (100%)	84 (100%)	0	100	100
45	r	93/93 (100%)	92 (99%)	1 (1%)	65	79
46	s	80/84 (95%)	79 (99%)	1 (1%)	61	76
47	t	83/85 (98%)	81 (98%)	2 (2%)	43	61
48	u	78/78 (100%)	78 (100%)	0	100	100
49	v	56/63 (89%)	56 (100%)	0	100	100
50	w	67/68 (98%)	67 (100%)	0	100	100
51	x	54/55 (98%)	54 (100%)	0	100	100
52	y	48/49 (98%)	48 (100%)	0	100	100
53	z	47/48 (98%)	47 (100%)	0	100	100
55	8	13/18 (72%)	13 (100%)	0	100	100
All	All	4565/4843 (94%)	4549 (100%)	16 (0%)	81	90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	K	129	VAL
7	d	110	THR
11	2	31	HIS
13	C	178	LEU
14	D	44	ARG
14	D	188	ARG
16	F	62	MET
19	I	85	ARG
34	f	120	LYS
34	f	150	ARG
35	g	3	ARG

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Mol	Chain	Res	Type
41	n	16	ARG
45	r	66	ILE
46	s	93	LEU
47	t	17	LYS
47	t	54	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
4	4	20	ASN
4	4	30	HIS
4	4	33	ASN
4	4	48	GLN
5	K	118	HIS
6	L	112	GLN
7	d	32	ASN
7	d	173	GLN
8	l	60	GLN
11	2	31	HIS
12	B	42	ASN
12	B	89	GLN
12	B	103	ASN
12	B	120	GLN
13	C	139	GLN
13	C	140	ASN
14	D	40	GLN
14	D	41	HIS
14	D	71	GLN
14	D	140	ASN
15	E	70	ASN
15	E	82	GLN
15	E	97	GLN
15	E	121	HIS
16	F	3	HIS
16	F	55	HIS
17	G	9	GLN
17	G	68	ASN
17	G	86	GLN
18	H	4	GLN
18	H	21	ASN
19	I	31	ASN
19	I	75	GLN

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Mol	Chain	Res	Type
19	I	110	GLN
20	J	58	ASN
22	N	4	GLN
22	N	35	ASN
22	N	60	GLN
22	N	66	GLN
23	O	50	HIS
23	O	80	GLN
24	P	29	ASN
28	T	13	GLN
28	T	20	HIS
28	T	84	ASN
29	U	64	ASN
32	c	25	HIS
32	c	90	ASN
32	c	197	ASN
33	e	90	GLN
33	e	165	HIS
34	f	27	GLN
35	g	22	GLN
35	g	30	ASN
35	g	73	ASN
35	g	104	ASN
36	h	2	GLN
37	i	128	ASN
37	i	138	GLN
38	j	3	GLN
41	n	29	HIS
42	o	10	GLN
42	o	12	GLN
43	p	37	GLN
44	q	6	GLN
44	q	12	HIS
44	q	66	HIS
45	r	40	ASN
46	s	92	ASN
47	t	40	ASN
48	u	24	ASN
48	u	49	ASN
50	w	6	GLN
51	x	15	ASN
51	x	20	ASN

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Mol	Chain	Res	Type
51	x	27	ASN
51	x	36	GLN
51	x	45	GLN
51	x	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	2749/2904 (94%)	305 (11%)	0
2	A	1516/1542 (98%)	206 (13%)	31 (2%)
30	X	5/6 (83%)	2 (40%)	0
31	b	118/120 (98%)	11 (9%)	0
54	Z	75/77 (97%)	22 (29%)	2 (2%)
All	All	4463/4649 (95%)	546 (12%)	33 (0%)

All (546) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	10	A
1	a	34	U
1	a	63	A
1	a	71	A
1	a	74	A
1	a	75	G
1	a	101	A
1	a	102	U
1	a	118	A
1	a	119	A
1	a	120	U
1	a	139	U
1	a	142	A
1	a	163	C
1	a	181	A
1	a	196	A
1	a	199	A
1	a	200	U
1	a	215	G
1	a	216	A
1	a	221	A
1	a	222	A
1	a	248	G

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Mol	Chain	Res	Type
1	a	272	A
1	a	278	A
1	a	282	A
1	a	285	G
1	a	286	U
1	a	289	G
1	a	294	A
1	a	311	A
1	a	329	G
1	a	330	A
1	a	357	C
1	a	361	G
1	a	362	A
1	a	386	G
1	a	404	A
1	a	405	U
1	a	411	G
1	a	412	A
1	a	451	U
1	a	481	G
1	a	491	G
1	a	503	A
1	a	504	A
1	a	505	A
1	a	509	C
1	a	532	A
1	a	533	G
1	a	543	G
1	a	544	C
1	a	545	U
1	a	546	U
1	a	549	G
1	a	563	A
1	a	573	U
1	a	575	A
1	a	586	A
1	a	603	A
1	a	614	A
1	a	615	U
1	a	627	A
1	a	637	A
1	a	645	C

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Mol	Chain	Res	Type
1	a	646	U
1	a	647	G
1	a	654	A
1	a	655	A
1	a	686	U
1	a	717	C
1	a	730	A
1	a	738	G
1	a	747	5MU
1	a	764	A
1	a	765	C
1	a	775	G
1	a	776	G
1	a	782	A
1	a	784	G
1	a	785	G
1	a	792	A
1	a	805	G
1	a	812	C
1	a	827	U
1	a	828	U
1	a	846	U
1	a	847	U
1	a	858	G
1	a	859	G
1	a	881	G
1	a	883	G
1	a	884	U
1	a	891	G
1	a	893	C
1	a	895	U
1	a	896	A
1	a	897	C
1	a	898	C
1	a	910	A
1	a	914	G
1	a	915	C
1	a	931	U
1	a	934	U
1	a	946	C
1	a	961	C
1	a	974	G

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Mol	Chain	Res	Type
1	a	983	A
1	a	984	A
1	a	985	C
1	a	996	A
1	a	1009	A
1	a	1012	U
1	a	1013	C
1	a	1022	G
1	a	1026	G
1	a	1033	U
1	a	1045	C
1	a	1046	A
1	a	1108	U
1	a	1110	G
1	a	1111	A
1	a	1112	G
1	a	1115	G
1	a	1116	G
1	a	1122	G
1	a	1128	G
1	a	1129	A
1	a	1132	U
1	a	1133	A
1	a	1134	A
1	a	1135	C
1	a	1142	A
1	a	1171	G
1	a	1227	G
1	a	1253	A
1	a	1256	G
1	a	1271	G
1	a	1272	A
1	a	1301	A
1	a	1321	A
1	a	1352	U
1	a	1365	A
1	a	1379	U
1	a	1383	A
1	a	1411	U
1	a	1416	G
1	a	1419	A
1	a	1421	G

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Mol	Chain	Res	Type
1	a	1428	C
1	a	1452	G
1	a	1453	A
1	a	1455	G
1	a	1482	G
1	a	1493	C
1	a	1497	U
1	a	1498	C
1	a	1509	A
1	a	1510	G
1	a	1515	A
1	a	1534	U
1	a	1535	A
1	a	1536	C
1	a	1537	G
1	a	1566	A
1	a	1569	A
1	a	1578	U
1	a	1585	C
1	a	1608	A
1	a	1609	A
1	a	1618	6MZ
1	a	1619	G
1	a	1647	U
1	a	1648	U
1	a	1649	G
1	a	1674	G
1	a	1715	G
1	a	1729	U
1	a	1730	C
1	a	1731	G
1	a	1733	G
1	a	1738	G
1	a	1764	C
1	a	1773	A
1	a	1782	U
1	a	1800	C
1	a	1801	A
1	a	1808	A
1	a	1809	A
1	a	1816	C
1	a	1829	A

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Mol	Chain	Res	Type
1	a	1847	A
1	a	1848	A
1	a	1858	A
1	a	1870	C
1	a	1871	A
1	a	1873	G
1	a	1906	G
1	a	1907	G
1	a	1913	A
1	a	1914	C
1	a	1929	G
1	a	1930	G
1	a	1937	A
1	a	1938	A
1	a	1939	5MU
1	a	1955	U
1	a	1967	C
1	a	1970	A
1	a	1971	U
1	a	1972	G
1	a	1991	U
1	a	1993	U
1	a	2020	A
1	a	2023	C
1	a	2031	A
1	a	2033	A
1	a	2043	C
1	a	2055	C
1	a	2056	G
1	a	2060	A
1	a	2061	G
1	a	2062	A
1	a	2069	G7M
1	a	2093	G
1	a	2198	A
1	a	2203	U
1	a	2204	G
1	a	2211	A
1	a	2212	A
1	a	2225	A
1	a	2238	G
1	a	2239	G

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Mol	Chain	Res	Type
1	a	2268	A
1	a	2273	A
1	a	2278	A
1	a	2283	C
1	a	2287	A
1	a	2305	U
1	a	2308	G
1	a	2312	U
1	a	2322	A
1	a	2324	U
1	a	2325	G
1	a	2333	A
1	a	2335	A
1	a	2336	A
1	a	2347	C
1	a	2350	C
1	a	2377	A
1	a	2383	G
1	a	2385	C
1	a	2402	U
1	a	2403	C
1	a	2406	A
1	a	2424	C
1	a	2425	A
1	a	2429	G
1	a	2430	A
1	a	2435	A
1	a	2441	U
1	a	2448	A
1	a	2459	A
1	a	2469	A
1	a	2476	A
1	a	2478	A
1	a	2491	U
1	a	2502	G
1	a	2505	G
1	a	2506	U
1	a	2518	A
1	a	2529	G
1	a	2535	G
1	a	2547	A
1	a	2566	A

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Mol	Chain	Res	Type
1	a	2567	G
1	a	2573	C
1	a	2574	G
1	a	2602	A
1	a	2603	G
1	a	2609	U
1	a	2613	U
1	a	2629	U
1	a	2663	G
1	a	2689	U
1	a	2690	U
1	a	2714	G
1	a	2716	C
1	a	2726	A
1	a	2744	G
1	a	2748	A
1	a	2750	A
1	a	2757	A
1	a	2765	A
1	a	2778	A
1	a	2790	U
1	a	2791	G
1	a	2798	U
1	a	2799	A
1	a	2820	A
1	a	2821	A
1	a	2873	A
1	a	2874	C
1	a	2883	A
1	a	2884	U
2	A	4	U
2	A	5	U
2	A	6	G
2	A	8	A
2	A	9	G
2	A	32	A
2	A	39	G
2	A	47	C
2	A	48	C
2	A	51	A
2	A	70	U
2	A	71	A

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Mol	Chain	Res	Type
2	A	74	A
2	A	83	C
2	A	84	U
2	A	85	U
2	A	86	G
2	A	87	C
2	A	88	U
2	A	94	G
2	A	95	C
2	A	120	A
2	A	122	G
2	A	131	A
2	A	141	G
2	A	144	G
2	A	164	G
2	A	166	U
2	A	182	A
2	A	183	C
2	A	197	A
2	A	202	G
2	A	204	G
2	A	226	G
2	A	240	G
2	A	245	U
2	A	247	G
2	A	251	G
2	A	266	G
2	A	267	C
2	A	271	C
2	A	280	C
2	A	281	G
2	A	289	G
2	A	321	A
2	A	328	C
2	A	329	A
2	A	339	C
2	A	347	G
2	A	352	C
2	A	354	G
2	A	367	U
2	A	372	C
2	A	406	G

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Mol	Chain	Res	Type
2	A	412	A
2	A	413	G
2	A	414	A
2	A	417	G
2	A	421	U
2	A	422	C
2	A	424	G
2	A	429	U
2	A	436	C
2	A	438	U
2	A	439	U
2	A	453	G
2	A	457	G
2	A	458	U
2	A	459	A
2	A	463	U
2	A	465	A
2	A	467	U
2	A	468	A
2	A	469	C
2	A	478	A
2	A	479	U
2	A	481	G
2	A	484	G
2	A	486	U
2	A	511	C
2	A	518	C
2	A	531	U
2	A	532	A
2	A	536	C
2	A	547	A
2	A	572	A
2	A	573	A
2	A	576	C
2	A	577	G
2	A	587	G
2	A	588	G
2	A	596	A
2	A	633	G
2	A	641	U
2	A	642	A
2	A	648	A

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Mol	Chain	Res	Type
2	A	650	G
2	A	653	U
2	A	665	A
2	A	721	G
2	A	723	U
2	A	724	G
2	A	734	G
2	A	746	A
2	A	748	G
2	A	755	G
2	A	777	A
2	A	793	U
2	A	794	A
2	A	815	A
2	A	817	C
2	A	890	G
2	A	914	A
2	A	926	G
2	A	934	C
2	A	935	A
2	A	960	U
2	A	966	2MG
2	A	969	A
2	A	975	A
2	A	976	G
2	A	977	A
2	A	984	C
2	A	992	U
2	A	993	G
2	A	994	A
2	A	996	A
2	A	1003	G
2	A	1004	A
2	A	1006	G
2	A	1007	U
2	A	1008	U
2	A	1009	U
2	A	1024	G
2	A	1027	C
2	A	1030	U
2	A	1031	C
2	A	1033	G

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Mol	Chain	Res	Type
2	A	1034	G
2	A	1035	A
2	A	1036	A
2	A	1039	G
2	A	1046	A
2	A	1065	U
2	A	1094	G
2	A	1095	U
2	A	1101	A
2	A	1129	C
2	A	1130	A
2	A	1132	C
2	A	1137	C
2	A	1139	G
2	A	1145	A
2	A	1146	A
2	A	1184	G
2	A	1196	A
2	A	1197	A
2	A	1211	U
2	A	1212	U
2	A	1213	A
2	A	1214	C
2	A	1225	A
2	A	1226	C
2	A	1227	A
2	A	1238	A
2	A	1256	A
2	A	1260	G
2	A	1275	A
2	A	1280	A
2	A	1286	U
2	A	1287	A
2	A	1300	G
2	A	1302	C
2	A	1317	C
2	A	1319	A
2	A	1320	C
2	A	1331	G
2	A	1338	G
2	A	1346	A
2	A	1353	G

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Mol	Chain	Res	Type
2	A	1363	A
2	A	1370	G
2	A	1378	C
2	A	1379	G
2	A	1381	U
2	A	1397	C
2	A	1398	A
2	A	1419	G
2	A	1429	A
2	A	1441	A
2	A	1447	A
2	A	1448	C
2	A	1451	U
2	A	1452	C
2	A	1453	G
2	A	1492	A
2	A	1493	A
2	A	1494	G
2	A	1497	G
2	A	1505	G
2	A	1506	U
2	A	1517	G
2	A	1529	G
2	A	1530	G
2	A	1533	C
2	A	1534	A
30	X	15	A
30	X	18	G
31	b	35	C
31	b	36	C
31	b	37	C
31	b	45	A
31	b	56	G
31	b	57	A
31	b	67	G
31	b	89	U
31	b	90	C
31	b	99	A
31	b	109	A
54	Z	4	G
54	Z	6	G
54	Z	7	G

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Mol	Chain	Res	Type
54	Z	8	U
54	Z	9	G
54	Z	14	A
54	Z	16	C
54	Z	17	C
54	Z	17(A)	U
54	Z	18	G
54	Z	19	G
54	Z	20	U
54	Z	21	A
54	Z	43	A
54	Z	46	G
54	Z	47	U
54	Z	51	C
54	Z	58	A
54	Z	61	C
54	Z	65	C
54	Z	69	C
54	Z	76	A

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	5	U
2	A	7	A
2	A	13	U
2	A	62	U
2	A	70	U
2	A	94	G
2	A	119	A
2	A	199	A
2	A	280	C
2	A	438	U
2	A	587	G
2	A	641	U
2	A	776	G
2	A	858	G
2	A	992	U
2	A	993	G
2	A	1006	G
2	A	1034	G
2	A	1035	A

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Mol	Chain	Res	Type
2	A	1124	G
2	A	1129	C
2	A	1137	C
2	A	1145	A
2	A	1211	U
2	A	1225	A
2	A	1239	A
2	A	1319	A
2	A	1320	C
2	A	1397	C
2	A	1447	A
2	A	1505	G
54	Z	7	G
54	Z	46	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	5MC	a	1962	1	18,22,23	0.40	0	26,32,35	0.65	0
1	5MU	a	1939	1	19,22,23	0.50	0	28,32,35	0.36	0
1	2MG	a	2445	1	23,26,27	0.54	0	32,38,41	0.40	0
1	2MG	a	1835	1	23,26,27	0.38	0	32,38,41	0.44	0
2	MA6	A	1519	2	23,26,27	0.42	0	34,38,41	0.80	1 (2%)
1	6MZ	a	1618	1	22,25,26	0.40	0	30,36,39	0.62	0
1	OMG	a	2251	1,54	23,26,27	0.46	0	33,38,41	0.45	0
6	D2T	L	89	6	7,9,10	1.01	0	6,11,13	1.77	3 (50%)
1	1MG	a	745	1	22,26,27	0.88	2 (9%)	33,39,42	0.44	0
2	2MG	A	1207	2	23,26,27	0.38	0	32,38,41	0.43	0
2	PSU	A	516	2	18,21,22	0.90	1 (5%)	22,30,33	0.68	0
2	5MC	A	967	2	18,22,23	0.36	0	26,32,35	0.56	0
1	PSU	a	1917	1	18,21,22	0.87	1 (5%)	22,30,33	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MEQ	d	150	7	8,9,10	0.59	0	5,10,12	0.89	0
1	OMC	a	2498	1	19,22,23	0.52	0	26,31,34	0.55	0
8	4D4	l	81	8	9,11,12	1.87	2 (22%)	8,13,15	1.29	0
1	PSU	a	746	1	18,21,22	0.98	1 (5%)	22,30,33	0.71	0
1	3TD	a	1915	1	18,22,23	0.85	1 (5%)	22,32,35	0.62	0
1	OMU	a	2552	1	19,22,23	0.50	0	26,31,34	0.48	0
2	2MG	A	1516	2	23,26,27	0.43	0	32,38,41	0.53	0
1	6MZ	a	2030	1	22,25,26	0.81	0	30,36,39	0.69	0
2	UR3	A	1498	2	19,22,23	0.42	0	26,32,35	0.69	0
2	MA6	A	1518	2	23,26,27	0.35	0	34,38,41	0.74	1 (2%)
1	PSU	a	2457	1	18,21,22	0.93	1 (5%)	22,30,33	0.63	0
1	PSU	a	1911	1	18,21,22	0.86	1 (5%)	22,30,33	0.60	0
8	MS6	l	82	8	5,7,8	0.23	0	2,7,9	0.27	0
2	4OC	A	1402	2	20,23,24	0.34	0	26,32,35	0.56	0
1	H2U	a	2449	1	18,21,22	0.70	0	21,30,33	0.98	2 (9%)
1	PSU	a	2580	1	18,21,22	1.03	1 (5%)	22,30,33	0.79	1 (4%)
1	PSU	a	2504	1	18,21,22	0.90	1 (5%)	22,30,33	0.71	1 (4%)
2	2MG	A	966	2	23,26,27	0.41	0	32,38,41	0.41	0
1	PSU	a	2604	1	18,21,22	1.01	2 (11%)	22,30,33	0.83	1 (4%)
2	G7M	A	527	2	23,26,27	0.78	1 (4%)	35,39,42	0.64	1 (2%)
1	PSU	a	2605	1	18,21,22	0.96	1 (5%)	22,30,33	0.92	1 (4%)
1	5MU	a	747	1	19,22,23	0.43	0	28,32,35	0.49	0
1	G7M	a	2069	1	23,26,27	0.80	0	35,39,42	0.71	0
5	IAS	K	119	5	6,7,8	1.36	1 (16%)	6,8,10	0.88	0
1	2MA	a	2503	1	22,25,26	0.55	0	33,37,40	0.76	1 (3%)
1	PSU	a	955	1	18,21,22	0.93	1 (5%)	22,30,33	0.69	0
2	5MC	A	1407	2	18,22,23	0.32	0	26,32,35	0.68	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	5MC	a	1962	1	-	1/7/25/26	0/2/2/2
1	5MU	a	1939	1	-	0/7/25/26	0/2/2/2
1	2MG	a	2445	1	-	0/9/27/28	0/3/3/3
1	2MG	a	1835	1	-	0/9/27/28	0/3/3/3
2	MA6	A	1519	2	-	2/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6MZ	a	1618	1	-	0/9/27/28	0/3/3/3
1	OMG	a	2251	1,54	-	0/9/27/28	0/3/3/3
6	D2T	L	89	6	-	5/7/12/14	-
1	1MG	a	745	1	-	0/7/25/26	0/3/3/3
2	2MG	A	1207	2	-	0/9/27/28	0/3/3/3
2	PSU	A	516	2	-	0/7/25/26	0/2/2/2
2	5MC	A	967	2	-	0/7/25/26	0/2/2/2
1	PSU	a	1917	1	-	0/7/25/26	0/2/2/2
7	MEQ	d	150	7	-	2/8/9/11	-
1	OMC	a	2498	1	-	0/9/27/28	0/2/2/2
8	4D4	l	81	8	-	1/11/12/14	-
1	PSU	a	746	1	-	1/7/25/26	0/2/2/2
1	3TD	a	1915	1	-	0/7/25/26	0/2/2/2
1	OMU	a	2552	1	-	0/9/27/28	0/2/2/2
2	2MG	A	1516	2	-	0/9/27/28	0/3/3/3
1	6MZ	a	2030	1	-	2/9/27/28	0/3/3/3
2	UR3	A	1498	2	-	0/7/25/26	0/2/2/2
2	MA6	A	1518	2	-	0/11/29/30	0/3/3/3
1	PSU	a	2457	1	-	0/7/25/26	0/2/2/2
1	PSU	a	1911	1	-	0/7/25/26	0/2/2/2
8	MS6	l	82	8	-	1/4/6/8	-
2	4OC	A	1402	2	-	0/9/29/30	0/2/2/2
1	H2U	a	2449	1	-	0/7/38/39	0/2/2/2
1	PSU	a	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	a	2504	1	-	0/7/25/26	0/2/2/2
2	2MG	A	966	2	-	0/9/27/28	0/3/3/3
1	PSU	a	2604	1	-	0/7/25/26	0/2/2/2
2	G7M	A	527	2	-	1/7/25/26	0/3/3/3
1	PSU	a	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	a	747	1	-	0/7/25/26	0/2/2/2
1	G7M	a	2069	1	-	2/7/25/26	0/3/3/3
5	IAS	K	119	5	-	0/7/7/8	-
1	2MA	a	2503	1	-	2/7/25/26	0/3/3/3
1	PSU	a	955	1	-	0/7/25/26	0/2/2/2
2	5MC	A	1407	2	-	0/7/25/26	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	l	81	4D4	CZ-NE	4.01	1.41	1.33
2	A	516	PSU	C6-C5	3.46	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1915	3TD	C6-C5	3.40	1.39	1.35
1	a	2504	PSU	C6-C5	3.32	1.39	1.35
1	a	1911	PSU	C6-C5	3.25	1.39	1.35
1	a	1917	PSU	C6-C5	3.25	1.39	1.35
2	A	527	G7M	C8-N7	2.99	1.38	1.33
1	a	2604	PSU	C6-C5	2.96	1.38	1.35
8	l	81	4D4	CZ-NH2	2.84	1.43	1.32
1	a	2580	PSU	C6-C5	2.81	1.38	1.35
5	K	119	IAS	CB-CG	2.74	1.56	1.49
1	a	2457	PSU	C6-C5	2.72	1.38	1.35
1	a	955	PSU	C6-C5	2.67	1.38	1.35
1	a	2605	PSU	C6-C5	2.45	1.38	1.35
1	a	2604	PSU	C4-C5	-2.43	1.37	1.44
1	a	745	1MG	C1'-N9	-2.34	1.40	1.47
1	a	746	PSU	C6-C5	2.34	1.38	1.35
1	a	745	1MG	C5-C6	-2.00	1.40	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1518	MA6	C2-N1-C6	3.11	119.11	111.75
2	A	1519	MA6	C2-N1-C6	3.05	118.96	111.75
1	a	2449	H2U	N3-C2-N1	2.61	119.42	116.65
6	L	89	D2T	OD1-CG-CB	-2.56	117.07	122.44
1	a	2503	2MA	C5-C4-N3	-2.40	124.49	127.19
1	a	2449	H2U	O2-C2-N1	-2.37	120.13	123.11
1	a	2580	PSU	C3'-C2'-C1'	2.25	104.26	101.64
1	a	2504	PSU	C2'-C3'-C4'	-2.19	98.39	102.64
6	L	89	D2T	OD2-CG-CB	2.18	117.86	113.15
6	L	89	D2T	O-C-CA	-2.15	119.14	124.78
1	a	2604	PSU	C2'-C3'-C4'	-2.11	98.55	102.64
1	a	2605	PSU	C2'-C3'-C4'	-2.01	98.74	102.64
2	A	527	G7M	N9-C8-N7	-2.00	107.25	112.21

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	89	D2T	O-C-CA-CB
6	L	89	D2T	CA-CB-CG-OD1
6	L	89	D2T	CA-CB-CG-OD2
6	L	89	D2T	SB-CB-CG-OD2

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Mol	Chain	Res	Type	Atoms
1	a	2030	6MZ	O4'-C4'-C5'-O5'
1	a	2030	6MZ	C3'-C4'-C5'-O5'
7	d	150	MEQ	OE1-CD-CG-CB
7	d	150	MEQ	NE2-CD-CG-CB
2	A	1519	MA6	C5-C6-N6-C10
6	L	89	D2T	CG-CB-SB-CB1
2	A	527	G7M	C3'-C4'-C5'-O5'
1	a	2069	G7M	O4'-C4'-C5'-O5'
2	A	1519	MA6	O4'-C4'-C5'-O5'
1	a	1962	5MC	O4'-C1'-N1-C6
1	a	746	PSU	O4'-C1'-C5-C6
1	a	2069	G7M	C4'-C5'-O5'-P
8	l	82	MS6	CB-CG-SD-CE
1	a	2503	2MA	O4'-C4'-C5'-O5'
8	l	81	4D4	O-C-CA-CB
1	a	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	1939	5MU	1	0
1	a	1915	3TD	2	0
1	a	2552	OMU	1	0
1	a	2030	6MZ	2	0
1	a	2604	PSU	1	0
5	K	119	IAS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

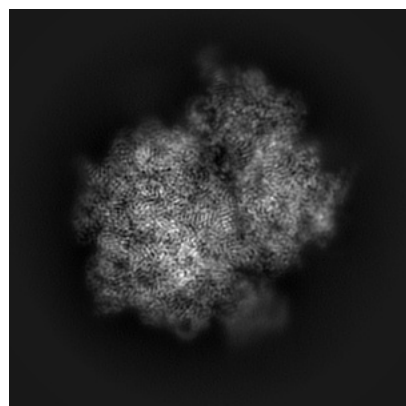
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55845. These allow visual inspection of the internal detail of the map and identification of artifacts.

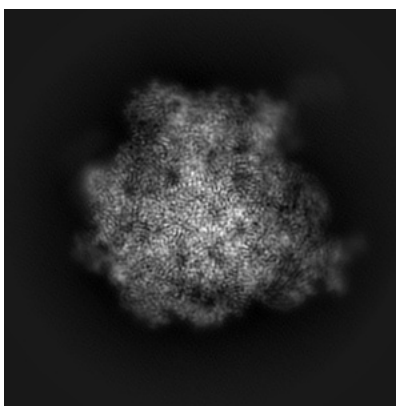
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

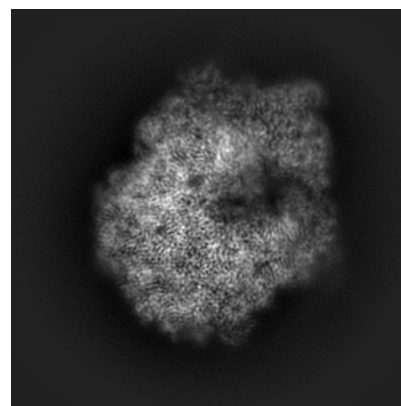
6.1.1 Primary map



X

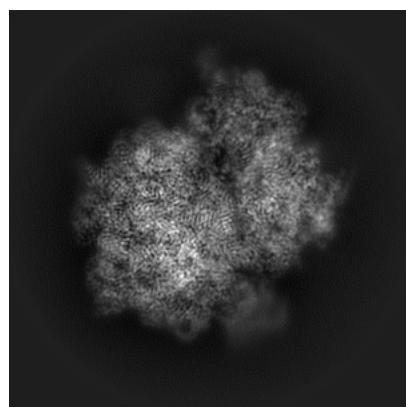


Y

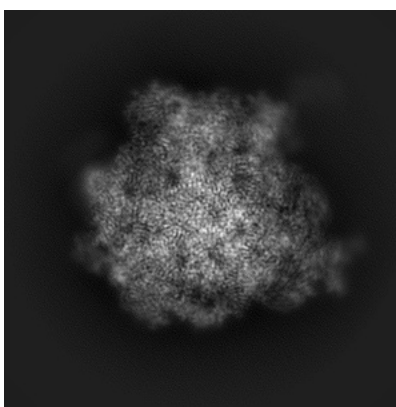


Z

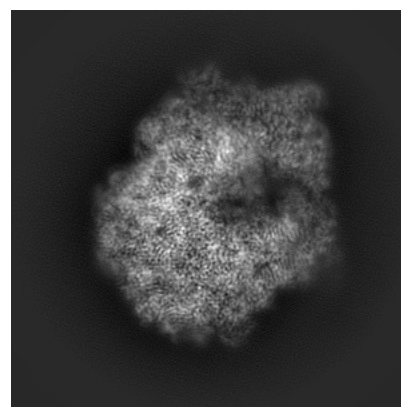
6.1.2 Raw map



X



Y

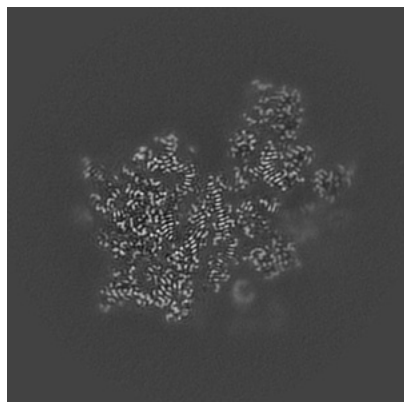


Z

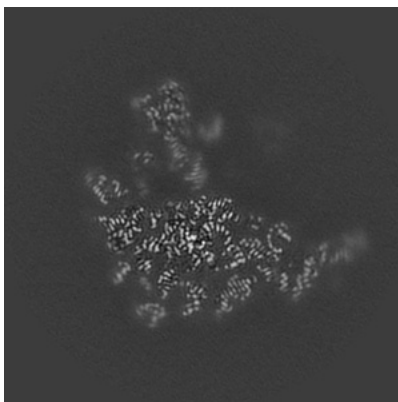
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

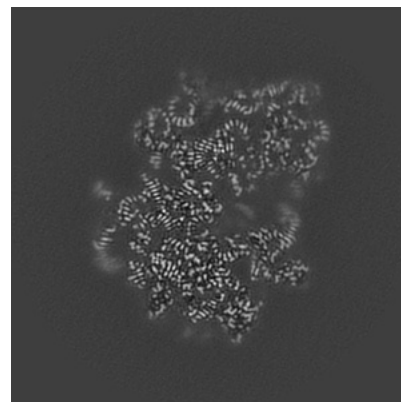
6.2.1 Primary map



X Index: 208

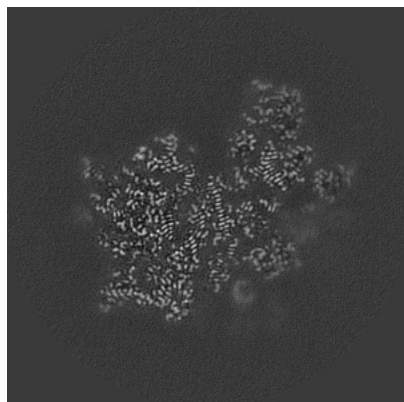


Y Index: 208



Z Index: 208

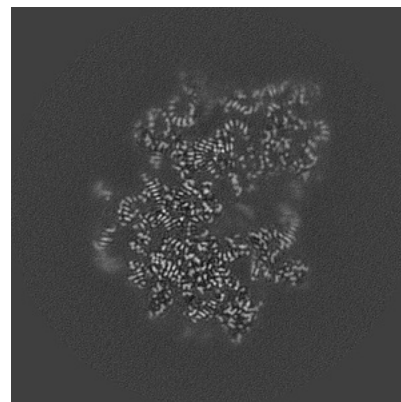
6.2.2 Raw map



X Index: 208



Y Index: 208

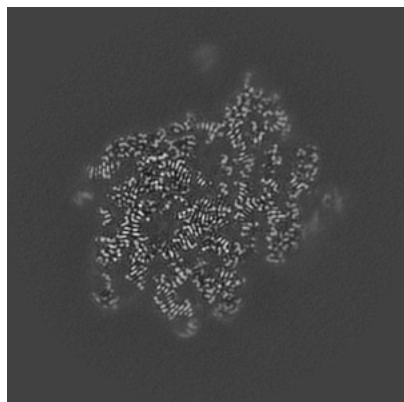


Z Index: 208

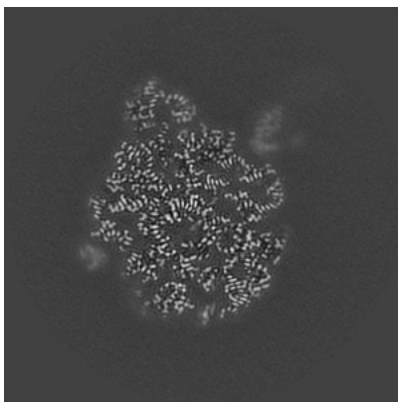
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

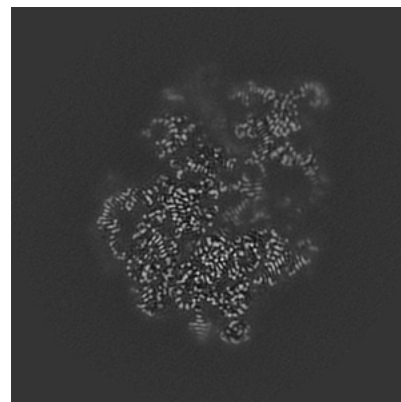
6.3.1 Primary map



X Index: 178

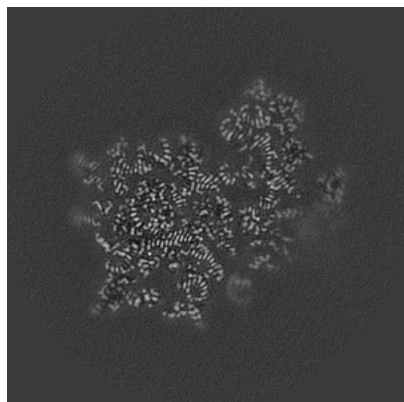


Y Index: 169

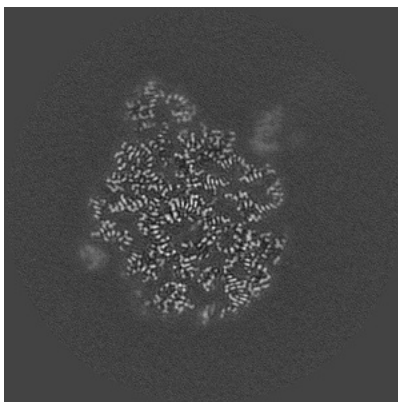


Z Index: 194

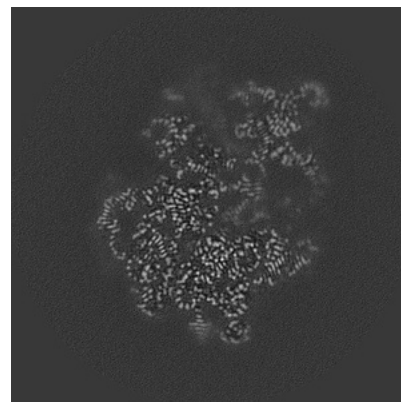
6.3.2 Raw map



X Index: 199



Y Index: 169

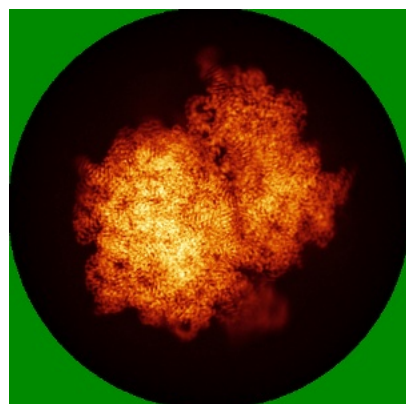


Z Index: 194

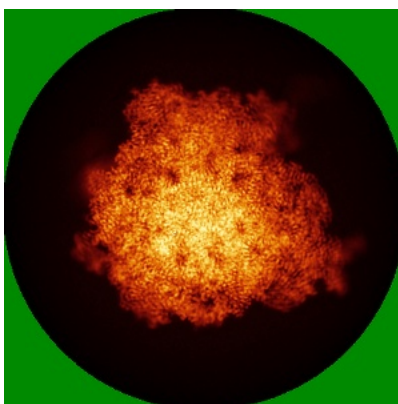
The images above show the largest variance slices of the map in three orthogonal directions.

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

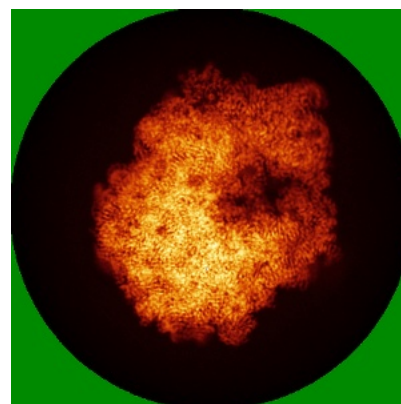
6.4.1 Primary map



X

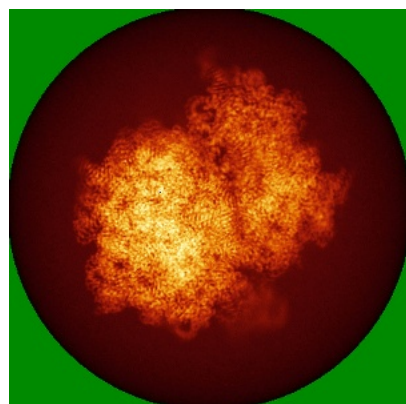


Y

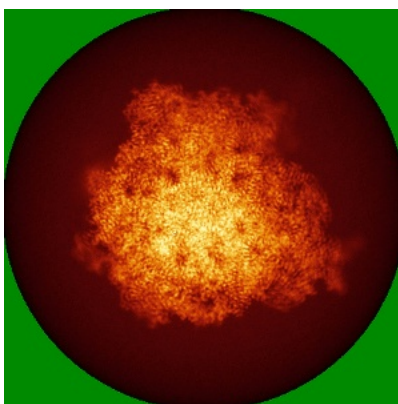


Z

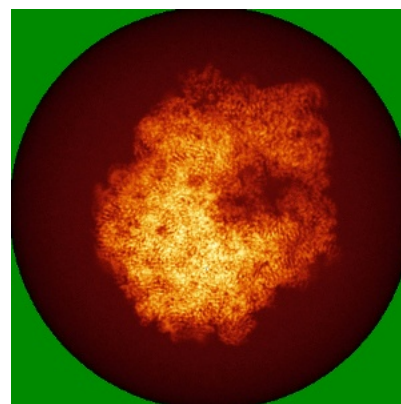
6.4.2 Raw map



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



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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



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.

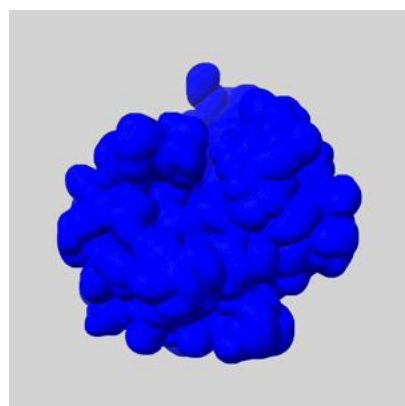
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

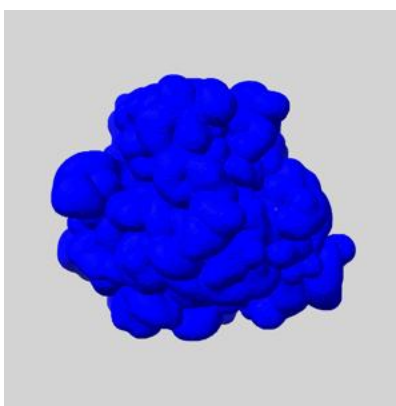
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

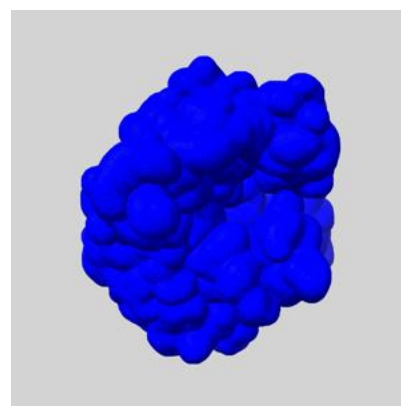
6.6.1 emd_55845_msk_1.map [i](#)



X



Y

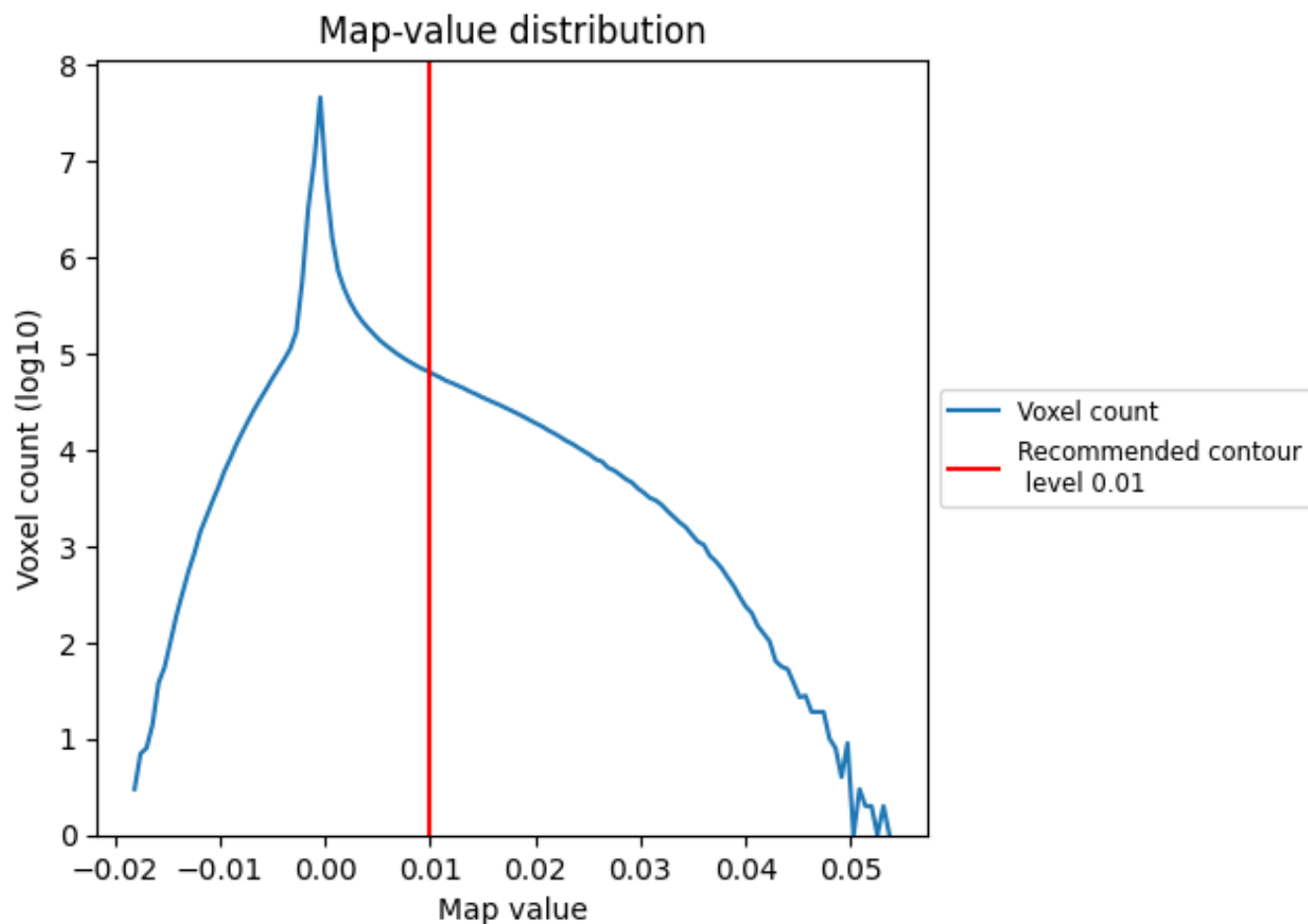


Z

7 Map analysis [i](#)

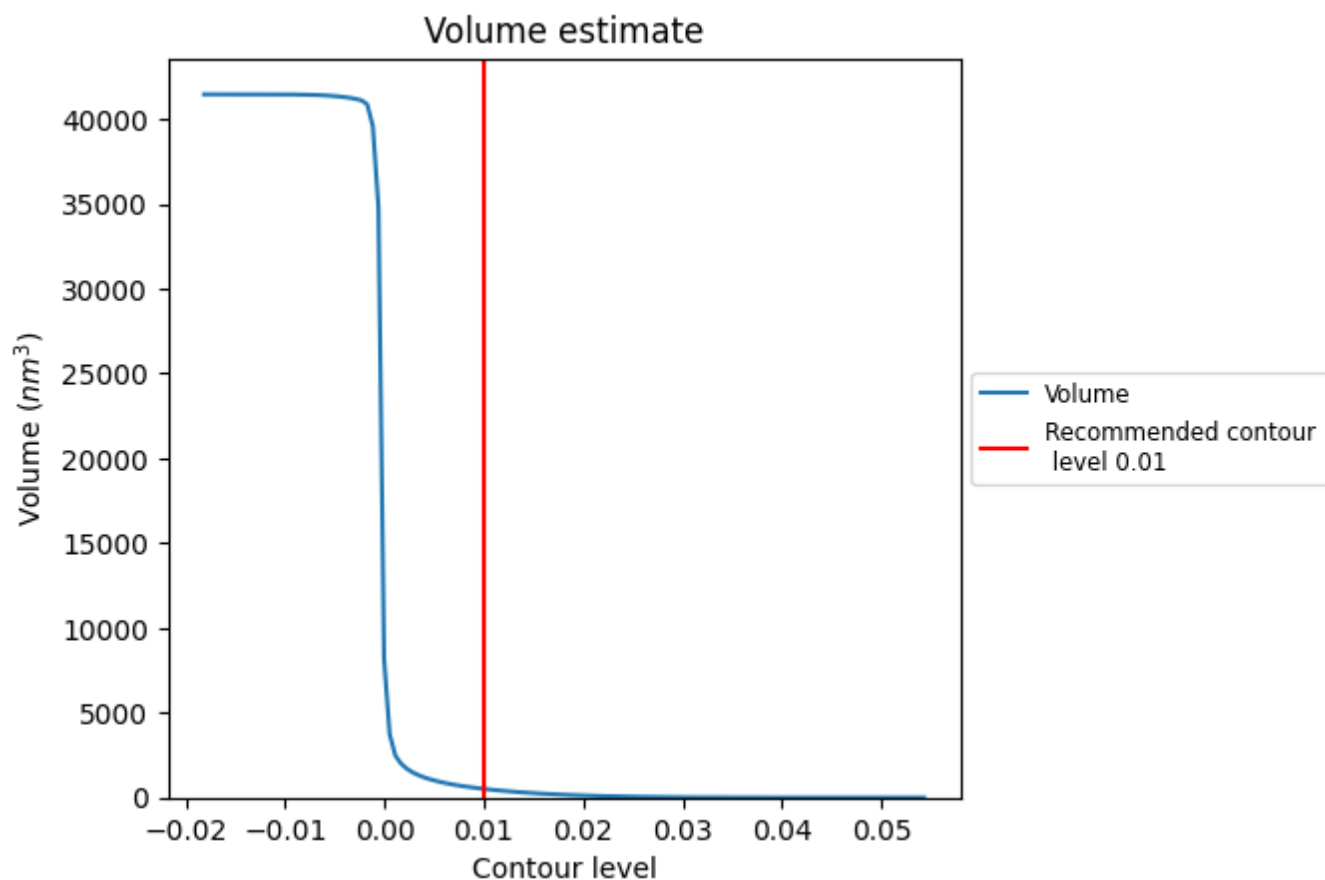
This section contains the results of statistical analysis of the map.

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.

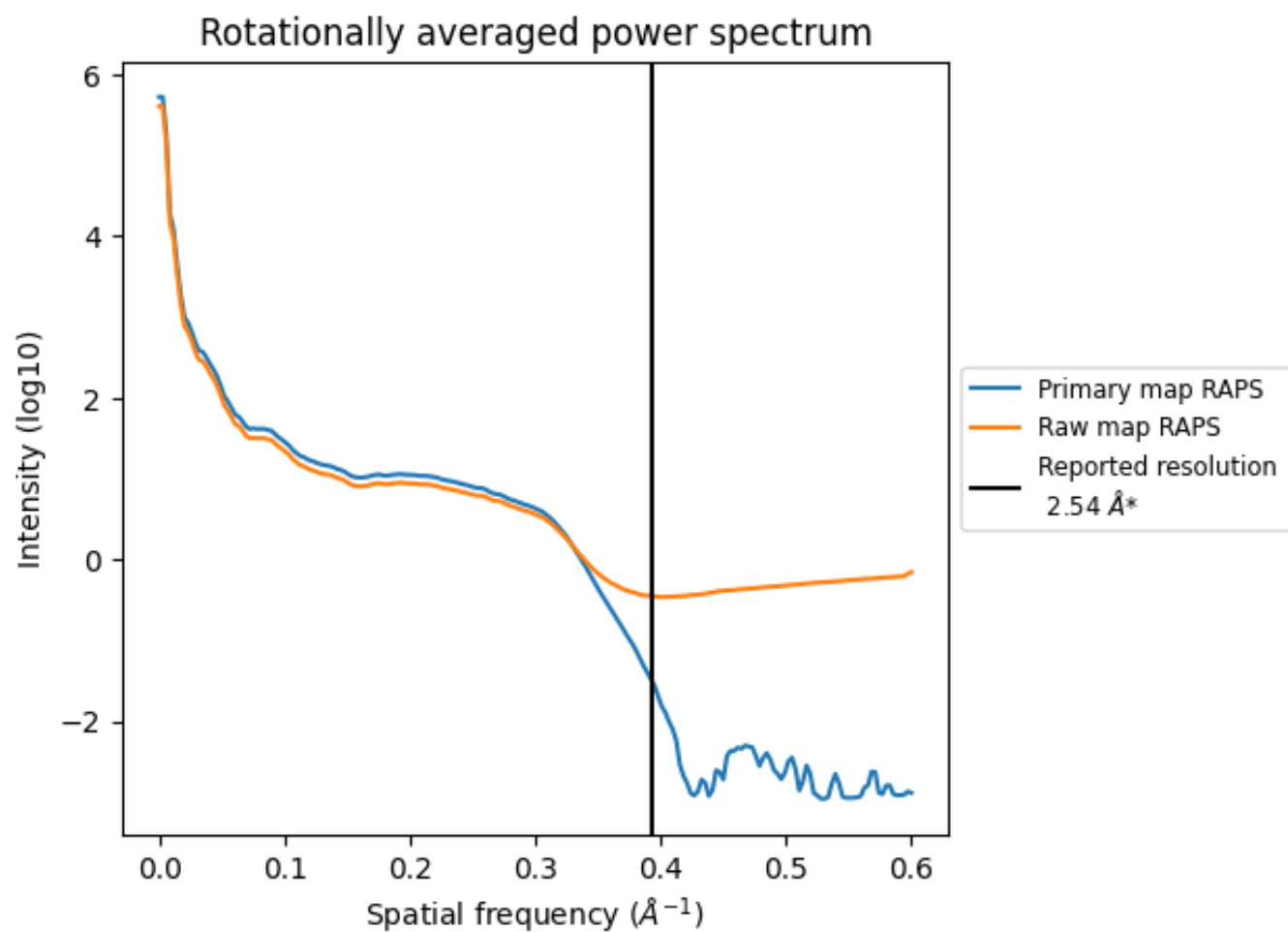
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 511 nm³; this corresponds to an approximate mass of 461 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 [i](#)

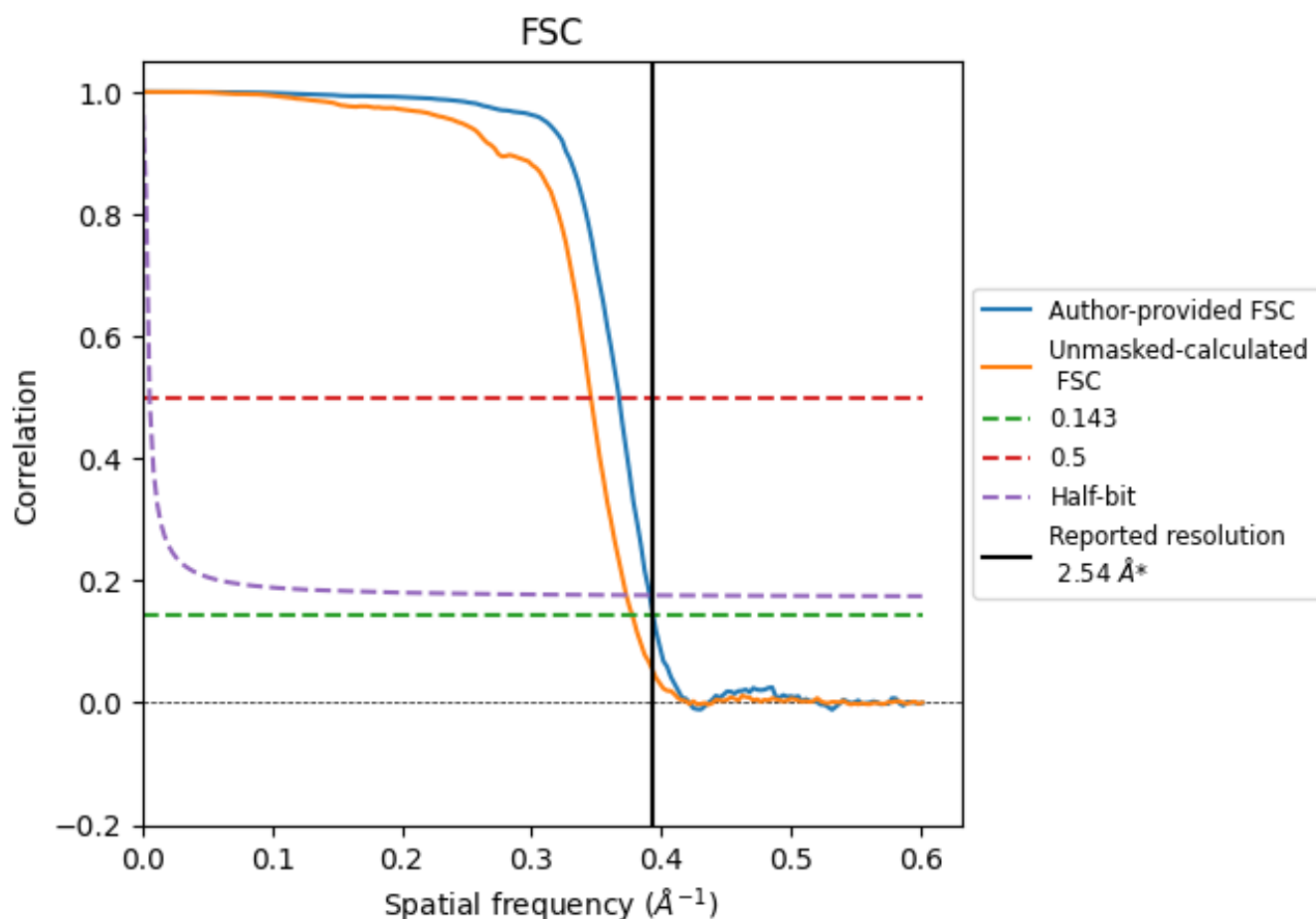


*Reported resolution corresponds to spatial frequency of 0.394 Å⁻¹

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 0.394 \AA^{-1}

8.2 Resolution estimates [i](#)

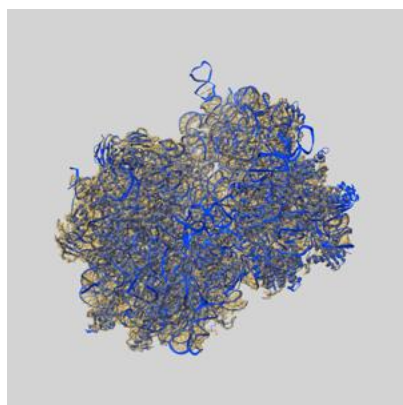
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	2.54	2.72	2.56
Unmasked-calculated*	2.65	2.89	2.68

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

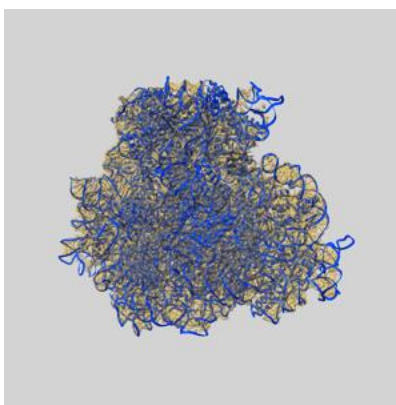
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55845 and PDB model 9TEX. Per-residue inclusion information can be found in section 3 on page 15.

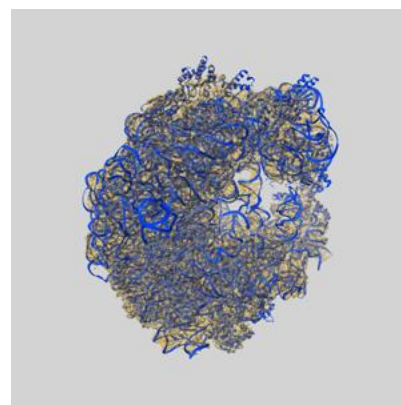
9.1 Map-model overlay [i](#)



X



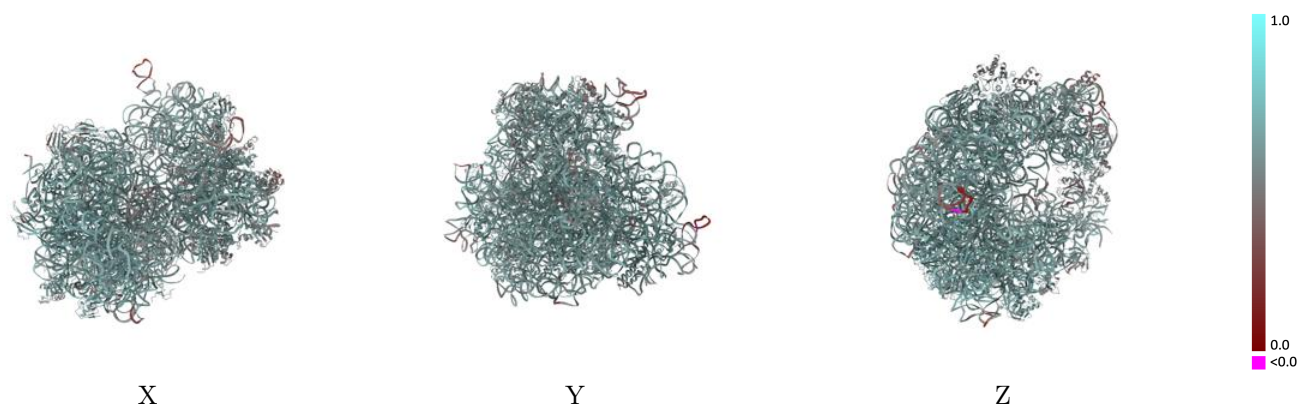
Y



Z

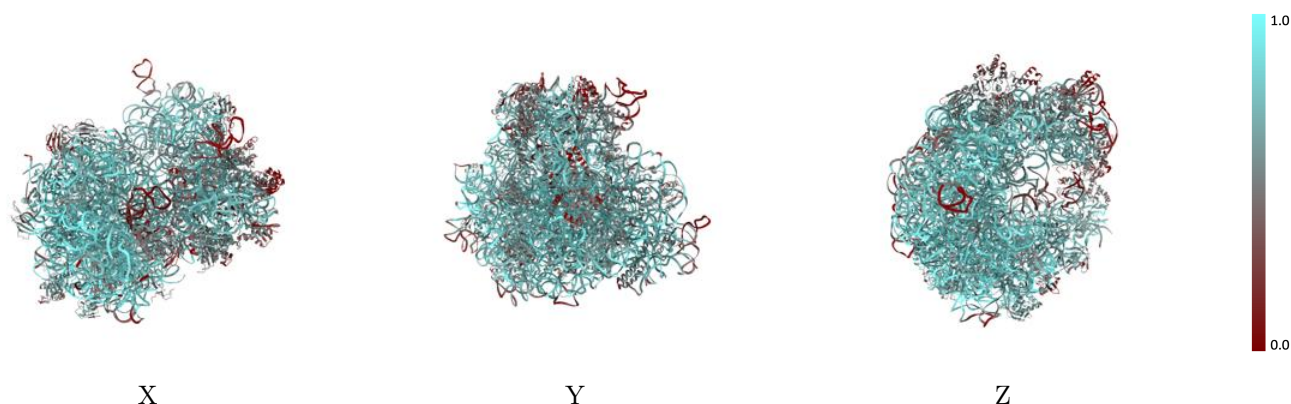
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



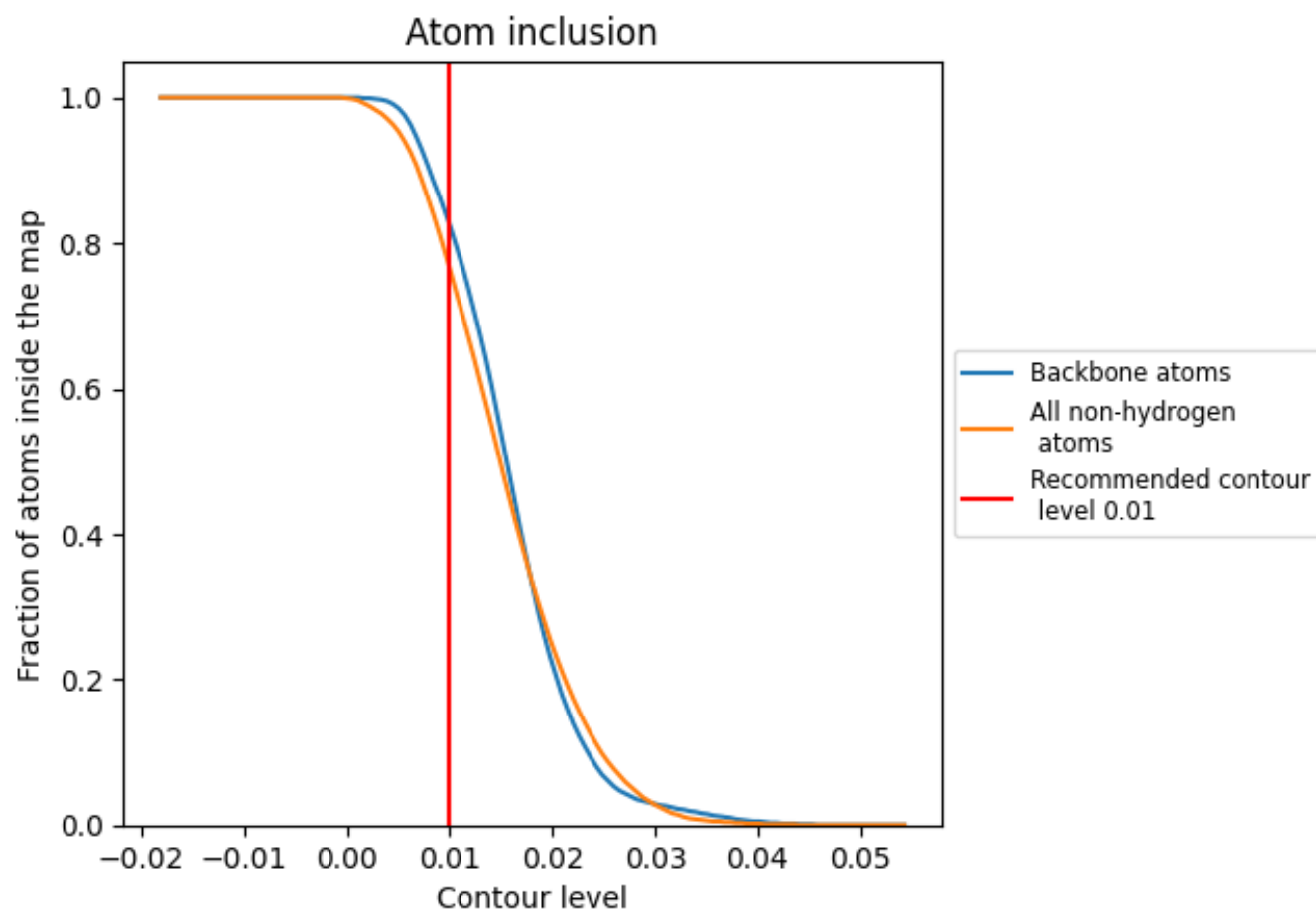
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 76% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7650	 0.6110
0	 0.6420	 0.6070
1	 0.8320	 0.6610
2	 0.8150	 0.6580
3	 0.6890	 0.6210
4	 0.2740	 0.5110
8	 0.6360	 0.6310
A	 0.7830	 0.6000
B	 0.3690	 0.5250
C	 0.5120	 0.5750
D	 0.5110	 0.5710
E	 0.6150	 0.6040
F	 0.4990	 0.5540
G	 0.4330	 0.5360
H	 0.5910	 0.5930
I	 0.4830	 0.5600
J	 0.3360	 0.5260
K	 0.5790	 0.5850
L	 0.5800	 0.6000
M	 0.4480	 0.5580
N	 0.5320	 0.5770
O	 0.5840	 0.5890
P	 0.5880	 0.5910
Q	 0.5110	 0.5760
R	 0.5780	 0.5780
S	 0.4080	 0.5500
T	 0.5360	 0.5750
U	 0.3420	 0.5200
X	 0.4960	 0.5600
Z	 0.4390	 0.5590
a	 0.8860	 0.6330
b	 0.7980	 0.6050
c	 0.7690	 0.6450
d	 0.7610	 0.6400
e	 0.6490	 0.6090



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Chain	Atom inclusion	Q-score
f	 0.4060	 0.5480
g	 0.4230	 0.5380
h	 0.5130	 0.5600
i	 0.7610	 0.6360
j	 0.7080	 0.6320
k	 0.7140	 0.6290
l	 0.7050	 0.6290
m	 0.8150	 0.6510
n	 0.6030	 0.5800
o	 0.7040	 0.6260
p	 0.7910	 0.6470
q	 0.7000	 0.6210
r	 0.7190	 0.6330
s	 0.6070	 0.6020
t	 0.5610	 0.5830
u	 0.6040	 0.5920
v	 0.7620	 0.6330
w	 0.7270	 0.6350
x	 0.5460	 0.5700
y	 0.6920	 0.6240
z	 0.7290	 0.6310